Survival probability of a diffusing test particle in a system of coagulating and annihilating random walkers

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We calculate the survival probability of a diffusing test particle in an environment of diffusing particles that undergo coagulation at rate λ_c and annihilation at rate λ_a. The test particle is annihilated at rate λ' on coming into contact with the other particles. The survival probability decays algebraically with time as $t^{-\theta}$. The exponent θ in $d<2$ is calculated using the perturbative renormalization group formalism as an expansion in $\epsilon=2-d$. It is shown to be universal, independent of λ', and to depend only on δ, the ratio of the diffusion constant of test particles to that of the other particles, and on the ratio λ_a/λ_c. In two dimensions we calculate the logarithmic corrections to the power law decay of the survival probability. Surprisingly, the logarithmic corrections are nonuniversal. The one-loop answer for θ in one dimension obtained by setting $\epsilon=1$ is compared with existing exact solutions for special values of δ and λ_a/λ_c. The analytical results for the logarithmic corrections are verified by Monte Carlo simulations.

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I. INTRODUCTION

The calculation of the survival probability of a test particle in reaction-diffusion systems has been studied in different contexts such as site persistence [1], walker persistence problems [2–6], polydispersity exponents in models of aggregation [6–9], and predator-prey models [10,11]. The approach to these problems has mostly been based on studying exactly solvable limiting cases or using the mean field approximation and its improvements such as the Smoluchowski approximation [12,13]. In recent years, field theoretic methods have proved successful in providing a general framework to understand these problems. In particular, the renormalization group analysis has been instrumental both in identifying the universal persistent features of reaction-diffusion systems and in extracting quantitative results about persistence exponents which could not be obtained using other methods [2,6,9,11,14–16]. In this paper, we apply field theoretic methods to the problem of the survival probability of diffusing test B particles in a background of diffusing A particles undergoing the reactions

$$A+A\xrightarrow{\lambda_c}A,$$

$$A+A\xrightarrow{\lambda_a}\varnothing,$$

$$A+B\xrightarrow{\lambda'}A. \tag{1}$$

The above reaction has been studied in the context of persistence. In one dimension and when B particles are stationary, calculating the survival probability of B particles is equivalent to calculating the fraction of spins that have not flipped up to time t in the q-state Potts model evolving via zero temperature Glauber dynamics, where $q=\lambda_c/\lambda_a+2$ [1]. The more general problem in which the B particles are mobile with a diffusion constant equal to δ times the diffusion constant of the A particles has been studied in Refs. [2,3,6,17]. The density of B particles then decays with time as $t^{-\theta(\delta,Q)}$, where $Q=(\lambda_c+\lambda_a)/(\lambda_c+2\lambda_a)$. As Q varies from $1/2$ to 1, the ratio λ_c/λ_a varies from 0 to ∞. The known results for $\theta(\delta,Q)$ are briefly reviewed below.

When the dimension d is greater than the upper critical dimension—two in this case—the decay exponents are obtained by solving the mean field rate equations with an appropriately renormalized lattice-dependent reaction rate. In dimensions $d\leqslant 2$, fluctuation effects become important, and $\theta(\delta,Q)$ is no longer given by the rate equations. Exact solutions are one way of calculating exponents in one dimension. When $\delta=0$, by mapping the calculation of the persistence probability to a calculation of empty interval probabilities in the $A+A\to A$ model, it was shown that [1]

$$\theta(0,Q)=\frac{2}{\pi^2}\left[\cos^{-1}\left(\frac{1-2Q}{\sqrt{2}}\right)\right]^2-\frac{1}{8},\quad d=1. \tag{2}$$

Attempts to generalize the methods used in Ref. [1] to arbitrary δ were successful only in determining the values of $(d\theta/dQ)|_{Q=0}$ and $(d\theta/d\delta)|_{\delta=0}$ [3]. Another solvable limit is $Q=1$, when annihilation is absent. In this case, the problem reduces to a three-particle problem which can be solved exactly to yield [18]

$$\theta(\delta,1)=\frac{\pi}{2\cos^{-1}[\delta/(1+\delta)]},\quad d=1. \tag{3}$$

More general ways of understanding the effects of fluctuation in low dimensional reaction-diffusion systems include the Smoluchowski approximation [12,13], which effectively reduces to the replacement of the reaction rates in the rate

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equations by diffusion-renormalized values, and the renormalization group formalism. The exponent $\theta(\delta,1/2)$ was calculated using the Smoluchowski approximation in Ref. [17]. The advantage of the Smoluchowski approximation is its computational simplicity. However, it is not clear how to improve this approximation in a systematic manner. Also, it was shown in Refs. [6,9] that, while this approach gives an answer close to the actual one for $Q=1/2$, it becomes increasingly worse as Q nears 1. The field theoretic approach using the renormalization group formalism currently provides the only systematic way of calculating the decay exponents below the critical dimension. The exponent $\theta(\delta,1/2)$ was calculated using field theoretic methods in Ref. [2]. However, the renormalization group scheme used was complicated and did not capture the right logarithmic corrections (see Sec. IV B for a more detailed discussion). $\theta(1,Q)$ was calculated as an expansion in $(2-d)$ in [6,9] in the context of domain wall persistence in the Potts model.

In this paper, we extend the formalism developed in Refs. [6,9] to calculate $\theta(\delta,Q)$ for arbitrary δ and Q to order ϵ, where $\epsilon=2-d$. In particular we show that

$$\theta=\frac{Q(1+\delta)}{2}\left[2-\epsilon\left\{\frac{3}{2}+\ln\frac{1+\delta}{2}+\frac{Q(1+\delta)f(\delta)}{2}\right\}+O(\epsilon^2)\right], \tag{4}$$

where

$$f(\delta)=1-2\delta+2\delta\ln\left(\frac{2}{1+\delta}\right)+(1-\delta^2)\int_{(\delta-1)/(\delta+1)}^{1}du\frac{\ln(1-u)}{u}. \tag{5}$$

The function $f(\delta)$ increases from $(1-\pi^2/4)$ to 0 as δ increases from 0 to ∞. In two dimensions, we calculate logarithmic corrections to the power law decay and show that

$$\langle b\rangle \sim t^{-Q(1+\delta)}\ln(t)^{\alpha}, \tag{6}$$

where $\langle b\rangle$ is the mean density of B particles and

$$\alpha=\frac{Q(1+\delta)}{2}\left[3+Q(1+\delta)f(\delta)+2\ln\frac{1+\delta}{2}\right]+2\pi Q(1+\delta)^2\left(\frac{1}{\lambda'}-\frac{2}{(1+\delta)(\lambda_a+\lambda_c)}\right), \tag{7}$$

with the function f as defined in Eq. (5). A surprising feature of Eq. (7) is its nonuniversality for finite reaction rates $\lambda,\lambda'<\infty$. In this case α explicitly depends on both reaction rates. This is contrary to the usual belief that below the upper critical dimension the kinetics is diffusion limited and hence one may set reaction rates to infinite. Most exact solutions make use of this simplifying assumption. The above result serves as a counterexample.

The rest of the paper is organized as follows. In Sec. II, the model is defined. In Sec. III, the rate equation approach is compared with the Smoluchowski approximation. The survival probability is calculated to one-loop precision. In Sec. IV, the renormalization group analysis of the problem is carried out and Eqs. (4), (6), and (7) are derived. The one-loop answer for θ is compared with the result of Smoluchowski approximation and also with known exact results in one dimension for special values of δ and Q. We also compare the analytical results with the results from numerical simulations. First, the predictions for the logarithmic corrections to the power law decay are confirmed numerically in the limit of instantaneous reactions. Second, the nonuniversality of logarithmic corrections for finite reaction rates is verified. Finally, we end with a summary and conclusions in Sec. V.

II. THE MODEL

Consider a d-dimensional hypercubic lattice whose sites may be occupied by A particles and B particles. Multiple occupancy of a site is allowed. Given a configuration of particles, the system evolves in time as follows. (i) At rate $D/(2d)$, an A particle hops to a nearest neighbor site. (ii) At rate $\delta D/(2d)$, a B particle hops to a nearest neighbor site. (iii) At rate λ_a, two A particles at the same site annihilate each other. (iv) At rate λ_c, two A particles at the same site coagulate together, thus reducing the number of A particles by 1. (v) At rate λ', a B particle is absorbed by an A particle at the same site. The initial numbers of $A(B)$ particles at the lattice sites are chosen independently from a Poisson distribution with intensity $a_0(b_0)$.

The action corresponding to the continuous limit of the model can be derived from the master equation using Doi's formalism [19–21]. We skip the derivation and give the final result. The action is

$$S=\int dt\int d^dx\Big(\overline{a}(\partial_t-\nabla^2)a+\overline{b}(\partial_t-\delta\nabla^2)b+\frac{\lambda}{2Q}\overline{a}a^2+\frac{\lambda}{2}\overline{a}^2a^2+\lambda'\overline{b}ab+\lambda'\overline{a}\overline{b}ab-(\overline{a}a_0+\overline{b}b_0)\delta(t)\Big) \tag{8}$$

where a and b are complex fields corresponding to A and B particles, the diffusion constant D has been set equal to 1, and

$$Q=\frac{\lambda_c+\lambda_a}{\lambda_c+2\lambda_a}, \tag{9}$$

$$\lambda=\lambda_a+\lambda_c. \tag{10}$$

The knowledge of all the correlation functions of the fields a,b allows one to construct all the correlation functions of local densities of A and B particles [22]. In particular, the mean density of A and B particles at $(\vec{x},t)$ is equal to $\langle a(\vec{x},t)\rangle$ and $\langle b(\vec{x},t)\rangle$, respectively, where $\langle\cdots\rangle$ denotes the functional average with respect to the functional measure Eq. (8).

The action can be brought into a more convenient form by rescaling the fields as follows: $(\overline{a},\overline{b})\to Q^{-1}(\overline{a},\overline{b}),(a,b)\to Q(a,b),(a_0,b_0)\to Q(a_0,b_0)$, and $(\lambda,\lambda')\to 2(\lambda,\lambda')$. Then

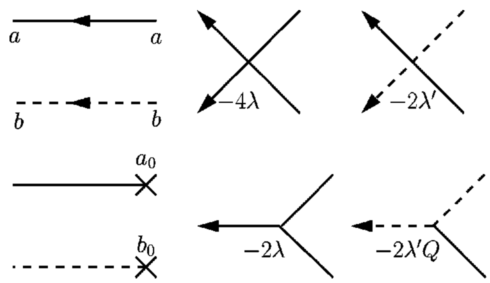

FIG. 1. Propagators and vertices of the theory.

$$S = \int dt \int d^d x \Big[\bar{a}(\partial_t - \nabla^2) a + \bar{b}(\partial_t - \delta\nabla^2) b + \lambda \bar{a} a^2 + \lambda \bar{a}^2 a^2 + 2\lambda' Q \bar{b} a b + 2\lambda' \bar{a}\bar{b} a b - (\bar{a} a_0 + \bar{b} b_0)\delta(t) \Big]. \quad (11)$$

The Feynman diagrams corresponding to the action in Eq. (11) are shown in Fig. 1.

We are interested in the mean density of B particles in the limit of large time, as the survival probability is proportional to the mean density. The evolution of mean density of A particles $\langle a \rangle$ is independent of the statistics of B particles and decays at large times t as [14]

$$\langle a \rangle \sim \begin{cases} t^{-d/2}, & d < 2, \\ t^{-1}\ln(t), & d = 2, \\ t^{-1}, & d > 2. \end{cases} \quad (12)$$

III. COMPUTATION OF THE PERSISTENCE EXPONENT USING MEAN FIELD AND SMOLUCHOWSKI APPROXIMATIONS

The perturbative expansion of $\langle b \rangle$ in powers of λ can be constructed using the Feynman diagrams shown in Fig. 1 [23]. Diagrammatically, $\langle a \rangle (\langle b \rangle)$ is the sum of all Feynman diagrams with one outgoing a (b) line, respectively. Clearly, there is an infinite number of diagrams contributing to $\langle a \rangle$ and $\langle b \rangle$. These diagrams can be grouped together according to the number of loops that they contain, thus giving rise to the loop expansion. Let $\epsilon = 2 - d$. A simple combinatorial argument shows that the contribution from a diagram with n loops is proportional to $g(t)^n$, where $g(t) = \lambda t^{\epsilon/2}$ [15]. When $\epsilon < 0$, the main contribution to $\langle a \rangle$ and $\langle b \rangle$ comes from properly renormalized tree level diagrams (diagrams without loops). When $\epsilon > 0$, the loop expansion fails since for large times $g(t)$ is no longer a small perturbation parameter. We therefore conclude that 2 is the upper critical dimension. For $d < 2$ we will use the formalism of perturbative renormalization group to convert the loop expansion into an ϵ expansion and calculate the scaling exponents as a series in ϵ.

A. Tree-level diagrams

In $d < 2$ and small times, tree diagrams give the main contribution to the survival probability. Let $\langle a \rangle_{\mathrm{mf}}$ and $\langle b \rangle_{\mathrm{mf}}$ be mean field densities given by the sum of contributions coming from tree diagrams with a single outgoing a line and b line, respectively. We denote $\langle a \rangle_{\mathrm{mf}}$ and $\langle b \rangle_{\mathrm{mf}}$ by thick solid lines and thick dashed lines, respectively. The integral equations satisfied by $\langle a \rangle_{\mathrm{mf}}$ and $\langle b \rangle_{\mathrm{mf}}$ are presented in diagrammatic form in Figs. 2(a) and 2(b) correspondingly. Analytically,

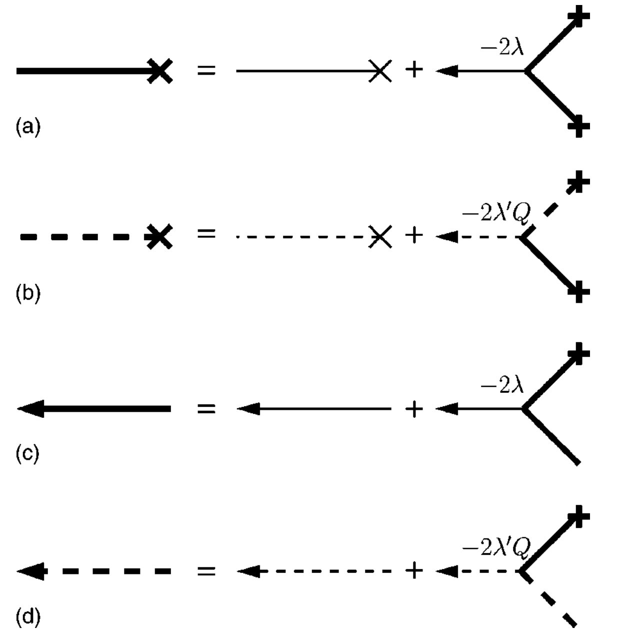

FIG. 2. Diagrammatic form of mean field equations for (a) mean particle density $\langle b \rangle$, (b) mean density of B particles $\langle b \rangle$, (c) $G^{\mathrm{NN}}_{\mathrm{mf}}$, and (d) $G^{\mathrm{PP}}_{\mathrm{mf}}$.

$$\langle a(t) \rangle_{\mathrm{mf}} = a_0 - \lambda \int_0^t dt' \langle a(t') \rangle^2_{\mathrm{mf}},$$

$$\langle b(t) \rangle_{\mathrm{mf}} = b_0 - 2\lambda' Q \int_0^t dt' \langle a(t') \rangle_{\mathrm{mf}} \langle b(t') \rangle_{\mathrm{mf}}.$$

After differentiating with respect to time, these equations can be rewritten in differential form as

$$\partial_t \langle a \rangle = -\lambda \langle a \rangle^2, \quad (13)$$

$$\partial_t \langle b \rangle = -2Q\lambda' \langle b \rangle \langle a \rangle, \quad (14)$$

in which one can easily recognize the rate equations of the model. Thus, the identification of tree-level truncation with mean field approximation is justified.

Equations (13) and (14) are easily solved, yielding

$$\langle a(t) \rangle_{\mathrm{mf}} = \frac{a_0}{1 + \lambda a_0 t}, \quad (15)$$

$$\langle b(t) \rangle_{\mathrm{mf}} = \frac{b_0}{(1 + \lambda a_0 t)^{2Q\lambda'/\lambda}}, \quad (16)$$

where a_0 and b_0 are the initial densities of A and B particles, respectively. Thus,

$$\theta(\delta,Q) = 2Q\frac{\lambda'}{\lambda}, \quad d > 2. \tag{17}$$

The result is explicitly dependent on λ', λ while being independent of δ and describes the reaction-limited regime of the problem. It should be mentioned here that the above result is valid only in the limit when the reaction rates are the smallest parameters in the problem, i.e., $\lambda, \lambda' \ll l_0^{d-2}$, where l_0 is the lattice spacing. In the other limit when the lattice spacing is the smallest parameter in the problem, the exponents get modified to [24]

$$\theta(\delta,Q) = Q(1+\delta), \quad l_0^{d-2} \ll \lambda, \lambda', \quad d > 2. \tag{18}$$

In order to estimate the validity of the mean field approximation in $d \leqslant 2$, the one-loop corrections to the mean field answer have to be evaluated. In calculating loop corrections to Eqs. (15) and (16), we are faced with the problem of summing over an infinite number of diagrams containing a given number of loops. This problem can be simplified by introducing mean field propagators, which are sums of all tree diagrams with one incoming line and one outgoing line. Expressed in terms of these mean field propagators, there are only a finite number of diagrams with a fixed number of loops.

Let $G_{\rm mf}^{\rm NN}$ and $G_{\rm mf}^{\rm PP}$ be mean field propagators. The integral equations satisfied by them are presented in diagrammatic form in Figs. 2(c) and 2(d). These equations have the following analytic forms:

$$G_{\rm mf}^{\rm NN}(\mathbf{2}|\mathbf{1}) = \tilde{G}_1(\mathbf{2}|\mathbf{1}) - 2\lambda\int_{t_1}^{t_2} dt \int_{\mathbf{R}^d} d\vec{x}\, \tilde{G}_1(\mathbf{2}|\vec{x},t) \times \langle a(t)\rangle G_{\rm mf}^{\rm NN}(\vec{x},t|\mathbf{1}), \tag{19}$$

$$G_{\rm mf}^{\rm PP}(\mathbf{2}|\mathbf{1}) = \tilde{G}_\delta(\mathbf{2}|\mathbf{1}) - 2\lambda' Q\int_{t_1}^{t_2} dt \int_{\mathbf{R}^d} d\vec{x}\, \tilde{G}_\delta(\mathbf{2}|\vec{x},t) \times \langle a(t)\rangle G_{\rm mf}^{\rm PP}(\vec{x},t|\mathbf{1}), \tag{20}$$

where $\mathbf{1} = (\vec{x}_1, t_1), \mathbf{2} = (\vec{x}_2, t_2)$, and $\tilde{G}_D$ is the Green's function of the linear diffusion equation with diffusion constant D. The solutions to these equations are

$$G_{\rm mf}^{\rm NN}(\mathbf{2}|\mathbf{1}) = \left(\frac{\langle a(t_2)\rangle_{\rm mf}}{\langle a(t_1)\rangle_{\rm mf}}\right)^2 \tilde{G}_1(\mathbf{2}|\mathbf{1}), \tag{21}$$

$$G_{\rm mf}^{\rm PP}(\mathbf{2}|\mathbf{1}) = \left(\frac{\langle a(t_2)\rangle_{\rm mf}}{\langle a(t_1)\rangle_{\rm mf}}\right)^{2Q\lambda'/\lambda} \tilde{G}_\delta(\mathbf{2}|\mathbf{1}). \tag{22}$$

B. Smoluchowski approximation

Before presenting the renormalization group calculation of $\theta(\delta,Q)$, we briefly discuss a method commonly used to study fluctuation effects in reaction-diffusion systems, namely, the Smoluchowski approximation. The essential idea of the Smoluchowski approach is to relate the reaction rates λ and λ' to the diffusion rates. One assumes that particles react instantaneously when they come within a fixed radius of each other (see [2,17] for a more detailed discussion). Knowing the first return probabilities of random walks, one obtains for $d < 2$

$$\lambda \sim \text{const} \times t^{d/2-1}, \tag{23}$$

$$\lambda' \sim \text{const} \times \left(\frac{1+\delta}{2}\right)^{d/2} t^{d/2-1}. \tag{24}$$

Note that the factor $(1+\delta)/2$, which often appears in our answers, is just the effective diffusion coefficient in the problem. In $d=2$ additional logarithmic corrections appear and

$$\lambda \sim \frac{\text{const}}{\ln(t)}, \tag{25}$$

$$\lambda' \sim \frac{\text{const} \times (1+\delta)}{2\ln\{[(1+\delta)/2]t\}}. \tag{26}$$

Replacing λ and λ' in Eqs. (13) and (14) by the effective reaction reaction rates, and solving for $\langle b\rangle$, we obtain

$$\langle b\rangle_S \sim \begin{cases} t^{-dQ[(1+\delta)/2]^{d/2}}, & d < 2, \\ \left(\dfrac{\ln(t)}{t}\right)^{Q(1+\delta)} [\ln(t)]^{Q(1+\delta)\ln[(1+\delta)/2]}, & d = 2, \end{cases} \tag{27}$$

where $\langle b\rangle_S$ denotes the mean density of B particles obtained from the Smoluchowski approximation. In order to obtain Eq. (27) we used the decay laws for the density of A particles as in Eq. (12), which also follow from the Smoluchowski approximation. In particular, the Smoluchowski theory's prediction for θ is

$$\theta_S(\delta,Q) = dQ\left(\frac{1+\delta}{2}\right)^{d/2}, \quad d < 2. \tag{28}$$

This answer for θ depends on δ, Q, and the space dimensionality d. It does not, however, depend on λ and λ'. Thus, unlike the mean field answer Eq. (17), it has the correct universality properties for a quantity describing reaction-diffusion systems in the diffusion-limited regime. However, the Smoluchowski result differs considerably from the correct result when Q nears 1. For example, in one dimension $\theta_S(1,1) = 1.0$ while $\theta(1,1) = 1.5$ [see Eq. (3)]. For more comparisons, see Sec. IV A. It is not clear how one can improve the Smoluchowski approximation. The renormalization group formalism, although more involved, provides a systematic way to go beyond the Smoluchowski approximation.

C. One-loop diagrams

The rate equation results do not depend on the diffusion coefficients of the particles or the dimensionality of the ambient space. These parameters appear in the one-loop corrections to the tree-level answers. Using the mean field propagators and densities, it is easy to classify all the one-loop diagrams contributing to $\langle b\rangle$. These are shown in Fig. 3 [25]. Skipping the computations, we present the final answers for contributions corresponding to each of the Feynman diagrams in the limit $a_0 \to \infty$:

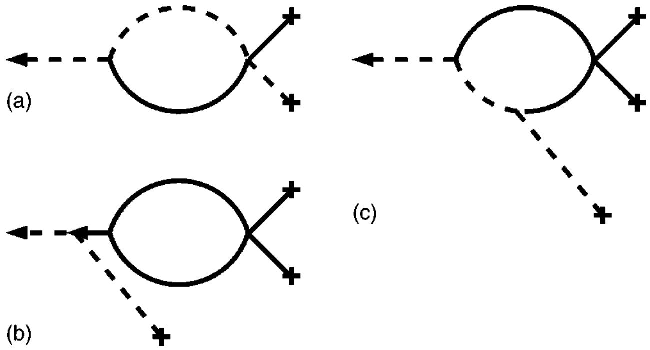

FIG. 3. One-loop corrections to the mean field result for $\langle b \rangle$.

$$(a) = \frac{32Q\lambda'^2 b_0 t^{\epsilon/2}}{\lambda(a_0\lambda t)^{2Q\lambda'/\lambda}[4\pi(1+\delta)]^{d/2}\epsilon^2(\epsilon+2)}, \qquad (29)$$

$$(b) = \frac{8Q^2\lambda'^2 b_0(1+\delta)t^{\epsilon/2}}{\lambda(a_0\lambda t)^{2Q\lambda'/\lambda}[4\pi(1+\delta)]^{d/2}\epsilon}[f(\delta)+O(\epsilon)], \qquad (30)$$

$$(c) = \frac{-256Q\lambda' b_0 t^{\epsilon/2}}{(a_0\lambda t)^{2Q\lambda'/\lambda}(8\pi)^{d/2}\epsilon^2(\epsilon+2)^2(\epsilon+4)}, \qquad (31)$$

where (a), (b), and (c) refer to the contributions from diagrams in Figs. 3(a)–3(c), respectively, and

$$f(\delta) = 1 - 2\delta + 2\delta \ln\left(\frac{2}{1+\delta}\right) + (1-\delta^2)\int_{(\delta-1)/(\delta+1)}^{1} du \frac{\ln(1-u)}{u}. \qquad (32)$$

Adding these one-loop contributions to the mean field answer Eq. (16), we obtain in the limit $a_0 \to \infty$

$$\langle b(t)\rangle = \frac{A}{t^{2Q\lambda'/\lambda}}\left[1 + \frac{8Q\lambda' t^{\epsilon/2}}{(4\pi)^{d/2}\epsilon}\left\{\frac{4\lambda'}{\lambda(1+\delta)^{d/2}}\frac{1}{\epsilon(\epsilon+2)} - \frac{32}{2^{d/2}}\frac{1}{\epsilon(\epsilon+2)^2(\epsilon+4)} + \frac{Q\lambda'(1+\delta)^{\epsilon/2}f(\delta)}{2\lambda}\right\}\right] + \text{two and higher loop corrections}, \qquad (33)$$

where $A = b_0/(a_0\lambda)^{2Q\lambda'/\lambda}$. We see that if $\lambda \sim \lambda'$, then the mean field answer Eq. (17) is correct in $d<2$ only if $Q\lambda t^{\epsilon/2} \ll 1$. Clearly, this condition breaks down in the limit of large times in $d<2$.

IV. PERTURBATIVE COMPUTATION OF $\theta(\delta,Q)$ NEAR $d=2$ USING THE RENORMALIZATION GROUP METHOD

In this section, we calculate the large time behavior of $\langle b \rangle$. The loop expansion for $\langle b(t)\rangle$ fails at large times in $d \leq 2$. To extract the large time behavior of $\langle b(t)\rangle$ in $d \leq 2$ we will use the formalism of the perturbative renormalization group.

The renormalization group formalism used in Refs. [6,9] for the case $\delta=1$ was based on the Callan-Symanzik equations for the mean density of B particles. There were two relevant couplings for the theory: the reaction rate λ and the initial density b_0. The anomalous dimension of $\langle b(t)\rangle$ was attributed to the renormalization of b_0.

This approach turns out to be very complicated when $\delta \neq 1$. This is due to the explicit dependence of the classical scaling dimension of $\langle b(t)\rangle$ on λ and λ'. Further complications arise due to noncommutativity of the $\epsilon \to 0$ and $a_0 \to \infty$ limits, which leads to an apparent order-$1/\epsilon^2$ singularity in the one-loop correction to $\langle b(t)\rangle$ [see Eq. (33)].

These problems are circumvented by analyzing the large time asymptotic behavior of the logarithmic derivative of $\langle b(t)\rangle$, rather than $\langle b(t)\rangle$ itself. It follows from Eq. (33) that

$$t\partial_t\{\ln[\langle b(t)\rangle]\} = \Pi(t), \qquad (34)$$

where

$$\Pi(t) = -2Q\frac{\lambda'}{\lambda} + \frac{4Q\lambda' t^{\epsilon/2}}{(4\pi)^{d/2}}\left\{\frac{4\lambda'}{\lambda(1+\delta)^{d/2}}\frac{1}{\epsilon(\epsilon+2)} - \frac{2^{-d/2}32}{\epsilon(\epsilon+2)^2(\epsilon+4)} + \frac{Q\lambda'(1+\delta)^{\epsilon/2}f(\delta)}{2\lambda}\right\} + O(\lambda^2). \qquad (35)$$

The large time asymptotic behavior of $\Pi(t)$ can be obtained by solving the Callan-Symanzik equation with initial conditions given by the right-hand side of Eq. (35) regularized at some reference time t_0 (see Ref. [22] for a review). The coefficients of the Callan-Symanzik equation are determined by the law of renormalization of all the relevant couplings of the theory. Power counting analogous to that carried out in Ref. [9] shows that there are only two relevant couplings of the theory which determine the large time behavior of $\Pi(t)$ in $d \leq 2$: the reaction rates λ and λ'. We mention here that $\Pi(t)$ is simply related to the polarization operator used in Ref. [9].

Let $g_0 = \lambda t_0^{\epsilon/2}$ and $g_0' = \lambda t_0^{\epsilon/2}$ be the dimensionless reaction rates. We choose t_0 in such a way that $g_0, g_0' \ll 1$. The way in which reaction rates get renormalized by interactions has been worked out in Ref. [2,14]. The renormalized reaction rates g_R and g_R' are related to g_0 and g_0' as follows:

$$g_R = \frac{g_0}{1+g_0/g_*}, \qquad (36)$$

$$g_R' = \frac{g_0'}{1+g_0'/g_*'}. \qquad (37)$$

Here g_* and g_*' are the nontrivial fixed points of the renormalization group flow in the space of effective coupling constants, and are given by

$$g_* = \frac{(8\pi)^{d/2}}{2\Gamma(\epsilon/2)}, \qquad (38)$$

$$g'_* = \frac{[4\pi(1+\delta)]^{d/2}}{2\Gamma(\epsilon/2)}, \tag{39}$$

where $\Gamma(x)$ is the Euler Gamma function. The renormalization of both coupling constants is due to the same physical effect—the recurrence of random walks in $d \leqslant 2$.

$\Pi(t_0)$ expressed in terms of g_R and g'_R has the following form:

$$\Pi(t_0) = -2Q\frac{g'_R}{g_R} + \frac{Qg'_R}{\pi}\left[\frac{g'_R(\gamma-1)}{g_R(1+\delta)} + \frac{5-2\gamma}{4} + \frac{Qg'_R f(\delta)}{2g_R} + O(\epsilon)\right] + O(g_R^2), \tag{40}$$

where γ is the Euler constant. $\Pi(t_0)$ regarded as a function of g_R and g'_R is nonsingular at $\epsilon=0$. As a result this expression is valid for $d \leqslant 2$. The lack of t_0 dependence of $\Pi(t)$ for $t > t_0$ is expressed by the following renormalization group (Callan-Symanzik) equation:

$$\left[t\frac{\partial}{\partial t} + \frac{\beta(g_R)}{2}\frac{\partial}{\partial g_R} + \frac{\beta(g'_R)}{2}\frac{\partial}{\partial g'_R}\right]\Pi(t) = 0, \tag{41}$$

where $\beta(g_R) = -2t_0\partial g_R/\partial t_0$ and $\beta(g'_R) = -2t_0\partial g'_R/\partial t_0$ are the beta functions

$$\beta(g_R) = \frac{g_R(g_R - g_*)\epsilon}{g_*}, \tag{42}$$

$$\beta(g'_R) = \frac{g'_R(g'_R - g'_*)\epsilon}{g'_*}. \tag{43}$$

We will now solve Eq. (41) with the initial condition given by Eq. (40) to obtain the large time asymptotic behavior of Π. We then extract the large time asymptotic behavior of $\langle b(t)\rangle$ by solving Eq. (34).

A. Survival probability in $d < 2$

At large times, the solutions of the Callan-Symanzik equation (41) are governed by the stable fixed points of the β functions. In $d < 2$, these are $g_R = g_*$ and $g'_R = g'_*$. It then follows that

$$\Pi(t) = -2Q(1+\delta) + \epsilon Q(1+\delta)\left[\ln\frac{1+\delta}{2} + \frac{3}{2} + Q\frac{1+\delta}{2}f(\delta)\right] + O(\epsilon^2, t^{-\epsilon/2}). \tag{44}$$

Substituting Eq. (44) into Eq. (34) and solving for $\langle b(t)\rangle$, we obtain the $O(\epsilon)$ result for θ:

$$\theta = \frac{Q(1+\delta)}{2}\left[2 - \epsilon\left\{\frac{3}{2} + \ln\frac{1+\delta}{2} + \frac{Q(1+\delta)f(\delta)}{2}\right\} + O(\epsilon^2)\right], \tag{45}$$

where the function $f(\delta)$ is as in Eq. (32).

We now compare the one dimensional result obtained by putting $\epsilon=1$ in Eq. (45) with exact results in one dimension for special values of δ and Q. The exact result for $\theta(0,Q)$ in one dimension is given in Eq. (2), while that for $\theta(\delta,1)$ is given in Eq. (3). Figures 4 and 5 show the results for $\delta=0$ and $Q=1$, respectively. The ϵ-expansion result is seen to compare very well with the exact result. On the other hand, the Smoluchowski results fail for Q larger than $1/2$ when $\delta=0$, and for all δ when $Q=1$. It should be noted that when δ becomes large the ϵ expansion will fail. This is because in deriving the ϵ expansion we wrote Eq. (28) as a series in ϵ to first order. This expansion fails when δ is large.

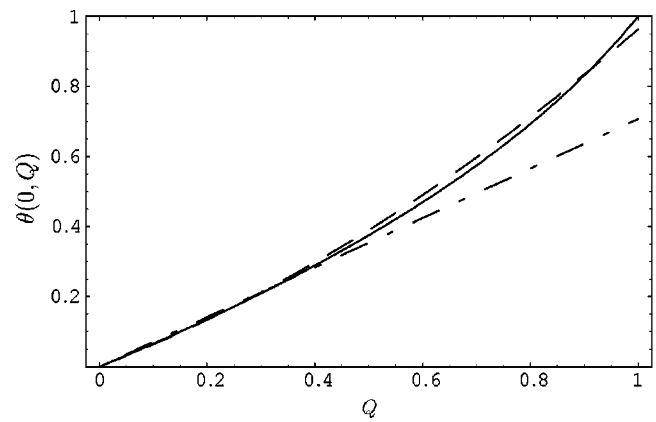

FIG. 4. The one-loop answer [Eq. (45)] is compared with the exact result in one dimension when $\delta=0$ [Eq. (2)]. The solid line corresponds to the exact answer, the dashed line to one loop, and the dot dashed line to the Smoluchowski result [Eq. (27)].

It is worth mentioning that, even though the persistence exponent turns out to be universal, the amplitude in the term governing corrections to scaling is nonuniversal. The corrections to $\Pi(t)$ due to nonconvergence to a fixed point have the form $C/t^{\epsilon/2}$, where the constant C depends on the bare reaction rates. Solving Eq. (34) with $\Pi(t)$ modified by these extra terms, we find corrections to scaling of the form $-(2C/\epsilon)t^{-\theta-\epsilon/2}$. In two dimensions a similar mechanism leads to nonuniversality of the logarithmic corrections (see Sec. IV B).

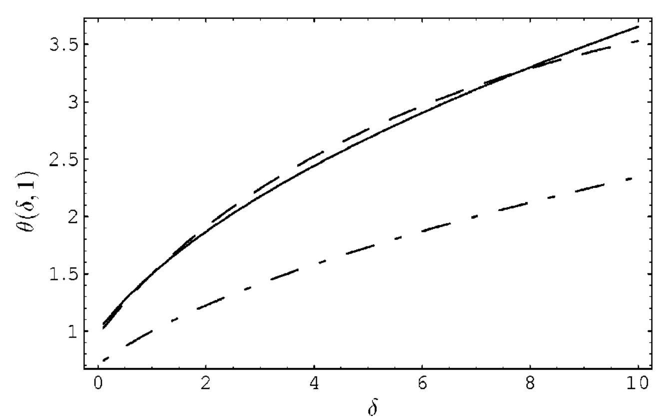

FIG. 5. The one-loop answer [Eq. (45)] is compared with the exact result in one dimension when $Q=1$ [Eq. (3)]. The solid line corresponds to the exact answer, the dashed line to one loop, and the dot dashed line to the Smoluchowski result [Eq. (27)].

B. Survival probability in $d=2$

The upper critical dimension of our model is 2. The nontrivial fixed points of the β functions Eqs. (42) and (43) vanish at $d=2$. It is then expected that the rate equation results give the correct large time behavior of the mean densities, perhaps modulo logarithmic corrections. This turns out to be incorrect. The complication comes from the fact that θ predicted by the mean field theory [see Eq. (17)] is nonuniversal and depends on the ratio of coupling constants g_R and g_R'. Each of these couplings is marginally relevant in two dimensions and flows under renormalization group transformations to 0 as $[\ln(t)]^{-1}$. Their ratio flows to a finite universal value which determines the algebraic decay of the survival probability. However, the deviation from this universal value vanishes with time as $C/\ln(t)$, where C is a nonuniversal constant. This results in nonuniversal logarithmic corrections to the universal power law decay of survival probability.

We need to solve the Callan-Symanzik equation (41) with coefficients calculated at $d=2$:

$$\beta(g)_{d=2} = \frac{g^2}{2\pi}, \tag{46}$$

$$\beta(g')_{d=2} = \frac{g'^2}{\pi(1+\delta)}. \tag{47}$$

Then Eq. (41) reduces to

$$\left[t\frac{\partial}{\partial t} + \frac{g_R^2}{4\pi}\frac{\partial}{\partial g_R} + \frac{g_R'^2}{2\pi(1+\delta)}\frac{\partial}{\partial g_R'}\right]\Pi(t) = 0, \tag{48}$$

which has to be solved with the initial condition given by Eq. (40) at $t=t_0, \epsilon=0$. The solution is

$$\Pi(t) = -Q(1+\delta) + \frac{2Q(1+\delta)}{\ln(t/t_0)}\left[\frac{3}{4} + \frac{Q}{2}f(\delta) + \pi(1+\delta) \times\left(\frac{1}{g_R'} - \frac{2}{(1+\delta)g_R}\right)\right] + O\left(\frac{1}{\ln^2(t)}\right). \tag{49}$$

The nonuniversal term in Eq. (49) is proportional to $1/g_R' - 2/[(1+\delta)g_R]$. It is convenient to express this amplitude in terms of bare couplings. In two dimensions,

$$\frac{1}{g_R'} - \frac{2}{(1+\delta)g_R} = \frac{1}{g_0'} - \frac{2}{(1+\delta)g_0} + \frac{\ln[(1+\delta)/2]}{2\pi(1+\delta)}. \tag{50}$$

In $d<2$, Eq. (50) has to be modified by omitting the logarithmic term on the right hand side.

Solving Eq. (34) with Eq. (49) substituted for the right hand side and taking Eq. (50) into account, one finds that

$$\langle b(t)\rangle = \text{const} \times \frac{[g_R \ln(t/t_0)]^{\alpha}}{(g_R t)^{Q(1+\delta)}}\left[1 + O\left(\frac{1}{\ln(t/t_0)}\right)\right], \tag{51}$$

where

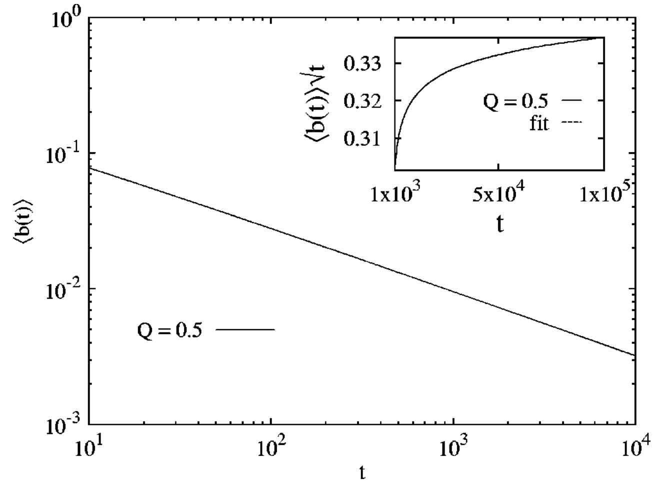

FIG. 6. The variation of the mean density of B particles in two dimensions with time. The simulations were done on a 3200×3200 lattice for $Q=0.5$ and $\delta=0$. The data have been averaged 1000 times. In the inset, the variation of $\langle b\rangle\sqrt{t}$ with time is shown. The power of the logarithm in the best fit is 0.23 ± 0.03. The fitted curve cannot be distinguished from the data.

$$\alpha = \frac{Q(1+\delta)}{2}\left[3 + Q(1+\delta)f(\delta) + 2\ln\frac{1+\delta}{2}\right] + 2\pi Q(1+\delta)^2\left(\frac{1}{\lambda'} - \frac{2}{(1+\delta)\lambda}\right). \tag{52}$$

Thus, in two dimensions, the power law exponent is universal and independent of λ and λ'. However, the logarithmic corrections are nonuniversal and depend on the microscopic reaction rates $\lambda'=g_0'$ and $\lambda=g_0$. However, most simulations are done in the limit when the reactions are instantaneous. In this limit, the nonuniversal term in Eq. (52) is zero.

The logarithmic corrections in Eq. (52) are different from the logarithmic corrections calculated for the $Q=1/2$ case in Ref. [2]. This discrepancy is due to the fact that only renormalized tree-level computations were done in [2], while to obtain the correct logarithmic dependence one-loop corrections have to be taken into account.

We also mention that, if one were to ignore the contribution from one-loop diagrams, then the logarithmic corrections would be identical with the logarithmic corrections obtained from the Smoluchowski approximation [see Eq. (27)], and will be different from the logarithmic corrections obtained from the renormalized tree level as in Ref. [2].

We now study logarithmic corrections numerically. First, consider the case when the microscopic reactions are instantaneous, i.e., $\lambda=\lambda'=\infty$. In this limit, the nonuniversal term in Eq. (52) is equal to zero. The Monte Carlo simulations were done for this case on a two-dimensional lattice of size 3200×3200 with periodic boundary conditions. As the reactions are instantaneous, the maximum number of particles at a site is 1. The simulations were done for $\delta=0$, i.e., immobile B particles. The results for $Q=0.5$ and $Q=1.0$ are shown in Figs. 6 and 7, respectively. For $Q=0.5, \alpha=0.23\pm0.03$, which compares well with the theoretical value of approximately 0.22 in Eq. (52). Note that the renormalized tree-level an-

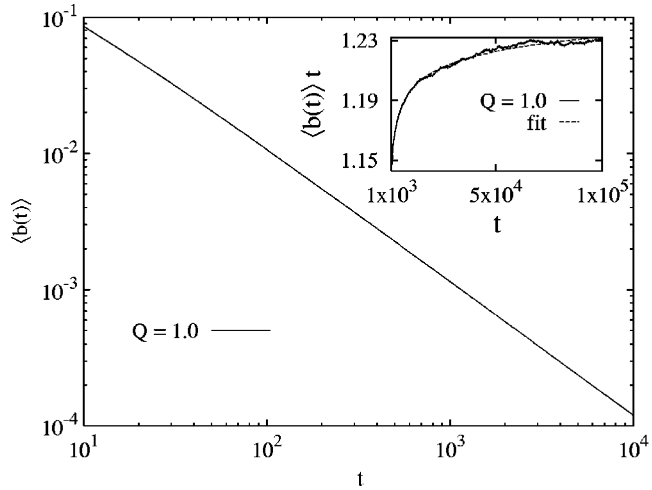

FIG. 7. The variation of the mean density of B particles in two dimensions with time. The simulations were done on a 3200×3200 lattice for $Q=1.0$ and $\delta=0$. The data have been averaged 1000 times. In the inset, the variation of $\langle b \rangle t$ with time is shown. The power of the logarithm in the best fit is 0.08 ± 0.04.

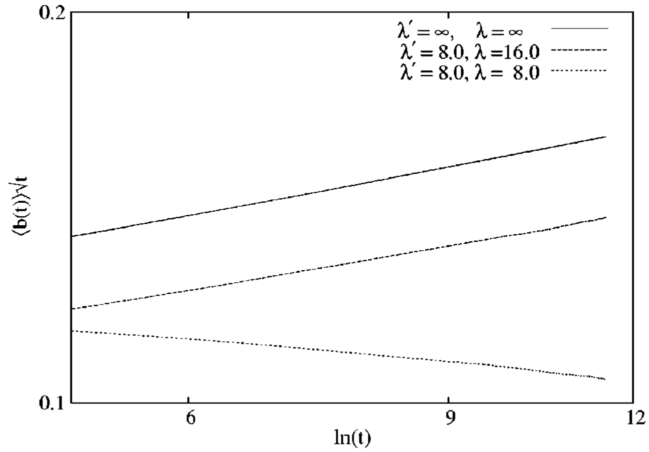

FIG. 8. The variation of the mean density of B particles in two dimensions with time. The simulations were done on a 900×900 lattice for $Q=0.5$ and $\delta=0$. The data have been averaged 1000 times.

swer is $\alpha=0.5$ [2]. For $Q=1.0$, the numerical value is 0.08 ± 0.04, which compares well with the theoretical value of approximately 0.07. This answer also deviates significantly from the renormalized tree-level value of 1.0.

Second, we study the logarithmic corrections for finite reaction rates to test the nonuniversal term in Eq. (52). In this case the lattice size is 900×900. The results for $\delta=0, Q=0.5$, and different reaction rates are shown in Fig. 8. If $\lambda=16, \lambda'=8$, then the nonuniversal term in Eq. (52) is zero and $\alpha \approx 0.22$ as in the case of infinite reaction rates. This is consistent with the dashed line in Fig. 8 being parallel to the solid line. If however, $\lambda=8, \lambda'=8$, then the theoretical value of α is -0.17. While the numerical precision of our experiment is insufficient for a reliable determination of the absolute value of α, its sign is negative, in line with the theoretical prediction.

V. SUMMARY AND CONCLUSIONS

In summary, we calculated the large time behavior of the survival probability of a test particle in a system of coagulating and annihilating random walkers in $d \leqslant 2$. In one dimension, this generalizes the site persistence problem in the q-state Potts model evolving via zero-temperature Glauber dynamics. The survival probability was shown to decay as a power law. In $d<2$, the exponent θ characterizing this power law was shown to be universal, in the sense that it depends only on δ and Q and is independent of λ, λ'. The renormalization group formalism provided a systematic way of calculating the survival probability for the entire parameter space.

In two dimensions, we computed the logarithmic corrections to the power law decay. It was shown that to compute the correct logarithmic factors one had to include contributions from one-loop diagrams and not just the tree-level diagrams as was done in earlier work. The behavior of the survival probability in two dimensions is surprising. First, the power law decay is universal and thus does not coincide with the rate equation result, even though $d=2$ is the upper critical dimension. Second, the logarithmic corrections to the power law are nonuniversal and depend on the reaction rates. This is contrary to the general expectation that kinetics of reaction-diffusion systems are diffusion limited below the upper critical dimension. Both the universality of the power law and the nonuniversality of logarithmic corrections in two dimensions can be traced to the fact that the rate equation exponent is given by the ratio of microscopic rates, which are both marginally relevant in two dimensions.

From the renormalization group point of view, by studying the logarithmic derivative of the mean density of B particles, we have considerably simplified the schemes used in Refs. [2,6,9]. While the exponents are calculated only up to first order in ϵ, the renormalization group method remains the only systematic way of computing the exponents when an exact solution is not available.

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[1] B. Derrida, V. Hakim, and V. Pasquier, Phys. Rev. Lett. **75**, 751 (1995).
[2] M. J. Howard, J. Phys. A **29**, 3437 (1996).
[3] C. Monthus, Phys. Rev. E **54**, 4844 (1996).
[4] S. N. Majumdar and S. J. Cornell, Phys. Rev. E **57**, 3757 (1998).
[5] S. J. O'Donoghue and A. J. Bray, Phys. Rev. E **65**, 051114 (2002).
[6] S. Krishnamurthy, R. Rajesh, and O. Zaboronski, Phys. Rev. E **68**, 046103 (2003).

[7] S. Cueille and C. Sire, Phys. Rev. E **55**, 5465 (1997).
[8] E. K. O. Hellén, P. E. Salmi, and M. J. Alava, Europhys. Lett. **59**, 186 (2002).
[9] S. Krishnamurthy, R. Rajesh, and O. Zaboronski, Phys. Rev. E **66**, 066118 (2002).
[10] S. Redner and P. L. Krapivsky, Am. J. Phys. **67**, 1277 (1999).
[11] J. Cardy and M. Katori, J. Phys. A **36**, 609 (2003).
[12] M. Smoluchowski, Z. Phys. Chem., Stoechiom. Verwandtschaftsl. **92**, 215 (1917).
[13] S. Chandrasekhar, Rev. Mod. Phys. **15**, 1 (1943).
[14] L. Peliti, J. Phys. A **19**, L365 (1986).
[15] B. P. Lee, J. Phys. A **27**, 2633 (1994).
[16] J. Cardy, J. Phys. A **28**, L19 (1995).
[17] P. L. Krapivsky, E. Ben-Naim, and S. Redner, Phys. Rev. E **50**, 2474 (1994).
[18] M. E. Fisher and M. P. Gelfand, J. Stat. Phys. **53**, 175 (1988).
[19] M. Doi, J. Phys. A **9**, 1465 (1976).
[20] M. Doi, J. Phys. A **9**, 1479 (1976).
[21] Y. B. Zel'dovich and A. A. Ovchinnikov, Sov. Phys. JETP **47**, 829 (1978).
[22] J. Cardy, http://www-thphys.physics.ox.ac.uk/users/JohnCardy/
[23] C. Itzykson and J. M. Drouffe, *Statistical Field Theory*, Cambridge Monographs on Mathematical Physics (Cambridge University Press, Cambridge, England, 1994).
[24] R. Rajesh and O. Zaboronski (unpublished).
[25] In listing the one-loop diagrams contributing to $\langle b \rangle$, we have been careful to avoid double counting. For instance, none of the diagrams in Fig. 3 has an A density line attached to a PP or NN propagator, since such contributions have already been accounted for in the definition of the mean field propagators.