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Renormalization group calculation for the reaction $kA \rightarrow \emptyset$

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Abstract. The diffusion-controlled reaction $kA \rightarrow \emptyset$ is known to be strongly dependent on fluctuations in dimensions $d \leqslant d_c = 2/(k-1)$. We develop a field-theoretic renormalization group approach to this system which allows explicit calculation of the observables as expansions in $\epsilon^{1/(k-1)}$, where $\epsilon = d_c - d$. For the density it is found that, asymptotically, $n \sim A_k t^{-d/2}$. The decay exponent is exact to all orders in ϵ, and the amplitude A_k is universal, and is calculated to second order in $\epsilon^{1/(k-1)}$ for $k = 2, 3$. The correlation function is calculated to first order, along with a long-wavelength expansion for the second-order term. For $d = d_c$ we find $n \sim A_k(\ln t/t)^{1/(k-1)}$ with an exact expression for A_k. The formalism can be immediately generalized to the reaction $kA \rightarrow \ell A$, $\ell < k$, with the consequence that the density exponent is the same, but the amplitude is modified.

1. Introduction

Diffusion-controlled chemical reactions are adequately described by mean-field-type rate equations in higher dimensions, but in lower dimensions the fluctuations become relevant [1,2]. For the reaction $kA \rightarrow \emptyset$ the critical dimension for fluctuations is conjectured to be $d_c = 2/(k-1)$ [3,4]. If $d > d_c$ the density $n(t)$ obeys the rate equation

$$\frac{\partial}{\partial t} n(t) = -\Gamma n(t)^k \tag{1}$$

with reaction rate constant Γ. This implies the density will decay asymptotically like $n \sim (\Gamma t)^{-1/(k-1)}$. For $d < d_c$ it is conjectured on the basis of scaling arguments [3,4], rigorous bounds [5], and exact results for $d = 1$ [6–10], that $n \sim t^{-d/2}$. For $d = d_c$ the mean-field power law with logarithmic corrections is expected.

In this paper we apply renormalization group (RG) methods to this system, with the goals of verifying the above conjectures and demonstrating universal quantities. The formalism developed can be used to calculate the density and correlation function perturbatively in $\epsilon^{1/(k-1)}$, where $\epsilon = d_c - d$. This formalism includes infinite sums for each order of $\epsilon^{1/(k-1)}$, since the initial density is a relevant parameter and must be summed to all orders.

Previous work in applying RG to this system was carried out by Peliti for the case $k = 2$ [11]. Using a field-theory formulation of this system, Peliti was able to confirm the conjectured decay exponent, and also demonstrate that the reactions $A + A \rightarrow \emptyset$ and $A + A \rightarrow A$ are in the same universality class with regard to the decay exponent and the upper critical dimension. Peliti also made the observations that the coupling constants can be exactly renormalized to all orders and that there is no wavefunction renormalization in the theory. The latter has the consequence that simple scaling arguments can be used to extract the decay exponent and the upper critical dimension. However, these scaling arguments

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are not capable of giving other universal quantities in the system, such as amplitudes or the asymptotic form of the correlation function. For these one must do the complete RG calculation.

Our formalism enables perturbative calculation of these quantities for general k. For example, we find that the density for $d < d_c$ is given by $n \sim A_k(\mathcal{D}t)^{-d/2}$ with

$$A_2 = \frac{1}{4\pi\epsilon} + \frac{2\ln 8\pi - 5}{16\pi} + O(\epsilon) \tag{2}$$

$$A_3 = \left(\frac{\sqrt{3}}{12\pi\epsilon}\right)^{1/2} + \frac{9\sqrt{2\pi}}{64} + O(\epsilon^{1/2}) \tag{3}$$

and for $d = d_c$

$$n(t) \sim \left(\frac{(k-2)!}{4\pi k^{1/(k-1)}}\right)^{1/(k-1)} \left(\frac{\ln t}{\mathcal{D}t}\right)^{1/(k-1)} . \tag{4}$$

where $\mathcal{D}$ is the usual diffusion constant.

Recent work in applying RG to this system includes that of Ohtsuki [12], in which the density is calculated, although with qualitatively different results than those above. First, Ohtsuki predicts that the amplitude for the asymptotic form of the density has the same reaction-rate constant dependence as the mean-field solution: $n \sim \Gamma^{-1}$ for $k = 2$. Second, the leading-order term in the ϵ-expansion for the density amplitude in [12] is of order unity. An RG scheme involving an external source of particles has been developed by Droz and Sasvári [13] which leads to scaling functions which confirm the decay exponent. Friedman *et al* attempted to calculate the density perturbatively, and concluded that it is necessary to perform a non-perturbative sum of all orders of n_0, the initial density, when calculating observables [14]. This infinite sum is exactly what we do in our calculation scheme. To our knowledge there has been no previous satisfactory, complete RG calculation.

A slightly different field-theory formalism for this system was developed in analogy with Bose-condensate calculations [15, 16]. This approach leads to a confirmation of the decay exponents as well. However, this method is not as readily generalized to an RG calculation as is the field-theory approach of Peliti.

The contents of this paper are as follows. In section 2 the system is defined via a master equation. This is then mapped to a second quantized representation, and in turn to a field theory. In section 3 the renormalization of the field theory and the calculation of observables is addressed. The latter requires summing infinite sets of diagrams, for which techniques are developed. With the formalism established, the density is then calculated in section 4, including correction terms and a discussion of the crossover timescales. An alternate method for calculating the leading-order amplitude, which does not involve RG, is discussed, and its apparent failure in the case $k = 2$. In section 5 the correlation function is calculated, and with it universal numbers for the fluctuations in particle number, both for the total system and for a small volume v. The local fluctuations in particle number are found to be divergent. Also the second moment of the correlation function is calculated, giving a correlation length scale. The case $d = d_c$ is addressed in section 6, and finally in section 7 a summary of these results is given, and the generalization to $kA \to \ell A$ is discussed.

2. The model

Consider a model of particles moving diffusively on a hypercubic lattice of size a, and having some probability of annihilating whenever k or more particles meet on a lattice site. This model is defined by a master equation for $P(\{n\}, t)$, the probability of particle configuration $\{n\}$ occurring at time t. Here $\{n\} = (n_1, n_2, \ldots, n_N)$, where n_i is the occupation number of the ith lattice site. The appropriate master equation is

$$\begin{aligned}\frac{\partial}{\partial t}P(\{n\},t) = \frac{\mathcal{D}}{a^2}\sum_i\sum_e\{(n_e+1)P(\ldots,n_i-1,n_e+1\ldots,t)-n_iP(\{n\},t)\}\\ +\lambda\sum_i\{(n_i+k)(n_i+k-1)\ldots(n_i+1)P(\ldots,n_i+k,\ldots,t)\\ -n_i(n_i-1)\ldots(n_i-k+1)P(\{n\},t)\}\end{aligned} \tag{5}$$

where i is summed over lattice sites, and e is summed over nearest neighbours of i. The first piece within curly brackets describes diffusion with diffusion constant $\mathcal{D}$, and the second describes annihilation with rate constant λ. The $P(\{n\}, 0)$ are given by a Poisson distribution for random initial conditions with average occupation number $\bar{n}_0$.

This master equation can be mapped to a second quantized-operator description, following a general procedure developed by Doi [17]. To summarize briefly, operators a and $a^\dagger$ are introduced at each lattice site, with commutation relations $[a_i, a_j^\dagger] = \delta_{ij}$. The vacuum ket is given by $a_i|0\rangle = 0$. The state ket of the system at time t is defined to be

$$|\phi(t)\rangle = \sum_{\{n\}} P(\{n\},t)\prod_i^N (a_i^\dagger)^{n_i}|0\rangle\,. \tag{6}$$

Then the master equation (5) can be written as

$$-\frac{\partial}{\partial t}|\phi(t)\rangle = \hat{H}|\phi(t)\rangle \tag{7}$$

with the non-Hermitian time-evolution operator

$$\hat{H} = -\frac{\mathcal{D}}{a^2}\sum_i\sum_e a_i^\dagger(a_e - a_i) - \lambda\sum_i(1-(a_i^\dagger)^k)a_i^k\,. \tag{8}$$

This has the formal solution $|\phi(t)\rangle = \exp(-\hat{H}t)|\phi(0)\rangle$.

To compute averages it is necessary to introduce the *projection state*

$$\langle| = \langle 0|\prod_i^N e^{a_i}\,. \tag{9}$$

Then for some observable $A(\{n\})$,

$$\langle\langle A(t)\rangle\rangle \equiv \sum_{\{n\}} A(\{n\})\,P(\{n\},t) = \langle|\hat{A}\exp(-t\hat{H})|\phi(0)\rangle \tag{10}$$

where $\hat{A}$ is the second quantized operator analogue of A. Note that $\langle|a_i^\dagger = \langle|$. Therefore any operator $\hat{A}$ represented in normal ordered form—where all the $a_i^\dagger$ have been commuted to the

left—can be written entirely in terms of the a_i. The operator corresponding to the density is simply a_i, while the correlation function $C(x_i, x_j)$ is given by $a_i^\dagger a_i a_j^\dagger a_j$ or $a_i\delta_{ij} + a_i a_j$. The importance of the δ-function term will be shown later when the renormalized correlation function is calculated.

The second quantized equation can in turn be mapped to a path integral, with variables ψ_i, $\hat{\psi}_i$ at each lattice site, via the coherent state representation [18, 19]. The action corresponding to (7) and (8) is

$$S[\hat{\psi}, \psi, t] = \sum_i \left[\int_0^t \mathrm{d}t \left\{ \hat{\psi}_i \partial_t \psi_i - \frac{\mathcal{D}}{a^2} \hat{\psi}_i \sum_e (\psi_e - \psi_i) - \lambda(1 - \hat{\psi}_i^k)\psi_i^k \right\} - \bar{n}_0 \hat{\psi}_i(0) - \psi_i(t) \right]. \tag{11}$$

The last two terms reflect the Poisson initial conditions and the projection state. The path integral form of (10) is then

$$\langle\langle A(t) \rangle\rangle = \mathcal{N} \int \prod_i \mathrm{d}\hat{\psi}_i \, \mathrm{d}\psi_i \, A(\psi(t)) \, \mathrm{e}^{-S[\hat{\psi}, \psi, t]}. \tag{12}$$

The normalization constant is given by $\mathcal{N}^{-1} = \int \prod_i \mathrm{d}\hat{\psi}_i \, \mathrm{d}\psi_i \, \mathrm{e}^{-S[\hat{\psi}, \psi, t]}$.

Next we take the continuum limit via $\sum_i \to \int \mathrm{d}^d x / a^d$, $\psi_i \to \psi(x)/a^d$, $\hat{\psi}_i \to \hat{\psi}(x)$, $\bar{n}_0 \to n_0 a^d$, and $\sum_e (\psi_e - \psi) \to a^2 \nabla^2 \psi$. The initial density is now n_0. The diffusion constant exhibits no singular behaviour in the renormalization of the theory, so it is absorbed into a rescaling of time, giving the action

$$S[\hat{\psi}, \psi, t] = \int \mathrm{d}^d x \left[\int_0^t \mathrm{d}t \left\{ \hat{\psi}(\partial_t - \nabla^2)\psi - \lambda_0(1 - \hat{\psi}^k)\psi^k \right\} - n_0 \hat{\psi}(0) - \psi(t) \right] \tag{13}$$

where $\lambda_0 = \lambda \mathcal{D}^{-1} a^{(k-1)d}$.

Treating (13) as a classical action gives the equations of motion

$$\frac{\delta S}{\delta \hat{\psi}(t')} = (\partial_{t'} - \nabla^2)\psi + k\lambda_0 \hat{\psi}^{k-1} \psi^k - n_0 \delta(t') = 0 \tag{14}$$

and

$$\frac{\delta S}{\delta \psi(t')} = -(\partial_{t'} + \nabla^2)\hat{\psi} + k\lambda_0(\hat{\psi}^k - 1)\psi^{k-1} - \delta(t' - t) = 0. \tag{15}$$

Assuming that ψ and $\hat{\psi}$ are spatially uniform gives the solution $\hat{\psi}(t' < t) = 1$ and (14) becomes

$$\frac{\partial}{\partial t}\psi = -k\lambda_0 \psi^k + n_0 \delta(t) \tag{16}$$

the mean-field rate equation. It is consistent that the rate constant is $k\lambda_0$, since λ_0 represents the rate at which the reaction occurs, and the resulting change in particle density is proportional to k. Consider shifting $\hat{\psi}$ by its classical solution: $\hat{\psi} \to 1 + \bar{\psi}$. The action which results is (up to an overall constant)

$$S[\bar{\psi}, \psi, t] = \int \mathrm{d}^d x \left[\int_0^t \mathrm{d}t \left\{ \bar{\psi}(\partial_t - \nabla^2)\psi + \sum_{i=1}^k \lambda_i \bar{\psi}^i \psi^k \right\} - n_0 \bar{\psi}(0) \right] \tag{17}$$

where $\lambda_i = \binom{k}{i}\lambda_0$. Note that the boundary terms introduced cancel the $\psi(t)$ term in (13).

Averages with respect to this action correspond to physical observables, and are denoted by double brackets. Single brackets are used for averages over the curly bracket part of (17). That is, for some observable A,

$$\langle\langle A(x,t)\rangle\rangle = \left\langle A(x,t)\, e^{n_0 \int d^d x\, \bar{\psi}(x,0)} \right\rangle . \tag{18}$$

This is already normalized, since $\langle \exp\{n_0 \bar{\psi}(p=0)\}\rangle = 1$.

The dimensions of the various quantities in (17), expressed in terms of momentum, are

$$[t] = p^{-2} \qquad [\bar{\psi}(x)] = p^0 \qquad [\psi(x)] = p^d \qquad [\lambda_i] = p^{2-(k-1)d} . \tag{19}$$

The couplings become dimensionless at the traditionally accepted value of the critical dimension, $d_c = 2/(k-1)$ [3,4]. The relative dimensions of ψ and $\bar{\psi}$ are arbitrary, but this choice is the most natural. Any other choice of dimensions would introduce n_0-dependence into the projection state, and cause the couplings λ_i to have different dimensions.

3. Renormalization of observables

The scheme developed for renormalizing the theory follows conventional RG analysis [20]. In this vein a renormalized coupling is introduced, and shown to have a stable fixed point of order ϵ. This is the small parameter of the theory, and not n_0, which implies that the computation of observables requires summing over an infinite set of diagrams, corresponding to all powers of n_0 in (18). This infinite sum must be grouped into sets of diagrams whose sums give a particular order of the coupling constant. It will be shown below that this grouping is given by the number of loops. That is, the infinite set of tree diagrams sum to give the leading-order term in the coupling, the one-loop diagrams the next-order term, and so on. However, before addressing the calculation of observables we turn to the renormalization of the theory.

3.1. Renormalization

To renormalize the theory all that is required is coupling-constant renormalization. This is because the set of vertices in (17) allow no diagrams which dress the propagator, implying there is no wavefunction renormalization. As a consequence the bare propagator is the full propagator for the theory.

To determine which couplings get renormalized one first needs to identify the primitively divergent vertex functions. A general correlation function with ℓ ψ's and m $\bar{\psi}$'s has the dimension

$$[\langle \psi(1)\ldots\psi(\ell)\bar{\psi}(\ell+1)\ldots\bar{\psi}(\ell+m)\rangle] = p^{d\ell} \tag{20}$$

where $(1) = (x_1, t_1)$. The Green's function $G^{(\ell,m)}(p_1, s_1, \ldots, p_{\ell+m}, s_{\ell+m})$ is calculated by Fourier and Laplace transforming the correlation function above, and factoring out overall p- and s-conserving δ-functions. The dimensions of this quantity are

$$[G^{(\ell,m)}] = p^{d+2-2\ell-(d+2)m} . \tag{21}$$

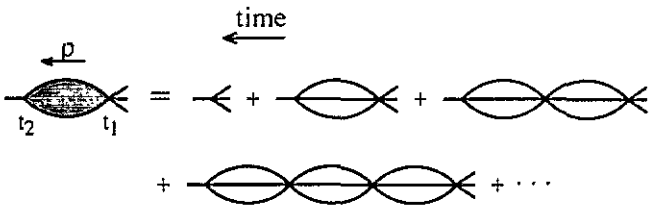

Figure 1. Sum of all the diagrams which contribute to $\lambda(p, t_2 - t_1)$. Shown here is the case $k = 3$, $i = 1$. These diagrams can be summed exactly, and are the same for all i.

The dimensions of the vertex functions $\Gamma^{(\ell,m)}$ are given by the Green's functions with the $\ell + m$ external propagators stripped off:

$$[\Gamma^{(\ell,m)}] = [G^{(\ell,m)}/(G^{(1,1)})^{\ell+m}] = p^{2-d(m-1)}. \tag{22}$$

The vertex functions with $m \leqslant k$ are those which are primitively divergent for $d \leqslant d_c$. Since vertices can only connect k $\bar{\psi}$'s to some number less than or equal to k ψ's, then it follows that the primitively divergent diagrams have $m = k$ and $\ell \leqslant k$.

A general $\bar{\psi}^i\psi^k$ vertex is renormalized by the set of diagrams shown in figure 1. In these diagrams the propagator $G_0(p, t) = \langle\psi(p, t)\bar{\psi}(-p, 0)\rangle = e^{-p^2 t}$ for $t > 0$, $G_0 = 0$ for $t < 0$, and is represented by a plain line. Note that this sum is the same for all i, that is, all vertices renormalize identically. This is a reflection of the fact that there is a only one coupling in the theory. These diagrams can be summed to all orders, as noted in [11]. In (p, t) space the temporally extended vertex function $\lambda(p, t_2 - t_1)$ is given by

$$\lambda(p, t_2 - t_1) = \lambda_0\delta(t_2 - t_1) - \lambda_0^2 I(p, t_2 - t_1) + \lambda_0^3 \int_{t_1}^{t_2} dt' I(p, t_2 - t')I(p, t' - t_1) - \cdots \tag{23}$$

where $I(p, t)$ is the $k - 1$ loop integral

$$I(p, t) = k! \int \prod_i^k \left(\frac{d^d p_i}{(2\pi)^d}\right)(2\pi)^d \delta\left(p - \sum_i^k p_i\right) \exp\left(-\sum_i^k p_i^2 t\right). \tag{24}$$

The δ-function can be written in integral form, which turns the integral into a product of k Gaussian integrals. This gives

$$I(p, t) = B_k t^{-(k-1)d/2} e^{-p^2 t/k} \tag{25}$$

where

$$B_k = \frac{k!}{k^{d/2}}\left(\frac{1}{4\pi}\right)^{(k-1)d/2}. \tag{26}$$

Taking the Laplace transform, $\lambda(p, s) = \int_0^\infty dt\, e^{-st}\lambda(p, t)$, makes (23) a geometric sum:

$$\lambda(p, s) = \frac{\lambda_0}{1 + \lambda_0 B_k \Gamma(\epsilon/d_c)(s + p^2/k)^{-\epsilon/d_c}} \tag{27}$$

where the d and k have been exchanged for ϵ and d_c. For a general $\bar{\psi}^i\psi^k$ vertex the λ_0 in the numerator is replaced by $\lambda_i = \binom{k}{i}\lambda_0$, and the denominator is unchanged. Therefore the small s and p form of the vertex function is independent of λ_0 for all i.

The vertex function (27) is used to define a renormalized coupling. Using the momentum κ as a normalization point, we define the dimensionless renormalized coupling to be $g_R = \kappa^{2\epsilon/d_c}\lambda(s, p)|_{s=\kappa^2, p=0}$, and the dimensionless bare coupling $g_0 = \kappa^{2\epsilon/d_c}\lambda_0$. The β function is defined by

$$\beta(g_R) \equiv \kappa\frac{\partial}{\partial\kappa}g_R = -\frac{2\epsilon}{d_c}g_R + \frac{2\epsilon}{d_c}B_k\Gamma\left(\frac{\epsilon}{d_c}\right)g_R^2. \tag{28}$$

It is exactly quadratic in g_R and has a fixed point $\beta(g_R^*) = 0$ at

$$g_R^* = \left\{B_k\Gamma(\epsilon/d_c)\right\}^{-1}. \tag{29}$$

The fixed point is of order ϵ. From the definition of g_R, equation (27), and equation (29), it follows that $g_R^{-1} = g_0^{-1} + g_R^{*-1}$, or

$$g_0 = \frac{g_R}{1 - g_R/g_R^*} = g_R + \frac{g_R^2}{g_R^*} + \cdots. \tag{30}$$

This will be used to exhange an expansion in g_0 calculated in perturbation theory for an expansion in g_R.

3.2. Calculation scheme

Next we develop a Callan–Symanzik equation for the theory. Given a correlation function

$$F^{(m)}(t, \lambda_0) \equiv \left\langle \psi(x, t)\left(\int \mathrm{d}^d y\, \bar{\psi}(y, t = 0)\right)^m \right\rangle \tag{31}$$

the lack of dependence on the normalization scale can be expressed via

$$\left[\kappa\frac{\partial}{\partial\kappa} + \beta(g_R)\frac{\partial}{\partial g_R}\right]F^{(m)}(t, \kappa, g_R) = 0. \tag{32}$$

From dimensional analysis $[F^{(m)}] = p^{d-md}$, implying

$$\left[\kappa\frac{\partial}{\partial\kappa} - 2t\frac{\partial}{\partial t} - d + md\right]F^{(m)} = 0. \tag{33}$$

We are interested in the density $n(t, n_0, g_R, \kappa) = \sum_m n_0^m F^{(m)}/m!$. Substituting (33) into (32), and summing to get the density gives the equation

$$\left[2t\frac{\partial}{\partial t} - dn_0\frac{\partial}{\partial n_0} + \beta(g_R)\frac{\partial}{\partial g_R} + d\right]n(t, n_0, g_R, \kappa) = 0. \tag{34}$$

This is solved by the method of characteristics, and has the solution

$$n(t, n_0, g_R, \kappa) = (\kappa^2 t)^{-d/2} n\left(\kappa^{-2}, \tilde{n}_0(\kappa^{-2}), \tilde{g}_R(\kappa^{-2}), \kappa\right) \tag{35}$$

with the characteristic equations for the running coupling and initial density,

$$2t\frac{\partial \tilde{n}_0}{\partial t} = -d\tilde{n}_0 \qquad \tilde{n}_0(t) = n_0 \tag{36}$$

$$2t\frac{\partial \tilde{g}_R}{\partial t} = \beta(\tilde{g}_R) \qquad \tilde{g}_R(t) = g_R\,. \tag{37}$$

Because of the simple form of the β function, the running coupling can be found exactly:

$$\tilde{n}_0(t') = (t/t')^{d/2} n_0 \tag{38}$$

$$\tilde{g}_R(t') = g_R^* \left(1 + \frac{g_R^* - g_R}{g_R (t/t')^{\epsilon/d_c}}\right)^{-1}\,. \tag{39}$$

One then sets $t' = \kappa^{-2}$ and plugs the result into (36). Notice that in the large-t limit $\tilde{g}_R \to g_R^*$.

In conventional RG analysis the mechanics developed above is used in the following way: one calculates an expansion in powers of g_0, and then converts this to an expansion in powers of g_R via (30). As long as the expansion coefficients are non-singular in ϵ, then the g_R expansion can be related to an ϵ-expansion via (35). That is, we substitute $t \to \kappa^{-2}$, $n_0 \to \tilde{n}_0$, $g_R \to \tilde{g}_R$, in the g_R expansion, and multiply by the overall factor shown in (35). Then for large t, $\tilde{g}_R \to g_R^*$ giving $n(t, n_0, \lambda_0)$ as an expansion in powers of ϵ. For a given coefficient in the g_R expansion we keep only the leading term for large n_0, since $\tilde{n}_0 \sim t^{d/2}$, and so the subleading terms in $\tilde{n}_0$ will correspond to sub-leading terms in t.

The identification of the leading terms in g_0 is less straightforward than it is in conventional RG calculations, since the sum over all powers of n_0 must be taken into account. For the density, tree diagrams are of order $g_0^i n_0^{1+i(k-1)}$ for integer i. Diagrams with j loops are of order $g_0^i n_0^{1+i(k-1)-j}$. Since the addition of loops makes the power of g_0 higher relative to the power of n_0, we hypothesize that the number of loops will serve as an indicator of the order of g_0. This will be shown to be the case via explicit calculation.

3.3. Tree diagrams

To calculate all possible diagrams of a given number of loops it is necessary to develop two tree-level quantities: the classical density and the classical-response function. The term classical means averaged with respect to the classical action, which is the action (17), but with only the $\bar{\psi}\psi^k$ vertex. The classical density is given by sum of all tree diagrams which terminate with a single propagator, as shown in figure 2, and is represented graphically by a broken line. These diagrams are evaluated in momentum space. From (18) it follows that the $\bar{\psi}(t=0)$ in the initial state all have $p = 0$, so all diagrams at tree level have $p = 0$.

Shown also in figure 2 is an exact graphical relation for the infinite sum, which is equivalent to the mean-field rate equation (16). This can be seen by considering the diagram in position space, and acting with $(\partial_t - \nabla^2)$, the inverse of the Green's function G_0, on either side of the diagrammatic equation. Note that the combinatoric factors involved in attaching the full-density lines to vertices is different than for propagators, which is discussed in the appendix. This equation has the exact and asymptotic (large-t) solutions

$$n_{cl}(t) = \frac{n_0}{(1 + k(k-1)n_0^{k-1}\lambda_0 t)^{1/(k-1)}} \sim \left(\frac{1}{k(k-1)\lambda_0}\right)^{1/(k-1)} t^{-1/(k-1)}\,. \tag{40}$$

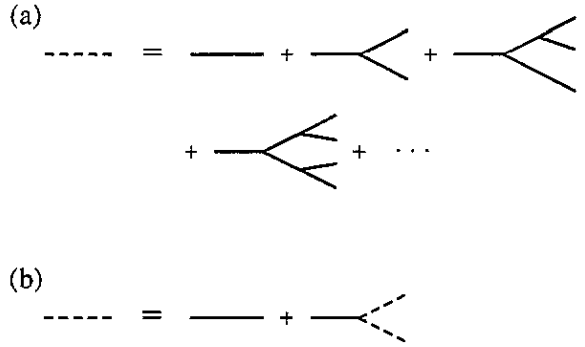

Figure 2. The classical density, represented as a broken line, is given by (*a*) the complete sum of tree diagrams, and (*b*) an integral equation. The latter is equivalent to the mean-field rate equation. Shown here is the case $k = 2$.

Figure 3. The response function, shown as a heavy line, is given as a sum of the bare propagator plus a term with a single vertex connecting $k-1$ full density lines, plus a term with two vertices, and so on. Shown here is $k = 3$. These diagrams can be summed exactly.

The asymptotic solution depends on the coupling strength, but not the initial density.

The response function is defined by

$$G(p, t_2, t_1) \equiv \langle\langle \psi(-p, t_2)\bar{\psi}(p, t_1)\rangle\rangle \tag{41}$$

and the classical response function is the above quantity with only tree diagrams included in the averaging. It is represented graphically by a heavy line, and is given by the sum of diagrams as shown in figure 3. Note that the only p-dependence is that of the bare propagator. That is, the density lines all carry no momentum. The time dependence of the propagators connecting the vertices cancels to leave only overall dependence on t_1, t_2. The vertices are now symmetric under interchange, so we can trade the requirement that they be ordered for a factor of $1/n_v!$, where n_v is the number of vertices. The sum of diagrams is then identified as the Taylor expansion of an exponential, giving

$$\begin{aligned} G_{cl}(p, t_2, t_1) &= e^{-p^2(t_2-t_1)} \exp\left\{-k^2\lambda_0 \int_{t_1}^{t_2} dt\, n_{cl}(t)^{k-1}\right\} \\ &= e^{-p^2(t_2-t_1)} \left(\frac{1 + k(k-1)n_0^{k-1}\lambda_0 t_1}{1 + k(k-1)n_0^{k-1}\lambda_0 t_2}\right)^{k/(k-1)} . \end{aligned} \tag{42}$$

The extra factor of k associated with each $-k\lambda_0$ vertex is a consequence of the combinatorics (see appendix). From (18) it follows that $\langle\langle \psi(t)\bar{\psi}(0)\rangle\rangle = \partial\langle\langle \psi(t)\rangle\rangle/\partial n_0$ or $G(p = 0, t, 0) = \partial n(t)/\partial n_0$. This relation should also hold for the classical density and response function, as is the case for the solution above.

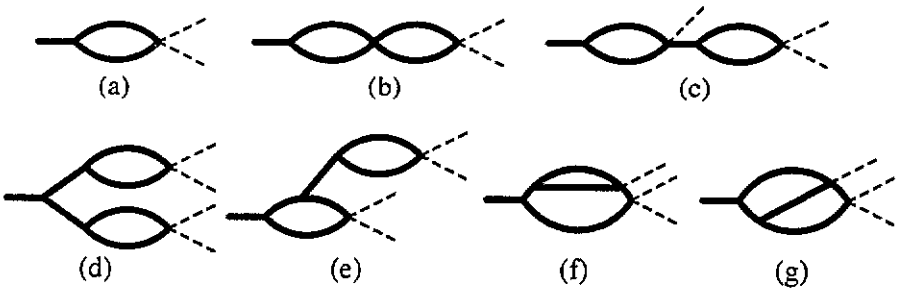

Figure 4. One- and two-loop diagrams for $k = 2$. By using the response function all such diagrams are included. Diagram (a) is used to calculate the amplitude correction.

4. Density calculation

With the classical or tree-level solutions of the previous section, and the renormalization scheme developed above, the asymptotic form of the density can now be calculated. The solution for the tree diagrams in terms of g_0, or λ_0, is given by (40). To leading order in g_R one just replaces λ_0 with $g_R\kappa^{2\epsilon/d_c}$. For large t the running coupling $\tilde{g}_R \to g_R^*$, which gives

$$n^{(0)}(t) = \frac{n_0}{(1 + k(k-1)n_0^{k-1} g_R^* t^{(k-1)d/2})^{1/(k-1)}}. \tag{43}$$

The superscript on the density refers to the number of loops in the calculation. The asymptotic form of this expression is

$$n^{(0)}(t) \sim \left(\frac{(k-2)!}{2\pi(k-1)k^{1/(k-1)}\epsilon}\right)^{1/(k-1)} t^{-d/2} + O(\epsilon^{1-1/(k-1)}). \tag{44}$$

The term in parentheses is the leading-order term in A_k, the amplitude of the $t^{-d/2}$ component of the density.

4.1. Amplitude corrections for $k = 2$

Next, the corrections from the higher-loop diagrams are calculated. It will be shown that adding a loop makes the sum of diagrams an order $g_R^{1/(k-1)}$ higher. At $k - 1$ loops the diagrams will contain a singularity in ϵ, caused by the appearance of the first primitively divergent diagram. However, this singularity is cancelled when the g_R^2 correction to g_0 in (30) is included in the tree diagram sum. In general the higher-order terms in (30) will cancel all divergences in the coefficients of the g_R expansion. This will be illustrated in the one-loop corrections for $k = 2$.

The infinite sum of all one-loop diagrams can be written in terms of the classical response function found above. The sum of diagrams is shown in figure 4. Expressing this graph in integral form

$$n^{(1)}(t, n_0, g_0, \kappa) = 2\int dt_2\, dt_1 \frac{d^d p}{(2\pi)^d} G_{cl}(0, t, t_2)(-2\lambda_0)G_{cl}(p, t_2, t_1)^2(-\lambda_0)n_{cl}(t_1)^2 \tag{45}$$

where the time integrals are over $0 < t_1 < t_2 < t$. Taking the large-n_0 limit of (45) to extract the asymptotic part gives

$$n^{(1)}(t, n_0, g_0, \kappa) = \frac{1}{t^2}\int dt_2\, dt_1 \frac{d^d p}{(2\pi)^d} t_2^{-2} e^{-2p^2(t_2 - t_1)} t_1^2 + O(n_0^{-1}). \tag{46}$$

Notice that this is independent of g_0, consistent with the prediction that the one-loop diagrams are of order g_R^0 and provide a correction to the leading term in (44). The integral can be done exactly. Expressing the leading piece in terms of g_R^*, and the rest as an expansion in ϵ:

$$n^{(1)}(t, n_0, g_0, \kappa) = t^{-d/2}\left(\frac{1}{2g_R^*} - \frac{2C+5}{16\pi} + O(\epsilon)\right) \tag{47}$$

where C is Euler's constant. The correction to the tree-level component due to the subleading term in $g_0(g_R)$ is

$$n^{(0)}(t, g_R) = \frac{1}{2g_R}t^{-d/2} - \frac{1}{2g_R^*}t^{-d/2} + O(g_R). \tag{48}$$

The singular parts of the g_R^0 coefficient cancel as advertised. Combining (47) and (48) and making use of the Callan–Symanzik solution (35) gives

$$A_2 = \frac{1}{4\pi\epsilon} + \frac{2\ln 8\pi - 5}{16\pi} + O(\epsilon). \tag{49}$$

The two-loop diagrams are also shown in figure 4. They all contribute to order g_R^1. Unfortunately, we are unable to evaluate diagrams (f, g) due to the complicated time dependence of the vertices, which prohibits calculation of the $O(\epsilon)$ term in A_2. The most singular of the diagrams, (b)–(d), are of order ϵ^{-2}. These diagrams can be calculated and the singular pieces cancel as expected.

Note that the asymptotic, or large-n_0, limits of the classical density and the classical response function are of order n_0^0, which implies that the asymptotic time dependence of the density, calculated to any number of loops, will be $t^{-d/2}$. Therefore the decay exponent is exact to all orders in ϵ.

The cancellation of the singularities which appear in the g_R expansion can be most easily understood by viewing the correction terms in (30) as counterterms introduced to cancel primitive divergences. That is, considering $\delta g_R = g_R^2/g_R^* + O(g_R^3)$, and calculating the first-order term in δg_R at tree level gives a diagram similar to figure 4(a), but with the counterterm in place of the loop. This diagram, when added to the one-loop diagram, cancels the singularity in the g_R^0 coefficient. Two-loop diagrams (b)–(f) can be viewed as primitively divergent loops added to the one-loop diagram (a). The order δg_R terms in the one-loop diagram are equivalent to diagrams (b)–(f) with a counterterm in place of the additional loop, and will cancel the divergences in these diagrams. Diagram (g) differs in that it is not a primitively divergent loop 'added on' to diagram (a), but it is also non-singular.

4.2. Amplitude corrections for $k = 3$

The one- and two-loop diagrams for $k = 3$ are shown in figure 5. The one-loop diagram contains no singularity, and gives the order g_R^0 correction to (44). The asymptotic piece is given by the integral

$$n^{(1)}(t, n_0, g_0, \kappa) = \frac{3}{2t^{3/2}}\int dt_2\, dt_1 \frac{d^d p}{(2\pi)^d} t_2^{-2}\, e^{-2p^2(t_2-t_1)} t_1^{3/2} + O(n_0^{-1}). \tag{50}$$

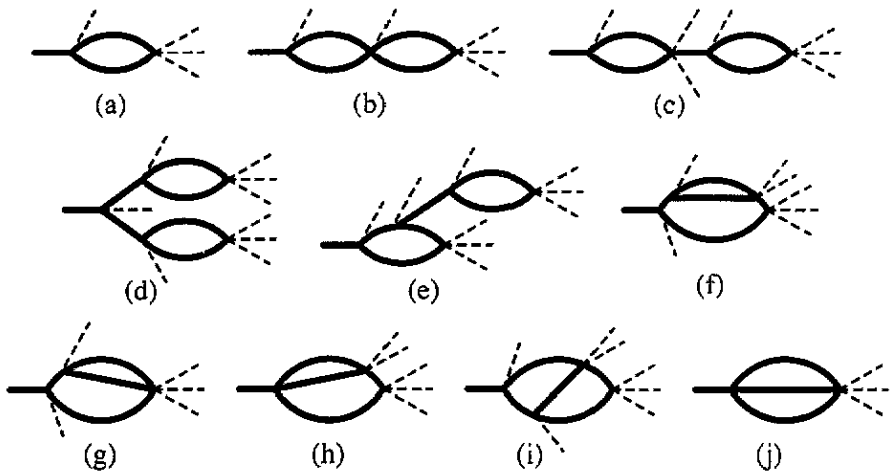

Figure 5. One- and two-loop diagrams for $k = 3$. Diagram (a) contains no ϵ singularity, and is used to calculate the amplitude correction.

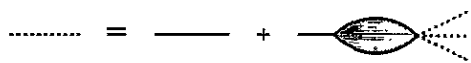

Figure 6. Exact diagrammatic equation for $n_{dt}(t)$, the sum of the dressed-tree diagrams.

Performing the integral and using (35) we find the amplitude

$$A_3 = \left(\frac{\sqrt{3}}{12\pi\epsilon}\right)^{1/2} + \frac{9\sqrt{2\pi}}{64} + O(\epsilon^{1/2}). \tag{51}$$

The two-loop diagrams are of order $g_R^{1/2}$, although, similar to the case of $k = 2$, we are unable to calculate diagrams (f)–(i). The only diagram with a singularity is (j) which can be calculated to demonstrate that the $g_R^{1/2}$ coefficient is non-singular, as expected.

4.3. Dressed tree calculation

There exists an alternate method for calculating the leading-order amplitude of the density which does not require using the RG formalism. However, there is a discrepancy between this method, the dressed-tree sum, and the RG in the case $k = 2$. We present the dressed-tree calculation below, and an explanation for why we believe the RG to be correct for $k = 2$.

Consider summing the most divergent diagrams for each power of λ_0 and n_0. This is equivalent to summing the dressed-tree diagrams, which are tree diagrams with all the vertices replaced by the temporally extended vertex function (23). The sum of these diagrams, $n_{dt}(t)$, satisfies the diagrammatic equation shown in figure 6, where n_{dt} is represented by a dotted line. As with the tree-diagram sum, acting on this equation with the propagator inverse $(\partial_t - \nabla^2)$ gives a differential equation

$$\partial_t n_{dt}(t) = n_0\delta(t) - k\int_0^t dt'\,\lambda(p = 0, t - t')n_{dt}(t')^k. \tag{52}$$

Laplace transforming the equation gives

$$sn(s) - n_0 = -k\lambda(0,s)n^k(s) \tag{53}$$

where $n(s) = \int_0^\infty dt\, e^{-st} n(t)$ and $n^k(s) = \int_0^\infty dt\, e^{-st} n(t)^k$. The transform of the vertex function $\lambda(0,s)$ is known exactly, and is given by (27). However, the equation is not algebraic in $n(s)$, making it difficult to obtain an exact solution. To proceed, we assume $n_{dt} \sim \tilde{A} t^{-\alpha}$, so that for small s, $n(s) \sim \tilde{A}\Gamma(1-\alpha)s^{\alpha-1}$. Also, $n^k(s) \sim \tilde{A}^k \Gamma(1-k\alpha)s^{k\alpha-1}$, and $\lambda(0,s) \sim s^{\epsilon/d_c}/(B_k\Gamma(\epsilon/d_c))$. The transform of $n_{dt}(t)^k$ is calculated by imposing a small-t regulator, which is justified as the transform of the exact solution does exist, and then taking the small-s limit. The amplitude which results is independent of the regulator. Substituting these in to (53) and taking the small-s limit of the equation gives $\alpha = d/2$, and the amplitude

$$\tilde{A}^{k-1} = \frac{B_k \Gamma\left(\frac{2\epsilon}{(k-1)}\right) \Gamma\left(\frac{(k-2)}{(k-1)} + \frac{\epsilon}{2}\right) \left(\frac{1}{(k-1)} - \frac{k\epsilon}{2}\right)}{k\,\Gamma\left(\frac{(k-2)}{(k-1)} + \frac{k\epsilon}{2}\right)}. \tag{54}$$

For $k \neq 2$ the non-singular Γ functions cancel to leading order in ϵ, with the result $\tilde{A} = A_k + O(\epsilon^0)$. However, for $k = 2$ all the Γ functions are singular, which has the consequence that $\tilde{A}_2 = 2A_2 + O(\epsilon^0)$. In light of this, it seems necessary to find an explanation why this particular set of diagrams sums to give the proper leading-order term for general k, but not for $k = 2$, if indeed the RG is giving the correct leading-order term.

Consider the set of dressed one-loop diagrams. That is, the set of diagrams given in figure 4(*a*) and figure 5(*a*), but again with each vertex replaced by the temporally extended vertex function. While it would be difficult to calculate this sum, it is possible to see a property specific to $k = 2$ that they have. The analogue of the classical densities in these diagrams is the dressed-tree density $n_{dt} \propto t^{-d/2}$. Therefore for general k there is a time integral over $t^{-kd/2}$, or $t^{-k/(k-1)-k\epsilon/2}$. This time integral will be in the form of a Laplace convolution integral, similar to (52). Using a regulated transform as before, the amplitude of the small-s limit will be proportional to $\Gamma\big((k-2)/(k-1) + k\epsilon/2\big)$. For $k \neq 2$ this is non-singular at $\epsilon = 0$, but for $k = 2$ it is of order ϵ^{-1}. Therefore these diagrams are part of the leading-order amplitude for $k = 2$. As a result, it would appear that the discrepancy is a consequence of the failure of the dressed-tree method, and not of the RG.

4.4. Crossovers

There are two crossover timescales in this system, one given by n_0 and one by λ_0. For the coupling constant crossover we consider the large-t expansion of (39)

$$\tilde{g}_R = g_R^* \left(1 - \lambda_0^{-1} t^{-\epsilon/d_c} + O(t^{-2\epsilon/d_c})\right). \tag{55}$$

Including the correction term in the density calculation will generate a λ_0-dependent term proportional to $t^{-d/2-\epsilon/d_c}$. From (55) it follows that the characteristic crossover time is given by $t_{\lambda_0} \sim (\epsilon/\lambda_0)^{d_c/\epsilon}$. In terms of the constants in the master equation, $t_\lambda \sim a^2 \mathcal{D}^{-1} (\epsilon \mathcal{D}/a^2\lambda)^{d_c/\epsilon}$. For small ϵ, or large λ_0, the time required to reach the fluctuation-dominated regime becomes small.

The n_0 crossover is calculated by keeping the order n_0^{-1} terms in the integrals performed above. These terms will pick up an extra factor of $t^{-d/2}$ when put into (35), so the exponent

of the leading n_0-dependent term in the density is t^{-d}. The characteristic crossover time is only weakly ϵ-dependent, and is given by $t_{n_0} \sim \mathcal{D}^{-1} n_0^{-2/d} = a^2 \mathcal{D}^{-1} \tilde{n}_0^{-2/d}$.

If the n_0 crossover occurs first, then for intermediate times $t_{n_0} \ll t \ll t_{\lambda_0}$ one would expect the system to obey the asymptotic form of the mean-field solution. That is, $n \sim [k(k-1)\lambda_0 t]^{-1/(k-1)}$. If the λ_0 crossover occurs first it is less clear what the behaviour in the intermediate regime will be. The contribution from the tree diagrams will be exactly (43), which does not become a power law until the n_0 crossover is reached. This is complicated even further by the higher-order diagrams.

5. Correlation function calculation

The density correlation function is given by

$$C(x,t) = \langle\langle \big(\psi(x,t) + \delta^d(x)\big)\psi(0,t) \rangle\rangle \tag{56}$$

where the δ-function is a consequence of the second quantized operators developed in section 2. A Callan–Symanzik equation for the correlation function can be developed in a similar fashion as before. Consider the function

$$F^{(m)}(p,t,\lambda_0) \equiv \int \mathrm{d}^d x\, \mathrm{e}^{-\mathrm{i}p\cdot x} \left\langle \big(\psi(x,t) + \delta^d(x)\big)\psi(0,t) \left(\int \mathrm{d}^d y\, \tilde{\psi}(y, t=0) \right)^m \right\rangle . \tag{57}$$

Dimensional analysis gives $[F^{(m)}] = p^{d-md}$. The correlation function $C(p,t)$ is given by $\sum_m n_0^m F^{(m)}/m!$. This leads to the equation

$$\left[2t\frac{\partial}{\partial t} - p\frac{\partial}{\partial p} - dn_0\frac{\partial}{\partial n_0} + \beta(g_\mathrm{R})\frac{\partial}{\partial g_\mathrm{R}} + d \right] C(p,t,n_0,g_\mathrm{R},\kappa) = 0 \tag{58}$$

which has the solution

$$C(p,t,n_0,g_\mathrm{R},\kappa) = (\kappa^2 t)^{-d/2} C\big(\tilde{p}(\kappa^{-2}), t=\kappa^{-2}, \tilde{n}_0(\kappa^{-2}), \tilde{g}_\mathrm{R}(\kappa^{-2}), \kappa\big) \tag{59}$$

with $\tilde{g}_\mathrm{R}$ and $\tilde{n}_0$ given by (38) and (39), and

$$\tilde{p}(t') = p\sqrt{\frac{t}{t'}} . \tag{60}$$

Again the calculation of the right-hand side of (59) is divided into the number of loops. First the connected and disconnected pieces are separated

$$C(p,t) = n(t) + g(p,t) + \delta^d(p) n(t)^2 . \tag{61}$$

The first term on the right-hand side is a consequence of the δ-function in (56), and is considered part of the connected correlation function. The disconnected tree-level graphs are of the order $g_0^i n_0^{2+i(k-1)}$, and represent the leading-order terms in the correlation function. This is reasonable, as the classical solution of this system corresponds to the absence of correlations. The connected tree-level diagrams, which are the leading terms in $g(p,t)$, are of order $g_0^i n_0^{1+i(k-1)}$ and represent the leading corrections due to fluctuations. The tree-level

and one-loop diagrams for $g(p,t)$ in the case $k = 2$ are shown in figure 7. Diagram (a) can be calculated explicitly to give the leading term

$$g(p,t) = -\frac{1}{4\pi\epsilon} t^{-d/2} f_2(p^2 t) + \mathrm{O}(\epsilon^0) \qquad f_2(x) = -\frac{\mathrm{e}^{-2x}}{4x^3} + \frac{1}{4x^3} - \frac{1}{2x^2} + \frac{1}{2x}. \tag{62}$$

The function $f_2(x)$ is regular at $x = 0$, with $f_2(0) = \frac{1}{3}$. For large x, $f_2(x) \sim 1/(2x)$.

We are unable to evaluate the one-loop diagrams analytically for general p, although it is possible to calculate an expansion in p^2, which we have done to order p^2. For the connected correlation function, $\bar{C}(p,t) = n(t) + g(p,t)$,

$$\bar{C}(p,t) = \left[\frac{1}{6\pi\epsilon} + \frac{9\ln 8\pi - 26}{108\pi} + \left(\frac{1}{24\pi\epsilon} + \frac{15\ln 8\pi - 19}{720\pi}\right) p^2 t + \ldots\right] t^{-d/2} + \mathrm{O}(\epsilon). \tag{63}$$

With the expansion above it is possible to calculate the second moment of $\bar{C}(x,t)$, giving a length scale for the correlations. For $\bar{C}(p,t) = A + Bp^2 + \cdots$ the second moment $-\xi^2 \equiv \int \mathrm{d}^d x\, x^2 \bar{C}(x,t) / \int \mathrm{d}^d x \bar{C}(x,t) = -2B/A$. The negative sign in the definition of ξ is required since the second moment is negative, indicating that the particles are negatively correlated at larger distances. For $k = 2$ the length ξ is given by

$$\xi_2 = \sqrt{t}\left(\frac{\sqrt{2}}{2} + \frac{73\sqrt{2}}{360}\epsilon + \mathrm{O}(\epsilon^2)\right). \tag{64}$$

The correlation function can be used to calculate the fluctuations in the density. For example, the fluctuations in the local density are given by integrating $C(p,t)$ over p. However, the p-independent term causes this integral to diverge. One can consider the fluctuations of the average particle number of fiducial volume v. This is given by

$$(\delta N_v)^2 = v \int_v \mathrm{d}x\, \bar{C}(x,t) = vn(t) + \mathrm{O}(v^2) \tag{65}$$

where translational invariance is assumed. The order v contribution originates from the δ-function in (56). For small v the fluctuations go as $\delta N_v \sim \sqrt{vn(t)}$, which is universal.

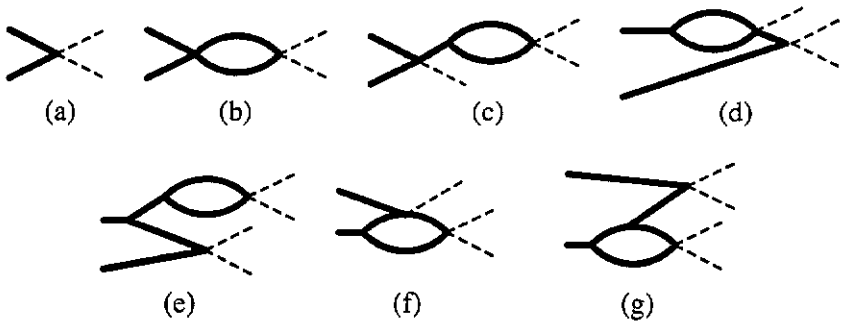

Figure 7. The diagrams for the connected correlation function at tree level and one loop, for $k = 2$.

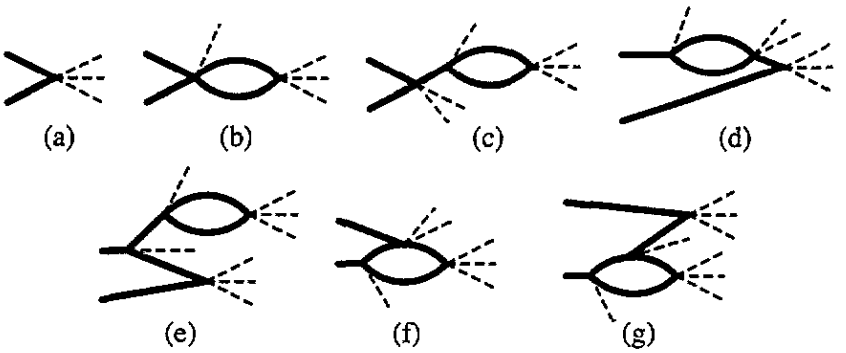

Figure 8. The diagrams for the connected correlation function at tree level and one loop, for $k = 3$.

Also, $\delta N_v/N_v \sim 1/\sqrt{vn(t)}$, which diverges as v goes to zero, consistent with the local fluctuations being divergent.

The fluctuations in the total number of particles is given by $V\bar{C}(p=0,t)$, where V is the volume of the system. When divided by the square of the average number of particles, $V^2n(t)^2$, this gives

$$\frac{(\delta N)^2}{N^2}V = \left(\frac{8\pi}{3}\epsilon - \frac{36\pi \ln 8\pi - 76\pi}{6}\epsilon^2 + O(\epsilon^3)\right)t^{-d/2}. \tag{66}$$

Note that all these fluctuation terms would be negative if the δ-function term were neglected. That is, $\langle\langle\psi(x)^2\rangle\rangle < 0$, a demonstration that the fields introduced via the path integral formulation of [18] are complex.

The diagrams contributing to $g(p,t)$ for $k = 3$ are shown in figure 8. The leading-order term for the connected part is

$$g(p,t) = -\left(\frac{\sqrt{3}}{12\pi\epsilon}\right)^{1/2} t^{-d/2} f_3(x) + O(\epsilon^0) \qquad f_3(x) = \frac{e^{-2x}3\sqrt{\pi}\,\mathrm{erfi}(\sqrt{2x})}{16\sqrt{2}x^{5/2}} - \frac{3}{8x^2} + \frac{1}{2x} \tag{67}$$

where $\mathrm{erfi}(x) = -i\,\mathrm{erf}(ix) = (2/\sqrt{\pi})\int_0^x dy\, e^{y^2}$. The function $f_3(x)$ is also regular, with $f_3(0) = \frac{2}{5}$ and $f_3(x) \sim 1/(2x)$ for large x.

The one-loop diagrams can be calculated as an expansion in p^2, with the net result

$$\bar{C}(p,t) = \left[\frac{3}{10}\left(\frac{\sqrt{3}}{3\pi\epsilon}\right)^{1/2} + \frac{81\sqrt{2\pi}}{1600} + \frac{288}{875}\sqrt{\frac{2}{\pi}} + \left(\frac{4}{35}\left(\frac{\sqrt{3}}{3\pi\epsilon}\right)^{1/2} + \frac{9\sqrt{2\pi}}{98} - \frac{27\,546}{42\,875}\sqrt{\frac{2}{\pi}}\right)p^2 t + \cdots\right]t^{-d/2} + O(\epsilon). \tag{68}$$

In this case the sign of the second moment of the correlation function depends on ϵ. For $\epsilon < 0.4$ the second moment is negative, and the resulting length scale is given by

$$\xi_3 = \sqrt{t}\left(\frac{4}{\sqrt{21}} + \left(\frac{2\sqrt{3}}{21}\right)^{1/2}\left(\frac{711\pi}{2240} - \frac{2217}{490}\right)\epsilon^{1/2} + O(\epsilon)\right). \tag{69}$$

The fluctuations in total particle number are given by

$$\frac{(\delta N)^2}{N^2}V = \left(\frac{6\sqrt{\pi}}{5}\epsilon^{1/2} + (2\pi\sqrt{3})^{1/2}\left(\frac{1152}{875} - \frac{189\pi}{400}\right)\epsilon + O(\epsilon^{3/2})\right)t^{-d/2}. \tag{70}$$

6. $d = d_c$

In general, when $d < d_c$, certain relevant parameters determine the critical exponents of the system. When $d = d_c$ these parameters become marginally irrelevant. In such a case the exponents are given by mean-field theory, but with logarithmic corrections. In our system the marginally irrelevant parameter is the coupling λ_0.

When $d = d_c$ the Callan–Symanzik solution (35) still holds, although with a different running coupling. The β function can be calculated either with a cutoff which is taken to infinity or by taking $\epsilon \to 0$ in (28) with the same result: $\beta(g_R) = 2B_k g_R^2$. This gives the running coupling

$$\tilde{g}_R(\kappa^{-2}) = \frac{g_R}{1 + g_R B_k \ln(\kappa^2 t)} . \tag{71}$$

For large t the coupling goes to zero, which is the only fixed point of the β function. Using the asymptotic form $\tilde{g}_R \sim \{B_k \ln(\kappa^2 t)\}^{-1}$ in the tree-level sum gives

$$n(t) \sim \left(\frac{(k-2)!}{4\pi k^{1/(k-1)}}\right)^{1/(k-1)} \left(\frac{\ln t}{t}\right)^{1/(k-1)} \left[1 + O\big((\ln t)^{-1/(k-1)}\big)\right] . \tag{72}$$

Higher-order terms in $\tilde{g}_R$ will give sub-leading time dependence, so this represents the full leading-order amplitude. Notice that the correction terms are only an order $(\ln t)^{-1/(k-1)}$ smaller, which will make time required to reach the asymptotic regime large.

The same procedure gives an exact expression for the leading term in the correlation function as well. For $k = 2$

$$\tilde{C}(p, t) = \frac{1}{8\pi}\big(1 - f_2(p^2 t)\big)\left(\frac{\ln t}{t}\right)[1 + O((\ln t)^{-1})] \tag{73}$$

and for $k = 3$

$$\tilde{C}(p, t) = \left(\frac{\sqrt{3}}{12\pi}\right)^{1/2}\big(1 - f_3(p^2 t)\big)\left(\frac{\ln t}{t}\right)^{1/2}[1 + O((\ln t)^{-1/2})] . \tag{74}$$

7. Summary and generalization to $kA \to \ell A$

With the RG calculation developed above we are able to calculate various universal quantities for this system. These include the amplitude of the asymptotic density for $d \leqslant d_c$, given by (49), (51), and (72), and the connected correlation function. Also universal are the fluctuations in total particle number and the fluctuations in particle number in a small volume v.

The density amplitude for $k = 2$ can be compared to the exact solution for $d = 1$ of $A_2 = (8\pi)^{-1/2} \approx 0.20$ [7]. Putting $\epsilon = 1$ in our expansion yields $A_2 = 0.08 + 0.03 + \cdots$. The agreement is less than satisfactory, indicating that the ϵ-expansion will not be quantitatively accurate to $\epsilon = 1$. However, the ϵ-expansion provides the only systematic derivation of universality and scaling.

Our results can be immediately generalized to a coagulation reaction $kA \to \ell A$, $\ell < k$. The only change in the field theory is the vertices λ_i in (17):

$$\lambda_i = \begin{cases} \lambda_0 \binom{k}{i} - \lambda_0 \binom{\ell}{i} & i \leqslant \ell \\ \lambda_0 \binom{k}{i} & i > \ell . \end{cases} \tag{75}$$

The renormalization follows identically. For example, the leading term in the amplitude, given by (44), is generalized to

$$A_{k,\ell} = \left(\frac{k}{k-\ell} \right)^{1/(k-1)} A_k + \mathrm{O}(\epsilon^0) . \tag{76}$$

This proportionality is not generally true for all terms in the ϵ expansion, although it does happen to hold when $k = 2$. To see this consider a rescaling $\psi \to b\psi$, $\tilde{\psi} \to \tilde{\psi}/b$, and $n_0 \to bn_0$ in the action (17). The only terms changed by such a rescaling are the couplings $\lambda_i \to b^{i-k}\lambda_i$, which for $k = 2$ is only the coupling λ_1. Starting from the theory $A + A \to \emptyset$ and making the scale transformation with $b = 2$ gives exactly the theory for $A + A \to A$. As a consequence, the density for $A + A \to A$, starting from an initial density of n_0, will for all times be exactly twice the density of the system $A + A \to \emptyset$ with initial density of $n_0/2$. This result agrees with the recent exact solution of a particular model of $A + A \to (\emptyset, A)$ in $d = 1$ [10], although it should be noted that this relation is not truly universal for all times, as it only holds when the irrelevant couplings are excluded. The asymptotic amplitude is universal, and so the relation $A_{2,1} = 2A_{2,0}$ is exact to all orders in ϵ, and independent of the initial densities.

For $k = 3$ such a simple relation does not hold. We can consider all three theories, $\ell = 0, 1, 2$, combined with relative strengths r_0, r_1, r_2, where $\sum_i r_i = 1$. The rescaling defined above will relate two systems with different r_ℓ in that the densities will be identical up to a rescaling. However, this rescaling only removes one degree of freedom from the two independent variables, so unlike $k = 2$, one cannot necessarily scale one theory into another. Considering r_0 and r_1, we find

$$r_0(b) = (1-b)^2 + b(2b-1)\bar{r}_0 + b(1-b)\bar{r}_1 \tag{77}$$

$$r_1(b) = (3-b)(b-1) + 2b(1-b)\bar{r}_0 + b^2\bar{r}_1 \tag{78}$$

where $\bar{r}_0, \bar{r}_1$ are the values of r_0, r_1 prior to rescaling. Consider the system which is purely $\ell = 0$, or $\bar{r}_0 = 1$, $\bar{r}_1 = \bar{r}_2 = 0$. For any $b \neq 1$ then $r_1(b) < 0$, which implies that there is no combination of systems with different ℓ which is equivalent to $\ell = 0$ up to a rescaling. This is not the case for the pure $\ell = 1$ system. This system can be rescaled from $b = 1$ to $b = \frac{3}{4}$. At the latter point one has $r_0 = \frac{1}{4}$, $r_1 = 0$, and $r_2 = \frac{3}{4}$, so this combination of systems, with an initial density of $3n_0/4$, will give exactly $\frac{3}{4}$ the density of the $\ell = 1$ system at all times. Similarly, starting with $\bar{r}_2 = 1$ the system can be rescaled from $b = 1$ to $b = \frac{3}{2}$. At the latter point $r_0 = \frac{1}{4}$, $r_1 = \frac{3}{4}$, and $r_2 = 0$.

It should be noted that the correlation function will not be identical up to a rescaling for any of the systems described above. This is a consequence of the fact that the correlation function contains both ψ and ψ^2 pieces.

While the reaction considered here is not as generally interesting as that of $A + B \to \emptyset$, it is a suitable starting point for developing the application of RG methods to these systems. A similar approach may be applicable to the reaction $mA + nB \to \emptyset$, a system where the universality classes appear to depend on the nature of the initial conditions [21–24].

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Appendix. Symmetry factors

Diagrams which contain the classical density or the classical response function are representations of infinite sums of diagrams. While they resemble ordinary perturbation theory diagrams, they differ in combinatorics. When calculating the Wick contraction combinatorics one treats propagators as distinguishable, although the resulting combinatoric factor is then cancelled by a factor which is absorbed into the definition of the coupling constant. Our diagrams differ from this in two ways. First, the classical density is attached to vertices as an indistinguishable object. This will be demonstrated below. Second, we have chosen to introduce in the coupling constants no pre-adjusted combinatoric factor. This is merely a matter of convention, and is motivated by the indistinguishability mentioned above, and by the direct relation of the coupling constant to the parameters used in the master equation.

The indistinguishability of the density lines can be demonstrated by considering the contraction of k ψ's, representing a vertex, with the infinite sum which is the initial state:

$$\begin{aligned}\langle\langle\psi^k\rangle\rangle_{\rm cl} &= \sum_{m=0}^{\infty} \frac{n_0^m}{m!} (\psi^k \bar{\psi}^m)_{\rm cl} \\ &= \sum_{m=0}^{\infty} \frac{1}{m!} \sum_{\substack{m_1,\ldots,m_k \\ m_1+\cdots+m_k=m}} C^m_{m_1,\ldots,m_k} \prod_{i=1}^{k} \left(n_0^{m_i} (\psi \bar{\psi}^{m_i})_{\rm cl} \right) \end{aligned} \tag{A.1}$$

where $C^m_{m_1,\ldots,m_k} = m!/(m_1!\ldots m_k!)$ is the number of ways to partition m objects into k distinct boxes. The sums can be replaced with unrestricted sums over $m_1 \ldots m_k$, and the above expression factors completely, giving

$$\langle\langle\psi^k\rangle\rangle_{\rm cl} = \langle\langle\psi\rangle\rangle_{\rm cl}^k \,. \tag{A.2}$$

The significance of (A.2) is that there is no $k!$ prefactor. The k classical density lines which are connected to the vertex are effectively indistinguishable.

In calculating the classical response function it is necessary to consider attaching one propagator and $k-1$ density lines to a ψ^k vertex. This brings in a factor of k, for the number of distinguishable ways the propagator can be attached. The remaining $k-1$ densities follow through the same combinatorics as that shown above, and contribute a factor of 1.

In general, where the classical response function appears in a diagram it can be treated as a propagator for combinatorics. The exception to this situation is in diagrams such as figures 4 and 5 (diagrams (*d*)). Here the symmetry of the two disconnected branches will result in the branches attaching as indistinguishable objects.

Note added. When $d = d_c$ the density amplitudes for $\ell \neq 0$ are given exactly by the relation $A_{k,\ell} = \left(\frac{k}{k-\ell}\right)^{1/(k-1)} A_k$. This is because the set of diagrams which contribute are the same as those which give the leading-order amplitude when $d < d_c$. These amplitude have recently been measured numerically for the reactions $3A \to A$ and $3A \to 2A$ with the results $A_{3,1} \approx 0.76$ and $A_{3,2} \approx 0.93$ [25]. Our calculations yield instead $A_{3,1} \approx 0.26$ and $A_{3,2} \approx 0.37$. This discrepancy has not been resolved.

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