Fluctuation-Induced First-Order Transition in a Nonequilibrium Steady State

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We present the first example of a phase transition in a nonequilibrium steady state that can be argued analytically to be first order. The system of interest is a two-species reaction-diffusion problem whose control parameter is the total density ρ. Mean-field theory predicts a second-order transition between two stationary states at a critical density $\rho = \rho_c$. We develop a phenomenological picture that instead predicts a first-order transition below the upper critical dimension $d_c = 4$. This picture is confirmed by hysteresis found in numerical simulations, and by the study of a renormalization-group improved equation of state. The latter approach is inspired by the Coleman–Weinberg mechanism in QED.

1. MOTIVATION

1.1. Fluctuation-Induced First-Order Transitions

In the realm of equilibrium critical phenomena it is well-known that systems which in high space dimension d undergo a second-order transition, may exhibit a first-order transition below their upper critical dimension $d = d_c$. Examples are spin systems with cubic anisotropy,[1–4] type-II superconductors,[5] and the three-state Potts model.[6] In equilibrium phenomena the phase diagram can be deduced from the analysis of the global extrema of a free energy functional. The global free energy minima correspond to stable phases. For $d < d_c$ this functional has to incorporate

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fluctuation effects. When fluctuations modify the energy landscape to the point of changing a second-order transition into a first-order one, one has a *fluctuation-induced* first-order transition. This phenomenon is also said to be due to the Coleman–Weinberg mechanism.[7] Indeed formally similar phenomena were first found in the study of the coupling of QED radiative corrections to a charged scalar field.

In nonequilibrium systems there is no such concept as a free energy; the steady state phase diagram cannot be deduced from a thermodynamic potential, and its statistical mechanics is not based on a partition function. The starting point, instead, is usually an evolution equation (often a master equation), whose stationary solutions are to be determined and yield the steady-state phase diagram. This indirect definition of the phase diagram renders analytic approaches very cumbersome. In the past twenty years techniques have been devised to find the steady states of such master equations and extract from them physical properties of interest (order parameter, correlation functions,...). These techniques include short time series expansion, numerical simulations, real-space renormalization and field-theoretic approaches. Nonequilibrium steady states (NESS) may undergo phase transitions in the same way as do equilibrium states. Several examples of *continuous* transitions in such systems have been found and well studied. To our knowledge, the only *first-order* transitions in NESS known today occur in the asymmetric exclusion model in one space dimension, as demonstrated analytically in ref. 8. This model belongs to the subclass of *driven diffusive systems:* due to an externally applied field these systems have a spatially anisotropic current carrying NESS. The occurrence of first order transitions in certain other driven diffusive systems[10] is also suggested by numerical simulations, or by mean field analyses. Finally, Schmittmann and Janssen[11] have argued field-theoretically that a similar fluctuation mechanism may induce a first-order longitudinal transition (high and low density stripes perpendicular to the driving field) in a driven diffusive system with a single conserved density. Some first-order transitions occurring in the NESS of reaction-diffusion processes have also appeared in some numerical studies of generalized directed percolation.[9]

The present study bears on the phase transition in the NESS of a diffusion-limited reaction between two species of particles. This system does *not* belong to the subclass of driven systems: it remains spatially isotropic under all circumstances.

We exhibit here, for the first time with analytic arguments, a *fluctuation-induced* first order transition in the steady-state of a reaction-diffusion process. We present an analytic procedure that allows to access the phase diagram of the system in a very explicit fashion. The outline of the article is as follows. In the next subsection we define the two-species

reaction-diffusion model. In Section 2 we recall some known properties of its phase diagram. We also introduce the field-theoretical formalism, which will be our main tool of analysis. Section 3 presents a heuristic approach to the first-order transition in terms of a nucleating and diffusing droplet picture. In Section 4 we report on numerical simulations on a two-dimensional system, in which a hysteresis loop is observed for the order parameter. This confirms the suspected existence of a first order transition below the critical dimension $d_c = 4$. Sections 5 through 8 contain the field-theoretic approach: the derivation of a renormalization group improved equation of state, valid in dimension $d = d_c - \varepsilon$, followed by the study of its solutions and of their stability with respect to spatial perturbations. We conclude with a series of possible applications.

1.2. Reaction-Diffusion Model

Particles of two species, A and B, diffuse in a d-dimensional space with diffusion constants D_A and D_B, respectively. Upon encounter an A and a B are converted into two B's at a rate k per unit of volume,

$$A + B \xrightarrow{k} B + B \tag{1}$$

Besides a B spontaneously decays into an A at a rate γ,

$$B \xrightarrow{\gamma} A \tag{2}$$

Denoting the local A and B densities by ρ_A and ρ_B, respectively, we can write the mean-field equations as

$$\begin{aligned}
\partial_t \rho_B &= D_B \, \Delta \rho_B - \gamma \rho_B + k \rho_A \rho_B \\
\partial_t \rho_A &= D_A \, \Delta \rho_A + \gamma \rho_B - k \rho_A \rho_B
\end{aligned} \tag{3}$$

The total particle density ρ, is a conserved quantity and will be the control parameter. In the initial state particles are distributed randomly and independently, with a given fraction of each species. Let ρ_A^{st} and ρ_B^{st} be the steady state values of the A and B particle density, respectively. Obviously their sum is equal to ρ. One easily derives from (3) that there exists a threshold density $\rho_c = \gamma/k$ such that for $\rho > \rho_c$ the steady state of the system is *active*, that is, has $\rho_B^{\mathrm{st}} > 0$, and that for $\rho < \rho_c$ it is absorbing, that is, has $\rho_B^{\mathrm{st}} = 0$. Hence ρ_B^{st} is the order parameter for this system, and an important question is how this quantity behaves at the transition point.

This model may be cast into the form of a field theory (and then turns out to generalize the field theory of the Directed Percolation problem).

It was shown by field-theoretic methods in refs. 12 and 13 that for $0 < D_A \leqslant D_B$ the transition between the steady states at $\rho = \rho_c$ is continuous. It is characterized by a set of critical exponents that differ from their mean-field values in $d < d_c = 4$. Whereas for $D_A \leqslant D_B$ the phase diagram may be obtained by convential tools of analysis, such as renormalization group approaches based on a field-theoretic formulation of the dynamics, the case $D_A > D_B$ cannot be analyzed along the same lines. In technical terms, the renormalization group flows away to a region where the theory is ill-defined. We interpret this as meaning that there is no continuous transition, and a natural idea, if one still believes in the existence of a transition, is the occurrence of a first-order one. The article is concerned with the case $D_A > D_B$.

2. FIELD-THEORETIC FORMULATION

2.1. Langevin Equations

There are at least two different ways to construct a field theory that describes a reaction-diffusion problem such as the one we just defined. One of them is to encode the stochastic rules for particle diffusion and reaction in a master equation for the probability of occurrence of a state of given local particle numbers at a given time. The master equation may be converted into an exactly equivalent field theory following methods that were pioneered by Peliti[14] and others. We will follow a different way of proceeding that has been widely employed, in particular, by Janssen and co-workers.[15] We postulate for the space and time dependent densities of the A and B particles two Langevin equations in which the noise terms have been deduced by heuristic considerations. The result of this approach differs from Peliti's up to terms that are irrelevant in the limit of large times and distances.

We switch now to the notation of field theory and denote by $\psi(\mathbf{r}, t)$ the coarse-grained B particle density and by $m(\mathbf{r}, t)$ the deviation from average of the coarse-grained total particle density. The deterministic part of the Langevin equations to be constructed should be the conventional mean-field reaction-diffusion PDE's of equation (3). Upon adding two noise terms η and ξ we get in the new notation, and after redefinition of several parameters,

$$\partial_t \psi = \lambda \, \Delta \psi - \lambda \tau \psi - \frac{\lambda g}{2} \psi^2 - \lambda f m \psi + \eta \tag{4}$$

$$\partial_t m = \Delta m + \lambda \sigma \, \Delta \psi + \xi \tag{5}$$

Here $\lambda = D_B/D_A$ is the ratio of the diffusion constants; τ is proportional to the deviation of the total density from its mean-field critical value γ/k; g, $\tilde{g}$ and f are proportional to the contamination rate k; and the parameter σ, which will play a key role in the present study, is proportional to $1 - (D_B/D_A)$.

For mathematical convenience we will want η and ξ to represent mutually uncorrelated Gaussian white noise. The noise η in the equation for ψ should vanish with ψ since $\psi = 0$ is an absorbing state. For the auto-correlation of η we therefore retain the first term of a hypothetical series expansion in powers of ψ. This procedure is best described in refs. 15, 12. The autocorrelation of ξ should be such that m is locally conserved. With these conditions the simplest possible expressions for the autocorrelations of η and ξ are, explicitly,

$$\langle \eta(\mathbf{r}, t)\, \eta(\mathbf{r}', t') \rangle = \lambda \tilde{g} \psi(\mathbf{r}, t)\, \delta^{(d)}(\mathbf{r} - \mathbf{r}')\, \delta(t - t')$$

$$\langle \xi(\mathbf{r}, t)\, \xi(\mathbf{r}', t') \rangle = 2 \nabla_{\mathbf{r}} \nabla_{\mathbf{r}'} \delta^{(d)}(\mathbf{r} - \mathbf{r}')\, \delta(t - t') \tag{6}$$

The Langevin equation (4) is to be understood with the Itô discretization rule. It is also possible to derive these equations *ab initio* by the operator formalism used in ref. 13.

Using the Janssen–De Dominicis formalism[16, 17] we obtain the physical observables as functional integrals over four fields $\bar{\psi}$, ψ, $\bar{m}$, m weighted by a factor $\exp(-S[\bar{\psi}, \psi, \bar{m}, m])$, with

$$S[\bar{\psi}, \psi, \bar{m}, m] = \int d^d x\, dt \left[\bar{\psi}(\partial_t + \lambda(\tau - \Delta))\, \psi + \bar{m}(\partial_t - \Delta)\, m \right. \tag{7}$$

$$\left. - (\nabla \bar{m})^2 - \lambda \sigma \bar{m}\, \Delta \psi + \frac{\lambda g}{2}\, \psi^2 \bar{\psi} - \frac{\lambda \tilde{g}}{2}\, \psi \bar{\psi}^2 + \lambda f \bar{\psi} \psi m \right]$$

It is possible (and sometimes more practical) to eliminate the fluctuating density field m and its response field $\bar{m}$, which yields an effective action for the $\bar{\psi}$, ψ fields alone.

2.2. Mean-Field Equation of State

Our starting point is the action describing the dynamics of the system in the presence of an arbitrary source of B particles $\lambda h(\mathbf{r}, t)$ in which the fluctuating density m and its response field $\bar{m}$ have been integrated out. It reads

$$S[\bar{\psi}, \psi] = \int d^d r \, dt \left[\bar{\psi}(\partial_t + \lambda(\tau - \Delta)) \psi + \frac{\lambda g}{2} \psi^2 \bar{\psi} - \frac{\lambda \tilde{g}}{2} \psi \bar{\psi}^2 - \lambda h \bar{\psi} \right]$$

$$- \int d^d r \, d^d r' \, dt \, dt' \left[\frac{(\lambda f)^2}{2} \bar{\psi}\psi(\mathbf{r}, t) \, C_0(\mathbf{r} - \mathbf{r}'; t - t') \, \bar{\psi}\psi(\mathbf{r}', t') \right.$$

$$\left. - \lambda^2 \sigma f \bar{\psi}\psi(\mathbf{r}, t) \, G_0(\mathbf{r} - \mathbf{r}'; t - t') \, \Delta\psi(\mathbf{r}', t') \right] \tag{8}$$

where the spatial Fourier transforms of G_0 and C_0 are

$$G_0(\mathbf{q}; t - t') = \Theta(t - t') \, e^{-\mathbf{q}^2(t - t')}, \qquad C_0(\mathbf{q}; t - t') = e^{-\mathbf{q}^2 |t' - t|} \tag{9}$$

We first look for an *a priori* inhomogeneous steady state (in terms of Fourier transforms, one takes the limit $\omega \to 0$) then one specializes the study to a homogeneous steady state (and one takes the limit $\mathbf{q} \to \mathbf{0}$). The limit of infinite times (corresponding to a system reaching a steady-state) and the limit of a homogeneous system do not commute. In the limit of a vanishing source term the mean-field equation of state for a homogeneous order parameter Ψ is found by imposing that

$$\lim_{\mathbf{q} \to \mathbf{0}} \lim_{\omega \to 0} \frac{\delta S}{\delta \bar{\psi}(\mathbf{q}, \omega)} [0, \Psi] = \lambda \Psi \left(\tau + \frac{\bar{g}}{2} \Psi \right) = 0 \tag{10}$$

with $\bar{g} \equiv g - 2\lambda \sigma f$. It is important to note that written in terms of the original parameters $\bar{g} > 0$ as long as $D_B/D_A > 0$ (the cases $D_B = 0$ or $D_A = 0$ would require a separate study). One may conclude that the steady state is active (a finite fraction of B's survive indefinitely) if $\tau > 0$, while the system eventually falls into an absorbing B-free state if $\tau < 0$. Mean-field therefore predicts a *continuous* transition between those states at $\tau = 0$, independently of the ratio of the diffusion constants.

2.3. Renormalization

In order to go beyond mean-field we have performed a one-loop perturbation expansion of the two and three-leg vertex functions. Renormalization is then required to extract physically relevant information from this expansion. We shall proceed within the framework of dimensional regularization and of the minimal subtraction scheme. In order to absorb the ε-poles in the vertex functions into a reparametrization of coupling constants and fields we introduce the renormalized quantities ψ_R, λ_R etc. defined by

$$\bar{\psi} = Z_{\bar{\psi}}^{1/2} \bar{\psi}_{\mathbf{R}} \qquad \psi = Z_{\psi}^{1/2} \psi_{\mathbf{R}} \qquad Z = (Z_{\bar{\psi}} Z_{\psi})^{1/2}$$

$$Z\lambda = Z_{\lambda} \lambda_{\mathbf{R}} \qquad Z_{\psi}^{1/2} \lambda \sigma = \lambda_{\mathbf{R}} \sigma_{\mathbf{R}}$$

$$Z_{\lambda} \tau = Z_{\tau} \tau_{\mathbf{R}} \qquad A_{\varepsilon}^{1/2} Z_{\lambda} f = Z_f f_{\mathbf{R}} \mu^{\varepsilon/2} \qquad Z_{\lambda} h = Z_{\psi}^{1/2} h_{\mathbf{R}} \tag{11}$$

$$A_{\varepsilon}^{1/2} Z_{\lambda} Z_{\psi}^{1/2} g = \sigma_{\mathbf{R}} \mu^{\varepsilon/2} (Z_g g_{\mathbf{R}} + W f_{\mathbf{R}}) \qquad A_{\varepsilon}^{1/2} Z_{\lambda} Z_{\bar{\psi}}^{1/2} \sigma_{\mathbf{R}} \tilde{g} = Z_{\tilde{g}} \tilde{g}_{\mathbf{R}} \mu^{\varepsilon/2}$$

It may be seen that the m and $\bar{m}$ fields two-point vertex functions in the action of Eq. (7) remain unrenormalized to all orders in perturbation theory, hence the absence of the related Z-factors. Here μ denotes an external momentum scale. The renormalization factors depend on $u = \tilde{g}_{\mathbf{R}} g_{\mathbf{R}}$, $v = f_{\mathbf{R}}^2$ and $w = f_{\mathbf{R}} \tilde{g}_{\mathbf{R}}$ and are at one-loop order given by

$$Z = 1 + \frac{u}{4\varepsilon} - \frac{2\lambda^2 v}{\varepsilon(1+\lambda)^2} - \frac{3\lambda+1}{2\varepsilon(1+\lambda)^2} w \tag{12}$$

$$Z_{\lambda} = 1 + \frac{u}{8\varepsilon} - \frac{2\lambda^2 v}{\varepsilon(1+\lambda)^3} - \frac{\lambda(1+4\lambda-\lambda^2)}{4\varepsilon(1+\lambda)^3} w \tag{13}$$

$$Z_{\tilde{g}} = 1 + \frac{u}{\varepsilon} - \frac{2\lambda(3\lambda+1)}{\varepsilon(1+\lambda)^2} v - \frac{2\lambda(2\lambda+1)}{\varepsilon(1+\lambda)^2} w \tag{14}$$

$$Z_g = 1 + \frac{u}{\varepsilon} - \frac{2\lambda(3\lambda+1)}{\varepsilon(1+\lambda)^2} v - \frac{\lambda(5\lambda+3)}{\varepsilon(1+\lambda)^2} w \tag{15}$$

$$Z_f = 1 + \frac{u}{2\varepsilon} - \frac{2v}{\varepsilon(1+\lambda)^2} - \frac{\lambda(2\lambda+1)}{\varepsilon(1+\lambda)^2} w \tag{16}$$

$$W = \frac{4v\lambda^2}{\varepsilon(1+\lambda)} + \frac{2w\lambda^2}{\varepsilon(1+\lambda)} \tag{17}$$

Since only Z is fixed by the renormalization conditions but not the individual factors $Z_{\bar{\psi}}$ and Z_{ψ} we may set $Z_{\psi} = 1$.

2.4. Renormalization Group and Fixed Points

From the above Z-factors and the definition of the renormalized couplings one finds the flow equations for the renormalized couplings. These read

$$\beta_u = \mu \left. \frac{du}{d\mu} \right|_{\text{bare}} = u \left(-\varepsilon + \frac{3u}{2} - \frac{2\lambda(5\lambda^2 + 5\lambda + 2) v}{(1+\lambda)^3} - \frac{2\lambda(4\lambda^2 + 5\lambda + 2) w}{(1+\lambda)^3} \right)$$
$$+ w \left(\frac{4v\lambda^2}{(1+\lambda)} + \frac{2\lambda^2 w}{1+\lambda} \right) \tag{18}$$

$$\beta_v = \mu \frac{dv}{d\mu}\bigg|_{\text{bare}} = v(-\varepsilon + 2\kappa) = v\left(-\varepsilon + \frac{3u}{4} - \frac{4v\lambda^3}{(1+\lambda)^3} - \frac{\lambda(9\lambda^2 + 8\lambda + 3)\,w}{2(1+\lambda)^3}\right)$$

(19)

$$\beta_w = \mu \frac{dw}{d\mu}\bigg|_{\text{bare}} = w\left(-\varepsilon + \frac{9u}{8} - \frac{2\lambda(4\lambda^2 + 2\lambda + 1)\,v}{(1+\lambda)^3} - \frac{3\lambda(9\lambda^2 + 8\lambda + 3)\,w}{4(1+\lambda)^3}\right)$$

(20)

$$\beta_\lambda = \mu \frac{d\lambda}{d\mu}\bigg|_{\text{bare}} = \zeta\lambda = \left(\frac{u}{8} - \frac{2\lambda^3 v}{(1+\lambda)^3} - \frac{\lambda(7\lambda^2 + 4\lambda + 1)\,w}{4(1+\lambda)^3}\right)$$

(21)

and the Wilson function is

$$\gamma = \mu \frac{d \ln Z}{d\mu}\bigg|_{\text{bare}} = -\frac{u}{4} + \frac{2\lambda^2 v}{(1+\lambda)^2} + \frac{\lambda(3\lambda + 1)\,w}{2(1+\lambda)^2}$$

(22)

In equations (18)–(22) all μ-derivatives are at fixed bare parameters. The renormalization group flow has three nontrivial fixed points: the well-known directed percolation fixed point with $v = w = 0$ and $u = u_{\text{DP}} = 2\varepsilon/3$, the symmetric ($w = 0$) fixed point $(u_s, v_s, \lambda_s) = (2\varepsilon, 27\varepsilon/64, 2)$ and the asymmetric fixed point $(u_a, v_a, w_a, \lambda_a)$ with

$$u_a = \frac{4\lambda_a \varepsilon}{2 + \lambda_a} \qquad v_a = \frac{1 + \lambda_a}{4\lambda_a}\varepsilon \qquad w_a = -(\lambda_a - 5)\,\varepsilon$$
$$\lambda_a^{-1} = (2 + \sqrt{3})^{1/3} + (2 - \sqrt{3})^{1/3} - 2$$

(23)

at leading order in ε. The continuous phase transitions described by these fixed points have already been studied in other publications.[12, 13] The symmetric fixed point ($w = 0$) is unstable with respect to the variable w. It corresponds to the case of equal diffusion constants $D_A = D_B$, whereas the asymmetric fixed point with $w < 0$ governs the critical behavior for $D_A < D_B$. Since the sign of w is conserved along the renormalization group flow the asymmetric fixed point cannot be reached for $w > 0$. Therefore there is no fixed point for $w > 0$ ($D_A > D_B$). In order to study the phase transition for $D_A > D_B$, which is the regime of interest, we consider in the next sections the solutions of the renormalization group flow in more detail. Figure 1 shows a plot of the steady-state density of B's as a function of τ (the deviation of the total density with respect to its mean-field critical value), for $\lambda = 1$ and $\lambda > 1$.
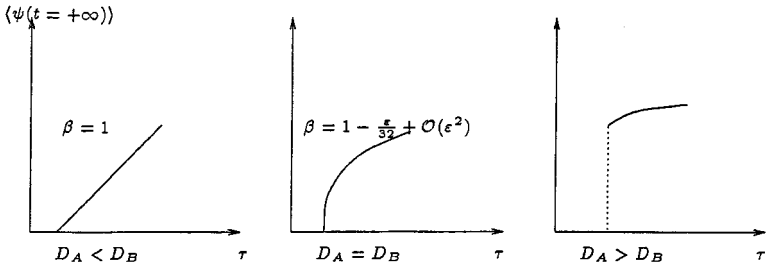
Fig. 1. Phase diagram in the $(\tau, \psi(t = \infty))$ plane (the ordinate is the steady-state density of B particles) for $\lambda > 1$, $\lambda = 1$ and a conjecture for $\lambda < 1$. Also shown is the order parameter exponent β.

Assuming the existence of a first-order transition for $\lambda < 1$ (which would make of $\lambda = 1$ a tricritical point), the jump of the order parameter across the transition point is related to the properties of the symmetric fixed point and should scale according to the tricritical scaling predictions developed by Lawrie and Sarbach,[18]

$$\rho_B(\tau_c^-) - \rho_B(\tau_c^+) \propto \sigma^{1/\delta}, \qquad \delta = -\frac{\gamma_s}{d + \gamma_s} \tag{24}$$

where γ_s is the Wilson function γ evaluated at the symmetric fixed point.

3. A PHENOMENOLOGICAL THEORY

3.1. What Happens When $D_B < D_A$?

In dimension $d < 4$ the renormalization group flow has no stable fixed point at finite coupling constants. Nevertheless, we still expect a phase transition. Here follows a heuristic argument leading to the conclusion that this is a first order transition. It is based, essentially, upon adding to the mean-field equations Eqs. (3) in an approximate way the fluctuations in the A particle density. Several steps in the argument are open to criticism but we expect it to provide the right qualitative picture.

Let us consider the system at total particle density ρ and write

$$\rho = \rho_c + \rho_0 \tag{25}$$

where ρ_c is the critical density. The mean-field values of the stationary A and B densities are $\rho_A^{\mathrm{mf}} = \rho_c$ and $\rho_B^{\mathrm{mf}} = \rho_0$, respectively.

We imagine the system divided into regions ("blocks") of volume L^d, where L is arbitrary. Consider a particular block. The instantaneous density in this block is a fluctuating variable that we denote by

$$\rho_L = \rho_c + \rho_0 + \delta\rho_L \tag{26}$$

where $\delta\rho_L$ is a random term of average zero.

We present the argument for the case $\rho_0 \ll \rho_c$, i.e., the average B density is much smaller than the average A density. Then the fluctuations of the total density are practically identical to those of ρ_A. We have in particular $\langle \delta\rho_L^2 \rangle = \rho_c L^{-d}$, so that the probability distribution of $\delta\rho_L$ is

$$P(\delta\rho_L) = C \exp\left(-\frac{L^d \delta\rho_L^2}{2\rho_c} \right) \tag{27}$$

A density fluctuation $\delta\rho_L$ will relax to zero diffusively, hence on a time scale

$$T_{\text{fl}, L} \sim \frac{L^2}{D_A} \tag{28}$$

We are now interested in fluctuations of ρ_L well below the critical density ("negative fluctuations"), say less than $\rho_c - \rho_1$. We have

$$\text{Prob}(\rho_L < \rho_c - \rho_1) \sim \exp\left(-\frac{L^d(\rho_0 + \rho_1)^2}{2\rho_c} \right) \tag{29}$$

Such a fluctuation will still have the decay time $T_{\text{fl}, L}$ given by (28) and therefore stay negative during a time

$$T_{\text{neg}, L} \sim \frac{\rho_1}{\rho_0 + \rho_1} \frac{L^2}{D_A} \tag{30}$$

In the meanwhile the local density of B particles will tend to zero with a relaxation time $T_{\text{rel}, L}$ which, according to the mean field equations, in the absence of B diffusion is given by

$$T_{\text{rel}, L} \sim \frac{1}{k\rho_1} \tag{31}$$

If ρ_1 is so large that $T_{\text{rel}, L} \lesssim T_{\text{neg}, L}$, then during the lifetime of the negative density fluctuation the B particles will become locally extinct. Upon combining (30) and (31) we find the condition for such a B extinguishing

density fluctuation. We now take ρ_1 exactly large enough for this condition to be satisfied, but not larger, since we want to take into account all extinguishing fluctuations. This leads to a relation between ρ_1 and L, *viz.*

$$\frac{\rho_1^2}{\rho_0 + \rho_1} = \frac{D_A}{kL^2} \tag{32}$$

We now ask what the typical time interval $T_{\text{int}, L}$ is between two such fluctuations in the same block. A rough estimate can be made as follows. The fraction f_- of time spent by the fluctuating density ρ_L below the value $\rho_c - \rho_1$ is equal to $f_- \equiv \text{Prob}(p_L < \rho_c - \rho_1)$, hence given by (29). This fraction is composed of short intervals of typical length $T_{\text{neg}, L}$ given by (30). The short intervals are separated by long ones of typical length $T_{\text{int}, L}$ that make up for the remaining fraction, $1 - f_-$, of time. Hence $T_{\text{neg}, L}/T_{\text{int}, L} = f_-/(1 - f_-)$. Using (29) and (30) we find

$$T_{\text{int}, L} \sim \frac{L^2}{D_A} \exp\left(\frac{L^d(\rho_1 + \rho_0)^2}{2\rho}\right) \tag{33}$$

where our replacing the prefactor $\rho_1/(\rho_0 + \rho_1)$ is without consequences for the remainder of the argument. The quantity $T_{\text{int}, L}$ is the decay time of the B population due to density fluctuations on scale L, in the absence of B diffusion. We now take into account the effect of this diffusion. The time $T_{B, L}$ needed for a B particle to diffuse over a distance of order L is

$$T_{B, L} \sim \frac{L^2}{D_B} \tag{34}$$

All B particles will be eliminated from the system by negative density fluctuations on scale L unless $T_{B, L} \lesssim T_{\text{int}, L}$. By comparing (33) and (34) we obtain for the existence of a stationary state with a nonzero B density the condition

$$f(L; \rho_0) \equiv \frac{L^d(\rho_1 + \rho_0)^2}{2\rho_c} \gtrsim \ln \frac{D_A}{D_B} \qquad \text{for all} \quad L \geqslant a \tag{35}$$

where a is the lattice parameter and with ρ_1 related to L by (32). The key point is now that when $D_B < D_A$, the inequality (35) can be satisfied only for ρ_0 above some threshold ρ_{0c} to be determined below. Therefore

$$\rho'_c = \rho_c + \rho_{0c} \tag{36}$$

is the new critical density. Since after having survived a negative density fluctuation any local B particle density will rapidly return to its average value ρ_0, there is at the new critical density a jump in ρ_B^{st} equal to

$$\Delta\rho_B^{\text{st}} = \rho_{0c} \tag{37}$$

We now determine the threshold value ρ_{0c}. Since the inequality (35) has to hold for all L, we first determine the minimum value of its LHS as a function of L. In practice the calculation is most easily done by using ρ_1 instead of L as the independent variable. The minimum occurs for $L = \xi_{\min}$ with

$$\xi_{\min}^2 = (2d)^{-2}(4+d)(4-d)\frac{D_A}{k\rho_0} \tag{38}$$

The values of ρ_1 and $f(L; \rho_0)$ at $L = \xi_{\min}$ are

$$\rho_{1,\min} = \frac{2d}{4-d}\rho_0 \tag{39}$$

$$f(\xi_{\min}; \rho_0) = (2\rho_c)^{-1}C_d(4-d)^{-2+d/2}\left(\frac{D_A}{k}\right)^{d/2}\rho_0^{2-d/2} \tag{40}$$

where $C_d = (2d)^{-d}(4+d)^{2+d/2}$. The condition $\xi_{\min} \geq a$ leads to

$$(4-d)\frac{D_A}{\rho_0 k a^2} \geq 1 \tag{41}$$

and can always be satisfied by choosing a small enough. Upon inserting (40) in (35) we find the critical value ρ_{0c} below which there cannot exist a phase with B particles:

$$\rho_{0c} = \text{cst.}\,\rho_c^{2/(4-d)}\left(\frac{D_A}{k}\right)^{-d/(4-d)}(4-d)\ln^{2/(4-d)}\frac{D_A}{D_B} \tag{42}$$

Consistency requires that (41) be satisfied when for ρ_0 we substitute ρ_{0c} taken from (42). This leads again to a condition that can always be satisfied for a sufficiently small, whatever the dimension d. Let ξ_* be the value of $\xi_{\min}$ at which the existence condition Eq. (35) of the B phase gets violated when $\rho_0 \to \rho_{0c}^+$. One readily finds

$$\xi_* = \left(\frac{D_A}{k\rho_c^{1/2}}\right)^{2/(4-d)}\ln^{-2/(4-d)}\frac{D_A}{D_B} \tag{43}$$

This is the spatial scale at which the instability sets in that causes the first order transition. We also have to check that $\rho_{0c} \ll \rho_c$, in order to be consistent with $\rho_0 \ll \rho_c$, which was assumed following Eq. (26). This condition is certainly satisfied in the limit $D_B \to D_A^-$, that we shall consider now. Setting as before

$$\sigma = 1 - \frac{D_B}{D_A} \tag{44}$$

we obtain from the preceding equations

$$\rho_{0c} \simeq \text{cst.}(4-d)\,\sigma^{2/(4-d)} \qquad (\sigma \to 0^+) \tag{45}$$

$$\xi_* = \left(\frac{D_A}{k\rho_c^{1/2}}\right)^{2/(4-d)} \sigma^{-2/(4-d)} \qquad (\sigma \to 0^+) \tag{46}$$

The relaxation time towards zero of the B density in the vicinity of the new critical density is

$$T_B \equiv T_{B,\,\xi_*}$$
$$\sim \sigma^{-4/(4-d)} \qquad (\sigma \to 0^+) \tag{47}$$

Comparison of Eq. (45) with the tricritical scaling predictions of the previous section leads, with $\varepsilon = 4 - d$, to the identification

$$\delta = \frac{\varepsilon}{2} \tag{48}$$

We expect that the exact theory gives power laws for the same quantities as the heuristic theory does, although with different exponents. One reason for this is the difficulty of correctly keeping track of the lattice parameter a.

3.2. A Nucleation Picture

Finally we would like to draw a parallel between the heuristic arguments developed above and the kinetics of first order transitions[19] in thermodynamic systems. In those systems the description is based on a nucleation picture: the transition from a metastable to a stable phase occurs as the result of fluctuations in a homogeneous medium. These fluctuations permit the formation of small quantities of a new phase, called nuclei. However the creation of an interface is an energetically unfavored process, so that below a certain size nuclei shrink and disappear. Nuclei having a size greater than a critical radius ξ_* will survive and eventually

expand. The analysis of the competition between bulk free energy and surface tension leads to an estimate of a critical nucleus size.

In the original reaction-diffusion problem there is of course no such concept as a bulk free energy or surface tension. Nuclei are analogous to regions that are free of B particles. Those analogies should not be over-interpreted: they merely reinforce the intuitive picture of the reaction-diffusion processes leading to the first-order transition.

4. SIMULATIONS IN TWO DIMENSIONS: A HYSTERESIS LOOP

In this section we present the results of simulations performed on a two-dimensional 500×500 lattice with periodic boundary conditions. At the beginning of the simulation particles are placed randomly and independently on the sites of the lattice, with an average density $\rho = 0.2$. The ratio of the B particle density to the total density is arbitrarily chosen equal to 0.3. The decay probability of the B particles is $\gamma = 0.1$ per time step, and the contamination probability is $k = 0.5$ per time step. These parameters are held fixed. The diffusion constants D_A and D_B are varied.

In each time step the reaction-diffusion rules are implemented by the following three operations.

1.   Each B particle is turned into an A with probability γ.

2.   Each A (B) particle moves with a probability $4D_A$ ($4D_B$); a moving particle goes to a randomly chosen nearest neighbor site.

3.   An A particle is contaminated with probability k by each of the B particles on the same site.

Then the new value of the average B density is evaluated and a new time step is begun. The process stops either when the system has fallen into its absorbing state or when the B density appears to have stabilized "(*active state*)." The latter situation is considered to be reached when the slope of $\rho_B(t)$, as measured from a linear fit to the last 100 time steps, is 10^{-5} times as small as the maximal variation of the density of those 100 points.

After this fixed density run we construct as follows a starting configuration for a new run in which the total density is increased by a factor 1.004. Two situations may occur. *If* at the end of the run just terminated the B particle density is *nonzero*, then we obtain the new starting configuration from the final one of the preceding run by randomly placing extra particles on the lattice while keeping the ratio of B's to the total number of particles constant. *If* at the end of the run just terminated the B particle density is zero, then we construct a new starting configuration with a B density equal to its value in the starting configuration of the preceding run.
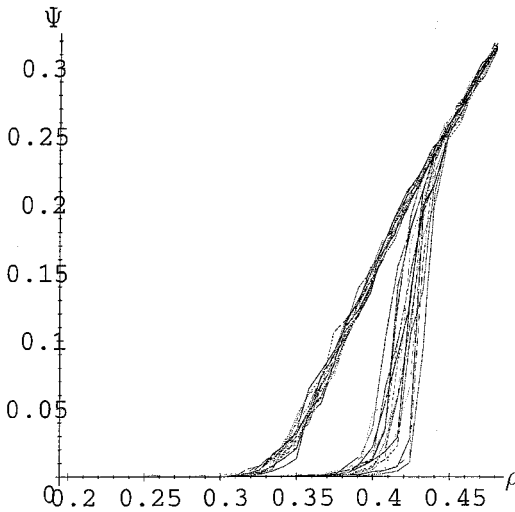
Fig. 2. The order parameter Ψ for $4D_A = 0.8$, and $4D_B = 0.1$, with $\gamma = 0.1$ and $k = 0.5$. The system cycles anticlockwise through a hysteresis loop.

A new run is carried out at the new density. This process is iterated until some upper value of the total density is reached, taken equal to $\rho = 0.5$ in the present simulations. After that we carried out a step-by-step decrease of the total density, using a reduction factor of 0.996 per step, until we reached again the total density $\rho = 0.2$ of the beginning of the simulation.

This whole procedure constitutes a simulation cycle. In this way we produced 21 cycles with different pseudo-random numbers. Figures 2 and 3 show the resulting order parameter curves in two different cases: in Fig. 2 we have $D_B < D_A$ and the system cycles counterclockwise through a hysteresis loop, signalling the occurrence of a first order transition. In Fig. 3 exactly the same simulation procedure does lead to some dispersion in the order parameter curves, but not to a clearcut hysteresis loop; in this case the transition is known to be continuous.

5. PERTURBATIVE CALCULATION OF THE EQUATION OF STATE

5.1. One-Loop Perturbation Expansion

In this section we determine the one-loop equation of state. We start from the dynamic functional of Eq. (7), in which we have included a particle
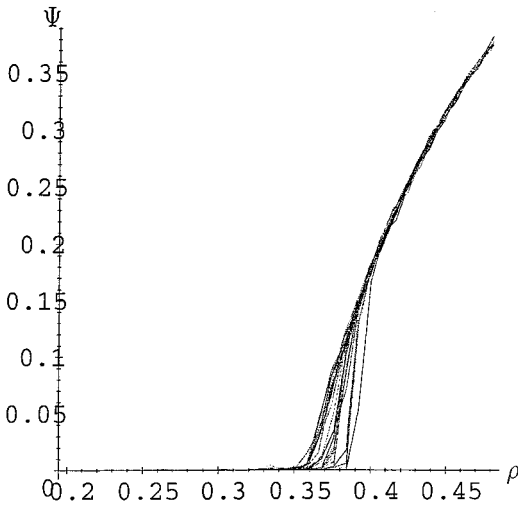
Fig. 3. Same as Fig. 2, but for $4D_A = 0.1$, and $4D_B = 0.8$. In this case the transition is known to be continuous and no hysteresis loop appears.

source term $-\int d^d r \, dt \, \lambda h(\mathbf{r}, t) \, \bar{\psi}(\mathbf{r}, t)$. The equations of motion for the fields are

$$0 = \frac{\delta S}{\delta \bar{m}} = \partial_t m - (\nabla^2 m + \lambda \sigma \, \nabla^2 \psi) + 2\nabla^2 \bar{m} \tag{49}$$

$$0 = \frac{\delta S}{\delta \bar{\psi}} = \partial_t \psi + \lambda(\tau - \nabla^2 + fm) \, \psi + \frac{\lambda g}{2} \, \psi^2 - \lambda \tilde{g} \psi \bar{\psi} - \lambda h \tag{50}$$

Note that the source term is not necessarily constant. Equations (49) and (50) are valid when they are inserted in averages. Taking the averages of (49) and (50) we find for the densities $M(\mathbf{r}) = \langle m(\mathbf{r}, t) \rangle$ and $\Psi(\mathbf{r}) = \langle \psi(\mathbf{r}, t) \rangle$ in a stationary state the exact equations

$$\nabla^2 M(\mathbf{r}) + \lambda \sigma \, \nabla^2 \Psi(\mathbf{r}) = 0 \tag{51}$$

$$\left[\tau - \nabla^2 + fM(\mathbf{r}) + \frac{g}{2} \, \Psi(\mathbf{r}) \right] \Psi(\mathbf{r}) + fC_{m\psi}(\mathbf{r}) + \frac{g}{2} \, C_\psi(\mathbf{r}) = h(\mathbf{r}) \tag{52}$$

with the correlation functions

$$C_{m\psi}(\mathbf{r}) = \langle (m - M(\mathbf{r}))(\psi - \Psi(\mathbf{r})) \rangle \qquad C_\psi(\mathbf{r}) = \langle (\psi - \Psi(\mathbf{r}))^2 \rangle \tag{53}$$

From Eq. (51) it follows that

$$M(\mathbf{r}) = -\lambda\sigma\Psi(\mathbf{r}) + c(\mathbf{r}) \tag{54}$$

where $c(\mathbf{r})$ is a harmonic function ($\nabla^2 c = 0$). Here we assume that c is constant. (It has to be constant in the thermodynamic limit if both M and Ψ are free of singularities and finite for $r \to \infty$.) If $\int_V \mathrm{d}^d r\, m(\mathbf{r}, t) = 0$ (which can always be achieved by a shift of τ) we get

$$c = \frac{\lambda\sigma}{V} \int_V \mathrm{d}^d r\, \Psi(\mathbf{r}) \tag{55}$$

where V denotes the volume of the system.

The mean field equation for the profile reads

$$\left[\tau + fc - \nabla^2 + \frac{\bar{g}}{2}\, \Psi_{mf}(\mathbf{r}) \right] \Psi_{mf}(\mathbf{r}) = h(\mathbf{r}) \tag{56}$$

where $\bar{g} = g - 2\lambda\sigma f$. Equation (56) shows that stability of the mean field theory requires that $\bar{g} \geqslant 0$. For negative $\bar{g}$ higher powers in ψ have to be taken into account in the functional S. We first consider an external field h which is constant within a sphere of radius R and vanishes for $r > R$. For simplicity we take the thermodynamic limit $V, R \to \infty$ in such a way that $R^d/V \to 0$. In this case the region outside the sphere acts as a reservoir for the homogeneous mode of the field m, and in (56) we can set $c = 0$ for $\tau > 0$.

To calculate the one-loop correction to the equation of state we shift the fields ψ and m by their average values and obtain

$$\begin{aligned} S[\bar{m}, M + m; \bar{\psi}, \psi + \Psi] \\ = S_0[\bar{\psi}; \Psi] + S_G[\bar{m}, m; \bar{\psi}, \psi; \Psi] + S_I[m; \bar{\psi}, \psi] \end{aligned} \tag{57}$$

with

$$S_0[\bar{\psi}; \Psi] = \int \mathrm{d}t \int \mathrm{d}^d r\, \lambda\bar{\psi} \left[\left(\tau - \nabla^2 + \frac{\bar{g}}{2}\, \Psi \right) \Psi - h \right] \tag{58}$$

where we have kept the full **r**-dependence of Ψ and expressed M in terms of Ψ. The Gaussian part of S reads

$$S_G[\bar{m}, m; \bar{\psi}, \psi; \Psi] = \int dt \int d^d r [\bar{m}(\partial_t m - \nabla^2(m + \lambda\sigma\psi)) - (\nabla\bar{m})^2$$
$$+ \bar{\psi}(\partial_t \psi + \lambda(\tau - \nabla^2 + (g - \lambda\sigma f) \Psi) \psi + \lambda f \Psi m)$$
$$- \tfrac{1}{2}\lambda\tilde{g}\Psi\bar{\psi}^2] \tag{59}$$

and the interaction part is

$$S_I[m; \bar{\psi}, \psi] = \int dt \int d^d r \lambda [fm\psi\bar{\psi} + \tfrac{1}{2}\psi(g\psi - \tilde{g}\bar{\psi}) \bar{\psi}] \tag{60}$$

The Gaussian propagators $G_\psi = \langle \psi\bar{\psi} \rangle$, $G_m = \langle m\bar{m} \rangle$, $G_{m\psi} = \langle m\bar{\psi} \rangle$ and $G_{\psi m} = \langle \psi\bar{m} \rangle$ follow from (59). They satisfy the differential equations

$$(\partial_t + \lambda(\bar{\tau} - \nabla^2)) G_\psi(\mathbf{r}, \mathbf{r}'; t - t') + \lambda f \Psi G_{m\psi}(\mathbf{r}, \mathbf{r}'; t - t') = \delta^{(d)}(\mathbf{r} - \mathbf{r}') \delta(t - t')$$
$$\tag{61}$$

$$(\partial_t - \nabla^2) G_{m\psi}(\mathbf{r}, \mathbf{r}'; t - t') - \lambda\sigma \nabla^2 G_\psi(\mathbf{r}, \mathbf{r}'; t - t') = 0 \tag{62}$$

$$(\partial_t - \nabla^2) G_m(\mathbf{r}, \mathbf{r}'; t - t') - \lambda\sigma \nabla^2 G_{\psi m}(\mathbf{r}, \mathbf{r}'; t - t') = \delta^{(d)}(\mathbf{r} - \mathbf{r}') \delta(t - t')$$
$$\tag{63}$$

$$(\partial_t + \lambda(\bar{\tau} - \nabla^2)) G_{\psi m}(\mathbf{r}, \mathbf{r}'; t - t') + \lambda f \Psi G_m(\mathbf{r}, \mathbf{r}'; t - t') = 0 \tag{64}$$

with $\bar{\tau} = \tau + (g - \lambda\sigma f) \Psi$. The Gaussian propagators can be used to determine the equal time correlation functions (53) to lowest nontrivial order:

$$C_{m\psi}(\mathbf{r}) = \int_0^\infty dt \int d^d r' [\lambda\tilde{g}\Psi(\mathbf{r}') G_{m\psi}(\mathbf{r}, \mathbf{r}'; t) G_\psi(\mathbf{r}, \mathbf{r}'; t)$$
$$+ 2(\nabla' G_m(\mathbf{r}, \mathbf{r}'; t))(\nabla' G_{\psi m}(\mathbf{r}, \mathbf{r}'; t)))] \tag{65}$$

$$C_\psi(\mathbf{r}) = \int_0^\infty dt \int d^d r' [\lambda\tilde{g}\Psi(\mathbf{r}')(G_\psi(\mathbf{r}, \mathbf{r}'; t))^2 + 2(\nabla' G_{\psi m}(\mathbf{r}, \mathbf{r}'; t))^2] \tag{66}$$

For constant Ψ the equations (61)–(64) can easily be solved by Fourier transformation. In this way one obtains for the fluctuation term in the equation of state (52)

$$fC_{m\psi} + \frac{g}{2} C_\psi = \int_{\mathbf{q}} \frac{\Psi}{\bar{\tau} + (1 + \lambda^{-1}) q^2} \left[\frac{1}{4} \tilde{g}g - f^2 + \frac{\bar{g}(\tilde{g}\lambda^{-1}q^2 + 2f^2\Psi)}{4(\tau' + q^2)} \right] \tag{67}$$

with $\tau' = \bar{\tau} - \lambda \sigma f \Psi$. After dimensional regularization the momentum integral becomes

$$fC_{m\psi} + \frac{g}{2} C_\psi = - \frac{A_\varepsilon \lambda \Psi}{2\varepsilon(1+\lambda)} \left(\frac{\lambda \bar{\tau}}{1+\lambda} \right)^{1-\varepsilon/2}$$

$$\times \left[\tilde{g}g - 4f^2 + \lambda^{-1}\tilde{g}\bar{g} + \frac{1+\lambda}{\lambda\bar{\tau}} \bar{g}(\tilde{g}\lambda^{-1}\tau' - 2f^2\Psi) \right.$$

$$\left. + \frac{\varepsilon}{2} \frac{(1+\lambda^{-1})^2 \tau'}{\bar{\tau}} \frac{\bar{g}(\tilde{g}\lambda^{-1}\tau' - 2f^2\Psi)}{\bar{\tau} - (1+\lambda^{-1}) \tau'} \ln \frac{(1+\lambda^{-1}) \tau'}{\bar{\tau}} + \mathcal{O}(\varepsilon^2) \right]$$

$$(68)$$

where $A_\varepsilon = (4\pi)^{-d/2} \Gamma(1+\varepsilon/2)/(1-\varepsilon/2)$.

5.2. Renormalized Equation of State

In order to absorb the ε-poles in the equation of state (52, 68) into a reparametrization of coupling constants and fields we make use of the renormalized quantities ψ_R, λ_R etc. introduced in Eqs. (11, 12).

The renormalized quantities satisfy the equation of state

$$h_R = \Psi_R \left\{ \tau_R + \frac{\bar{g}_R}{2} \Psi_R + \frac{\lambda_R}{4(1+\lambda_R)} \left[((1+\lambda_R^{-1}) u - 4v - 2w) \right. \right.$$

$$\times \frac{\bar{\tau}_R}{1+\lambda_R^{-1}} \ln \frac{\mu^{-2}\lambda_R \bar{\tau}_R}{1+\lambda_R} + \frac{(\lambda_R^{-1}u - 2w) \tau'_R - 2v\bar{g}_R \Psi_R}{\bar{\tau}_R - (1+\lambda_R^{-1}) \tau'_R}$$

$$\left. \left. \times \left(\bar{\tau}_R \ln \frac{\mu^{-2}\lambda_R \bar{\tau}_R}{1+\lambda_R} - (1+\lambda_R^{-1}) \tau'_R \ln(\mu^{-2}\tau'_R) \right) \right] \right\}$$

where $\bar{g}_R = g_R - 2\lambda_R f_R$, $\bar{\tau}_R = \tau_R + (g_R - \lambda_R f_R) \Psi_R$ and $\tau'_R = \tau_R + \bar{g}_R \Psi_R$ are the renormalized counterparts of $\bar{g}$, $\bar{\tau}$ and τ', respectively. For $f_R = v = w = 0$ we recover the one loop-equation of state for directed percolation.[22] To simplify the writing in equation (69) the geometrical factor A_ε, the momentum scale μ and σ_R have been absorbed into a rescaling of Ψ_R and h_R, i.e.,

$$A_\varepsilon^{-1/2}\mu^{\varepsilon/2}\sigma_R \Psi_R \to \Psi_R \qquad \text{and} \qquad A_\varepsilon^{-1/2}\mu^{\varepsilon/2}\sigma_R h_R \to h_R \qquad (70)$$

Hereafter we will drop the index "R" since only renormalized quantities will be used.

6. FLOW EQUATIONS

6.1. Renormalization Group for the Equation of State

The renormalizability of the field theory implies a set partial differential equations for the vertex functions. These are the renormalization group equations which follow from the independence of the bare vertex functions on the momentum scale μ. To investigate the equation of state in the critical region we need the one-point vertex function $\Gamma^{(1,0)}$ which is (up to a factor λ) equal to $h(\tau, \Psi; u, v, w, \rho; \mu)$. The renormalization group equation for h reads

$$\left[\mu \frac{\partial}{\partial \mu} + \beta_u \frac{\partial}{\partial u} + \beta_v \frac{\partial}{\partial v} + \beta_w \frac{\partial}{\partial w} + \beta_\lambda \frac{\partial}{\partial \lambda} + \kappa \tau \frac{\partial}{\partial \tau} + \zeta - \gamma \right]$$
$$\times h(\tau, \Psi; u, v, w, \lambda; \mu) = 0 \tag{71}$$

with the β-functions given in Section 2.

6.2. Scaling Form of the Equation of State

The renormalization group equation Eq. (71) can be solved by characteristics with the result

$$h(\tau, \Psi; u, v, w, \lambda; \mu)$$
$$= Y_h(\ell)^{-1} (\mu\ell)^{2+d/2} h(Y_\tau(\ell)(\mu\ell)^{-2} \tau, (\mu\ell)^{-d/2} \Psi;$$
$$u(\ell), v(\ell), w(\ell), \lambda(\ell); 1) \tag{72}$$

where

$$\frac{da(l)}{d \ln \ell} = \beta_a(u(\ell), v(\ell), w(\ell), \lambda(\ell)) \qquad \text{for} \quad a = u, v, w, \lambda \tag{73}$$

$$\frac{d \ln Y_\tau(\ell)}{d \ln \ell} = \kappa(u(\ell), v(\ell), w(\ell), \lambda(\ell)) \tag{74}$$

$$\frac{d \ln Y_h(\ell)}{d \ln \ell} = \gamma(u(\ell), v(\ell), w(\ell), \lambda(\ell)) - \zeta(u(\ell), v(\ell), w(\ell), \lambda(\ell)) \tag{75}$$

are the characteristics with the initial conditions $u(1) = u$, $v(1) = v$, $w(1) = w$, $\lambda(1) = \lambda$ and $Y_\tau(1) = Y_h(1) = 1$. Some solutions of the flow equations (73) are depicted in Fig. 4. For small initial values of $w \propto D_A - D_B$
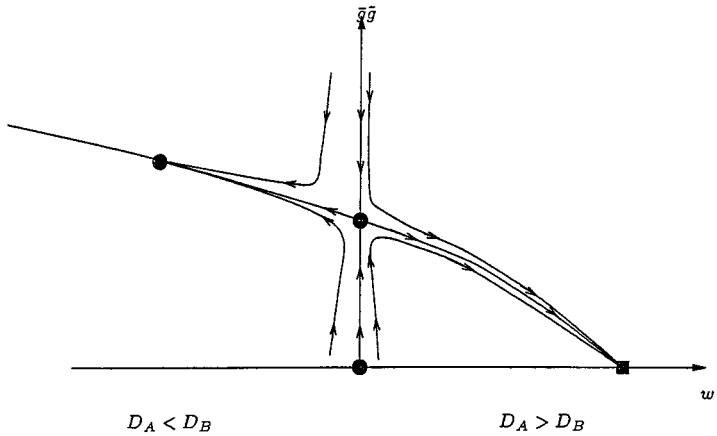
Fig. 4. Flow diagram in the $(\bar{g}\tilde{g}, w)$ plane. The leftmost black dot stands for the $D_A < D_B$ fixed point while the one lying on the $w = 0$ axis stands for the symmetric $D_A = D_B$ fixed point. They both describe second order transitions. Typical trajectories have been drawn. Those starting close to the symmetric fixed point but with an initial positive w eventually flow away from the symmetric fixed point.

the trajectories first approach the unstable manifold of the symmetric fixed point ($w = 0$) before they flow away. The unstable manifold leaves the stability region of the mean field theory ($\bar{g} > 0$, or $u - 2\lambda w > 0$) at the point $(u_*, v_*, w_*, \lambda_*)$. The numerical solution of the flow equations yields $u_* = 12.32\varepsilon$, $v_* = 2.104\varepsilon$, $w_* = 22.11\varepsilon$, and $\lambda_*^{-1} = 3.589$. The intersection point of the unstable manifold with the stability edge $\bar{g} = 0$ is of special interest since the perturbatively improved mean field theory should be a good approximation for small $\bar{g}$ (as will be discussed in the next section). Therefore the phase transition for very small $w > 0$ is governed by the equation of state at the point $(u_*, v_*, w_*, \lambda_*)$. In the following we shall denote by ℓ_* the value of the flow parameter at which $u(\ell_*) - 2\lambda(\ell_*) w(\ell_*) = 0$ and by $\xi_* = e^{\ell_*}$ the related length scale. One can identify ξ_* with its heuristic counterpart defined in Eq. (43). The flow equations are too complicated to be solved analytically for all ℓ, however it is possible, using scaling arguments, to predict that, as $\sigma \to 0^+$, $\xi_* \propto \sigma^{2/\gamma_s}$, a form also proposed in Eq. (46).

7. A FIRST-ORDER TRANSITION FOR $D_A > D_B$

In this section we study the mean field equation of state with the one-loop fluctuation correction (69) for small values of the coupling $\bar{g} \ll g$. Our motivation is an analogy of our reaction diffusion system with spin systems

with cubic anisotropy. Using a modified Ginzburg criterion for systems with cubic anisotropy Rudnick[3] (see also ref. 4) has shown that the fluctuation corrected mean field approximation should give reliable results if the values of the coupling coefficients are close to the stability edge of the mean field theory. In the case of the reaction diffusion system with $D_A > D_B$ the stability edge is given by $\bar{g} = 0$.

Now assume that we start with a very small value of the coupling w and choose the flow parameter $\ell = \ell_*$ in (72). After the ℓ-dependent prefactors $Y_\tau(\ell_*) \ell_*^{-2}$ etc. have been absorbed into a rescaling of τ, h, and Ψ the improved mean field equation of state takes the simple form

$$h = \Psi \left[\tau + \frac{u_* - 4v_*}{4(1 + \lambda_*^{-1})^2} \left(\tau + \frac{g_*}{2} \Psi \right) \ln \frac{\tau + g_* \Psi/2}{\mu^2 (1 + \lambda_*^{-1})} + \mathcal{O}(\text{two loop}) \right] \qquad (76)$$

with $(u_* - 4v_*)/(4(1 + \lambda_*^{-1})^2) = 0.04635\varepsilon > 0$.

In the limit $h \to 0^+$ the absorbing state with $\Psi = 0$ is a solution of the equation of state for all τ. For $\tau < \tau_{\text{spinod}}$ with

$$\tau_{\text{spinod}} = \mu^2 e^{-1} \frac{u_* - 4v_*}{4(1 + \lambda_*^{-1})} = \mathcal{O}(\varepsilon) \qquad (77)$$

there is also a solution with $\Psi > 0$ and $\partial\Psi/\partial h > 0$ (see Fig. 5). To see this one should anticipate that when the order parameter is of the order of its value at τ_{spinod} one has

$$\frac{\tau_{\text{spinod}}}{g_* \Psi} = \mathcal{O}(\varepsilon) \qquad (78)$$
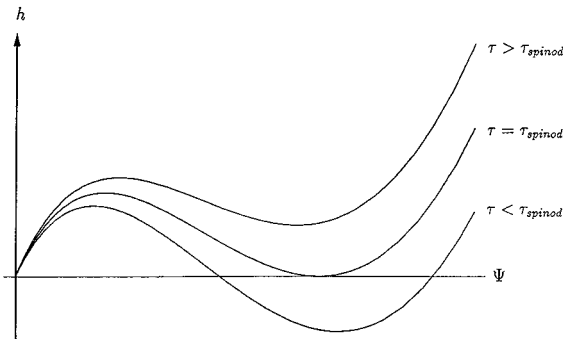

Fig. 5.   Sketch of the function $h(\tau, \Psi)$, Eq. (76).

and to leading order the reasoning is carried out on

$$h = \Psi \left[\tau + \frac{u_* - 4v_*}{4(1 + \lambda_*^{-1})^2} \frac{g_*}{2} \Psi \ln \frac{g_* \Psi}{2(1 + \lambda_*^{-1}) \mu^2} \right] \tag{79}$$

Solving the latter equation for $h = 0$ and $\partial h / \partial \Psi = 0$ yields, to leading order in ε,

$$\Psi_{\text{spinod}} = \frac{8(1 + \lambda_*^{-1})^2}{u_* - 4v_*} \frac{\tau_{\text{spinod}}}{g_*}, \qquad \tau_{\text{spinod}} = \mu^2 e^{-1} \frac{u_* - v_*}{4(1 + \lambda_*^{-1})} \tag{80}$$

which *a posteriori* justifies working on the approximation Eq. (79). Since the susceptibility $\chi = \partial \Psi / \partial h$ (the response of the order parameter to par- ticule injection) is positive the new solution is at least metastable for all $\tau < \tau_{\text{spinod}}$. The open question is for which range of τ the solution is stable, i.e., stable also with respect to nucleation processes. If we could derive the equation of state from a free energy this question would be easy to answer: a metastable solution is a *local* minimum of the free enemy while a stable solution is a *global* minimum. However, since there is no free energy for the reaction diffusion system we have to look for a different stability criterion, e.g., the form of density profiles. By analogy with equilibrium systems we expect that the solution with $\Psi > 0$ is stable below a coexistence "tem- perature" (in our case we should talk about a coexistence density) τ_{coex} with $0 < \tau_{\text{coex}} < \tau_{\text{spinod}}$.

8. DERIVING τ_{coex} FROM A DENSITY PROFILE

If τ is so large that Eq. (76) has only the trivial solution $\Psi = 0$ the den- sity $\Psi(\mathbf{r})$ generated by a local source $h(\mathbf{r})$ decays rapidly with increasing distance from the region in which $h(\mathbf{r})$ is nonzero. Consider for instance a plane particle source with

$$h(\mathbf{r}) = h_0 \, \delta(r_\perp) \tag{81}$$

where $r_\perp$ is the coordinate perpendicular to the source. For simplicity assume that $h_0 \to \infty$. For large $r_\perp$ the profile [i.e., the solution of (52)] will become independent of $r_\perp$ and tend to either (a) $\Psi = 0$ if τ is sufficiently large or (b) the nonzero solution of (76). In the thermodynamic limit the whole profile $\Psi(\mathbf{r})$ is uniquely determined by the source $h(\mathbf{r})$ since Ψ has to be finite for $r_\perp \to \pm \infty$. In the case (a) we can conclude that $\tau > \tau_{\text{coex}}$ whereas (b) occurs for $\tau < \tau_{\text{coex}}$.

In order to calculate a density profile perturbatively one usually starts with the mean field profile and assumes that the fluctuation corrections are small (of the order ε, say). In the present case this procedure would not lead to the desired result since the nonzero solution of the equation of state for $\tau < \tau_{\text{spinod}}$ is of the order ε^0. It can therefore not be derived as a small correction to Ψ_{mf}. Instead we have to compute the *equation for the density profile* perturbatively and then study the asymptotic behavior of its solutions. This means that we need the correlation functions $C_{m\psi}(\mathbf{r}; \{\Psi\})$ and $C_{\psi}(\mathbf{r}; \{\Psi\})$ in equation (52) for a general function $\Psi(\mathbf{r})$. Of course, we cannot compute these functions exactly but it is possible to derive a systematic gradient expansion for $C_{m\psi}$ and C_{ψ}.

We first compare the leading ε-orders in equation (52) (with $M = -\lambda\sigma\Psi$): Since we expect that the coexistence point to be located in the parameter range $0 < \tau \leqslant \tau_{\text{spinod}} = \mathcal{O}(\varepsilon)$ we may set $\tau = \mathcal{O}(\varepsilon)$. The limit of a very weak first order transition is governed by the point $(u_*, v_*, w_*, \lambda_*)$ which means that $\bar{g} = 0$ and that the combination $fC_{m\psi} + (g/2)\, C_{\psi}$ is of order $\mathcal{O}(\varepsilon)$. Comparing the terms on the l.h.s. of (52) therefore yields $(\nabla^2\Psi)/\Psi = \mathcal{O}(\varepsilon)$, i.e., gradients of Ψ may be considered as small quantities when we calculate $C_{m,\psi}$ and C_{ψ}. Using the Taylor series

$$\Psi(\mathbf{r}') = \Psi(\mathbf{r}) + \sum_{N=1}^{\infty} \frac{1}{N!} \sum_{\alpha_1\cdots\alpha_N} (r'-r)_{\alpha_1} \cdots (r'-r)_{\alpha_N} \partial_{\alpha_1} \cdots \partial_{\alpha_N} \Psi(\mathbf{r}) \qquad (82)$$

for the profile one arrives at a gradient expansion for $C_{m\psi}$ and C_{ψ} of the form

$$C_{\psi}(\mathbf{r}, \{\Psi\}) = C_{\psi}(\Psi(\mathbf{r})) + \sum_{N=1}^{\infty} \frac{1}{N!} \sum_{\alpha_1\cdots\alpha_N} C_{\psi;\,\alpha_1\cdots\alpha_N}(\Psi(\mathbf{r}))\, \partial_{\alpha_1} \cdots \partial_{\alpha_N} \Psi(\mathbf{r}) \qquad (83)$$

At leading order in ε only the first term on the r.h.s. of (83) contributes, i.e., we may simply replace Ψ in (68) by the profile $\Psi(\mathbf{r})$ and use the result in Eq. (52). After application of the renormalization group as before and absorbing ℓ-dependent prefactors the equation for the profile becomes

$$h(\mathbf{r}) = \Psi(\mathbf{r}) \left[\tau + \frac{u_* - 4v_*}{4(1 + \lambda_*^{-1})^2} \left(\tau + \frac{g_*}{2}\, \Psi(\mathbf{r}) \right) \ln \frac{\tau + g_*\, \Psi(\mathbf{r})/2}{\mu^2(1 + \lambda_*^{-1})} \right]$$

$$- \nabla^2\Psi(\mathbf{r}) + \mathcal{O}(\varepsilon^2) \qquad (84)$$

In order to extend this result to the next order in ε one has to (i) compute $C_{m\psi}$ and C_{ψ} for constant Ψ to two-loop order and (ii) take into account
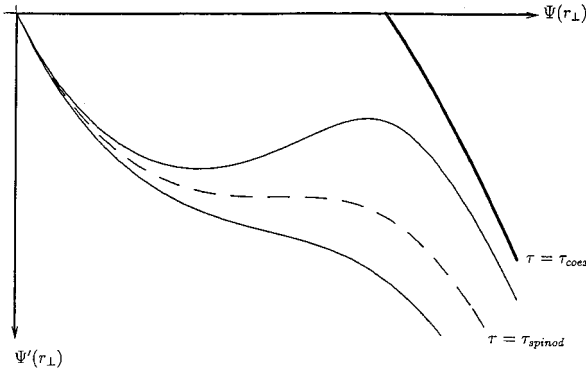
Fig. 6. Derivative of the density profile $\Psi'(r_\perp)$ as a function of $\Psi(r_\perp)$ for $\tau \geqslant \tau_{\text{coex}}$. The boundary condition at $r_\perp = 0^+$ is given by $\Psi'(0) = -h_0/2$.

the $\nabla^2\Psi$-correction in the gradient expansion (83) to one-loop order. In this way the $\nabla^2\Psi$-term in (84) may receive a Ψ-dependent correction.

For $h(\mathbf{r}) = h_0\,\delta(r_\perp)$ Eq. (84) can be integrated once after multiplication of both sides with $\Psi'(r_\perp)$. In Fig. 6 the result is depicted for various values of τ. There is a value $\tau_{\text{coex}} < \tau_{\text{spinod}}$ such that the profile does not tend to zero for $r_\perp \to \pm\infty$ if $\tau \leqslant \tau_{\text{coex}}$. As discussed above τ_{coex} is the coexistence point below which the active phase becomes a stable solution of the equation of state. Again one works with Eq. (79). In practice one has to solve the system composed of Eq. (79) with $h = 0$ along with its integrated counterpart

$$0 = \frac{\tau_{\text{coex}}}{2}\,\Psi_{\text{coex}}^2 + \frac{u_* - 4v_*}{24(1+\lambda_*^{-1})^2}\,g_*\,\Psi_{\text{coex}}^3\left[\ln\frac{g_*\,\Psi_{\text{coex}}}{2\mu^2(1+\lambda_*^{-1})} - \frac{1}{3}\right] \quad (85)$$

The explicit calculation yields $\Psi_{\text{coex}} = 12(1+\lambda_*^{-1})^2\,\tau_{\text{coex}}/((u_* - 4v_*)\,g_*)$ (which also justifies the use of the simplified equation of state Eq. (79)), with

$$\tau_{\text{coex}} = \mu^2 e^{-2/3}\frac{u_* - 4v_*}{6(1+\lambda_*^{-1})} = 0.93\tau_{\text{spinod}} \quad (86)$$

$\tau_{\text{coex}}/\tau_{\text{spinod}}$ is not a universal number, but the susceptibility ratio χ_+/χ_- with

$$\chi_+ = \lim_{h\to 0}\frac{\partial\Psi}{\partial h}\bigg|_{\Psi=0,\,\tau_{\text{coex}}} \qquad \chi_-\lim_{h\to 0}\frac{\partial\Psi}{\partial h}\bigg|_{\Psi>0,\,\tau_{\text{coex}}} \quad (87)$$

is universal. To one-loop order one finds

$$\frac{\chi_+}{\chi_-} = \frac{1}{2} + \mathcal{O}(\varepsilon) \tag{88}$$

This result is analogous to the universality of the magnetic susceptibility ratio found by Rudnick[3] and Arnold and Yaffe.[4]

9. CONCLUSIONS AND PROSPECTS

9.1. A Heuristic Functional for the Steady State Phase Diagram

In this paragraph we would like to build *a posteriori* a functional of the order parameter field $\Psi(\mathbf{r})$ describing the phase diagram in the stationary state of the system. We emphasize that the following is only valid to one loop order. We define $F[\Psi]$ by

$$F[\Psi] = \int \mathrm{d}^d r \left[\frac{1}{2}(\nabla\Psi)^2 + \int_0^{\Psi(\mathbf{r})} \mathrm{d}\psi \, \Gamma^{(1,0)}[0, \psi] \right] \tag{89}$$

By construction of course $\delta F/\delta \Psi = 0$ is equivalent to the equation of state Eq. (79). It is instructive to plot F as a function of Ψ for various values of τ (see Fig. 7). There it appears possible to deduce the phase diagram from the global minima of $F[\Psi]$. However the route leading to the functional $F[\Psi]$ follows a series of field-theoretic detours. The suggestive notation F, which reminds of a free energy (in the equilibrium statistical mechanics sense) is however misleading. For instance it could not be used as an effective Landau hamiltonian for the calculation of a Gibbs partition function describing fluctuations directly in the steady state. This functional is a remarkably compact and intuitive way of summarizing the properties of the steady state phase diagram. In particular the spinodal point τ_{spinod} appears as the point below which F develops a second minimum. Below τ_{coex} that minimum becomes the global minimum. To one loop order the equilibrium vocabulary can therefore be used carelessly.

9.2. Summary

In the course of this work we have elaborated a phenomenological description of a fluctuation-induced first-order transition taking place in a nonequilibrium steady state, the first one of this sort. We have in parallel
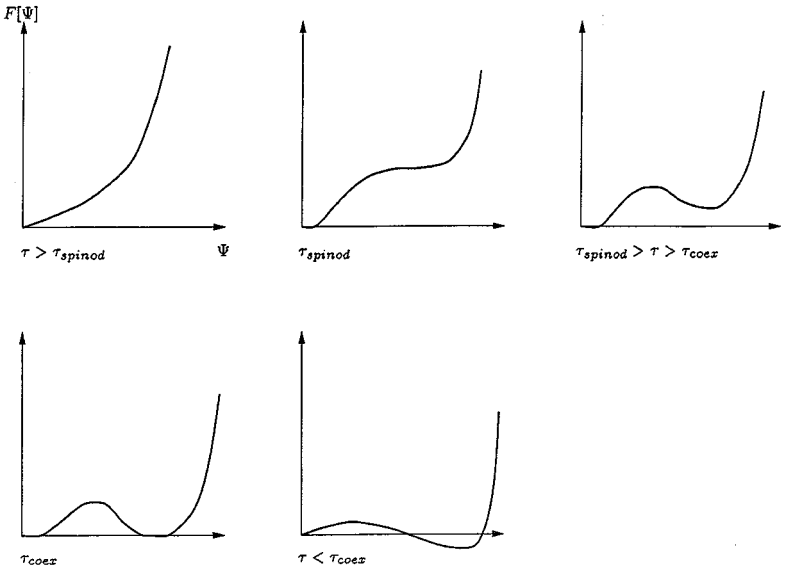
Fig. 7. $F[\Psi]$ as a function of Ψ for decreasing values of τ. We identify the spinodal point as the value of τ. below which F develops a local nonzero minimum and the coexistence point as the point at which the two minima become degenerate.

applied field-theoretic techniques to derive an effective (renormalization-group improved) equation of state that incorporates those fluctuations. This yields a PDE for the order parameter in the steady state. Performing a study of the stability (against space fluctuations of the order parameter) of the solutions of this PDE has led us to a complete description of the phase diagram. We have identified in this nonequilibrium situation a concept analogous to the point of spinodal decomposition consistent with our phenomenological description.

9.3. Possible Applications

Among the many nonequilibrium systems that appear in the literature, driven diffusive systems lend themselves to an analytic treatment by techniques similar to those of the present article.[23] In a number of such systems though, a significant portion of the phase space (in terms of control parameters) escapes conventional analysis. In some cases we believe that the reason is the occurrence of fluctuation-induced first order transition, such as in ref. 10. It would be quite interesting to see how both the technical argument and the heuristics can be extended to those systems. This will be the subject of future work.

APPENDIX

There are two ways to proceed in order to obtain the equation of state to one-loop order. In this appendix we follow the route familiar from static critical phenomena. We use the action Eq. (8) as the starting point of our analysis. The first task is to determine the one-loop expression of the effective potential Γ.

$$\Gamma[\bar{\psi}, \psi] = S[\bar{\psi}, \psi] + \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} \frac{d\omega}{2\pi} \ln \det S''(\mathbf{q}, \omega)[\bar{\psi}, \psi] \qquad (90)$$

with the matrix S'' defined by

$$S''(\mathbf{q}, \omega) = \begin{pmatrix} \dfrac{\delta^2 S}{\delta\bar{\psi}(-\mathbf{q}, -\omega)\,\delta\psi(\mathbf{q}, \omega)} & \dfrac{\delta^2 S}{\delta\bar{\psi}(-\mathbf{q}, -\omega)\,\delta\bar{\psi}(\mathbf{q}, \omega)} \\ \dfrac{\delta^2 S}{\delta\psi(-\mathbf{q}, -\omega)\,\delta\psi(\mathbf{q}, \omega)} & \dfrac{\delta^2 S}{\delta\psi(-\mathbf{q}, -\omega)\,\delta\bar{\psi}(\mathbf{q}, \omega)} \end{pmatrix} \qquad (91)$$

$$S''_{11}(\mathbf{q}, \omega) = \lambda(\mathbf{q}^2 + \bar{\tau}) - i\omega - \lambda\tilde{g}\Psi - \lambda^2\sigma f\Psi \frac{\mathbf{q}^2}{\mathbf{q}^2 - i\omega} - 2\frac{(\lambda f)^2 \mathbf{q}^2}{\mathbf{q}^4 + \omega^2} \Psi\bar{\psi} \qquad (92)$$

$$S''_{12}(\mathbf{q}, \omega) = -\frac{2(\lambda f)^2 \mathbf{q}^2}{\mathbf{q}^4 + \omega^2} \Psi^2 - \lambda\tilde{g}\Psi \qquad (93)$$

$$S''_{21}(\mathbf{q}, \omega) = -\frac{2(\lambda f)^2 \mathbf{q}^2}{\mathbf{q}^4 + \omega^2} \bar{\psi}^2 - 2\frac{\lambda^2\sigma f q^4}{q^4 + \omega^2} \bar{\psi} + \lambda g\bar{\psi} \qquad (94)$$

$$S''_{22}(\mathbf{q}, \omega) = \lambda(\mathbf{q}^2 + \bar{\tau}) + i\omega - \lambda\tilde{g}\Psi - \lambda^2\sigma f\Psi \frac{\mathbf{q}^2}{\mathbf{q}^2 + i\omega} - 2\frac{(\lambda f)^2 q^2}{\mathbf{q}^4 + \omega^2} \Psi\bar{\psi} \qquad (95)$$

For a homogeneous source term h the equation of state for a homogeneous order parameter Ψ now follows from the requirement that

$$\frac{\delta\Gamma}{\delta\bar{\psi}}[0, \Psi] = 0 \qquad (96)$$

It is a tedious but straightforward task to find the one-loop correction to $\Gamma^{(1, 0)}$ in the form of an integral over momentum and frequency. Writing

$$\Gamma^{(1, 0)}[\bar{\psi} = 0, \psi = \Psi] = -\lambda h + \lambda\Psi(\tau + \tfrac{1}{2}\bar{g}\Psi) + \delta\Gamma^{(1, 0)} \qquad (97)$$

one finds

$$\delta\Gamma^{(1,0)} = -\lambda^2 \int \frac{d^d q}{(2\pi)^d} \frac{d\omega}{2\pi} \left(\mathbf{q}^2 + \bar{\tau} - \frac{1}{2} g \Psi\right) (\tilde{g}(\mathbf{q}^4 + \omega^2) + 2\lambda f^2 \mathbf{q}^2 \Psi)$$
$$\times \left[(\omega^2 - iA\omega - B)(\omega^2 + iA\omega - B)\right]^{-1} \quad (98)$$

where we have defined the auxiliary variables

$$A \equiv (\lambda + 1)\, \mathbf{q}^2 + \lambda\bar{\tau}, \qquad B \equiv \mathbf{q}^2 \lambda(\mathbf{q}^2 + \tau') \quad (99)$$

Upon using the following integration formulas,

$$\int \frac{d\omega}{2\pi} \frac{1}{\omega^2 \pm iA\omega - B} = 0, \qquad \int \frac{d\omega}{2\pi} \frac{1}{|\omega^2 \pm iA\omega - B|^2} = \frac{1}{2AB} \quad (100)$$

Eq. (98) simplifies into

$$\delta\Gamma^{(1,0)} = -\frac{\lambda}{2} \int \frac{d^d q}{(2\pi)^d} \left[\left(\mathbf{q}^2 + \bar{\tau} - \frac{1}{2} g \Psi\right) \left(\tilde{g}\left(\mathbf{q}^2 + \frac{\tau'}{1+\lambda^{-1}}\right) + \frac{2f^2}{1+\lambda^{-1}} \Psi\right) \right]$$
$$\times \left[(\mathbf{q}^2 + \tau') \left(\mathbf{q}^2 + \frac{\bar{\tau}}{1+\lambda^{-1}}\right) \right]^{-1} \quad (101)$$

The above expression can be cast in a form suitable to perform the **q**-integrals:

$$\delta\Gamma^{(1,0)} = -\frac{1}{2} \lambda\tilde{g} \int \frac{d^d q}{(2\pi)^d}$$
$$+ \frac{\lambda\Psi}{4((1+\lambda^{-1})\, \tau' - \bar{\tau})} \left[\tilde{g}(\lambda^{-1}g - 2\sigma f)\, \tau' - 2f^2\bar{g}\Psi\right] \int \frac{d^d q}{(2\pi)^d} \frac{1}{\mathbf{q}^2 + \tau'}$$
$$+ \frac{\lambda\Psi}{4(1+\lambda^{-1})((1+\lambda^{-1})\, \tau' - \bar{\tau})} \left[2\tilde{g}\sigma f\bar{\tau} - (1+\lambda^{-1})\, g\tilde{g}\lambda\sigma f \Psi\right.$$
$$\left. - 4\lambda f^2\bar{\tau} + 2g(1+\lambda^{-1})\, f^2\Psi\right] \int \frac{d^d q}{(2\pi)^d} \frac{1}{\mathbf{q}^2 + \bar{\tau}/(1+\lambda^{-1})} \quad (102)$$

We use dimensional regularization to compute the momentum integrals:

$$\int \frac{d^d q}{(2\pi)^d} \frac{1}{\mathbf{q}^2 + \tau'} = -\frac{2}{\varepsilon} \tau'^{\,1-\varepsilon/2} A_\varepsilon$$
$$\int \frac{d^d q}{(2\pi)^d} \frac{1}{\mathbf{q}^2 + \bar{\tau}/(1+\lambda^{-1})} = -\frac{2}{\varepsilon} \left(\frac{\bar{\tau}}{1+\lambda^{-1}}\right)^{1-\varepsilon/2} A_\varepsilon \quad (103)$$

In terms of renormalized quantities the equation of state has the form

$$
\begin{aligned}
h_{\mathbf{R}} = \Psi_{\mathbf{R}} \Bigg\{ &\tau_{\mathbf{R}} + \frac{\bar{g}_{\mathbf{R}}}{2}\,\Psi_{\mathbf{R}} + \frac{1}{4(1+\lambda_{\mathbf{R}}^{-1})} \Bigg[\big((1+\lambda_{\mathbf{R}}^{-1})\,u - 4v - 2w\big) \\
&\times \frac{\bar{\tau}_{\mathbf{R}}}{1+\lambda_{\mathbf{R}}^{-1}} \ln \frac{\mu^{-2}\bar{\tau}_{\mathbf{R}}}{1+\lambda_{\mathbf{R}}^{-1}} \\
&+ \frac{(\lambda_{\mathbf{R}}^{-1}u - 2w)\,\tau_{\mathbf{R}}' - 2v\bar{g}_{\mathbf{R}}\,\Psi_{\mathbf{R}}}{\bar{\tau}_{\mathbf{R}} - (1+\lambda_{\mathbf{R}}^{-1})\,\tau_{\mathbf{R}}'} \\
&\times \bigg(\bar{\tau}_{\mathbf{R}} \ln \frac{\mu^{-2}\bar{\tau}_{\mathbf{R}}}{1+\lambda_{\mathbf{R}}^{-1}} - (1+\lambda_{\mathbf{R}}^{-1})\,\tau_{\mathbf{R}}' \ln(\mu^{-2}\tau_{\mathbf{R}}') \bigg) \Bigg] \Bigg\}
\end{aligned}
\tag{104}
$$

which is Eq. (69).

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