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LETTER TO THE EDITOR

Critical fluctuations around non-equilibrium steady states

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Abstract. Scaling and renormalisation-group concepts are used to derive phenomenological Langevin equations for non-equilibrium steady states. For the Schlögl model we unambiguously identify the critical Langevin equation in $4-\varepsilon$ dimensions simply by requiring that the correct mean-field limit be reproduced. Our approach should therefore be applicable to models for which only the mean-field behaviour is well established.

Non-equilibrium phase transitions (Haken 1975) have attracted a great deal of attention in recent years. Particularly for chemical systems, although there is broad agreement on the nature of the instabilities, a conventional treatment of the critical fluctuations is hampered by the absence of a simple phenomenological Langevin equation. In this letter we study the Schlögl (1972) model which is perhaps the simplest prototype for a non-equilibrium continuous phase transition. Using scaling and renormalisation-group ideas we find that we may unambiguously identify the Langevin equation which controls the critical fluctuations, by simply demanding that it reproduce the correct mean-field behaviour which is known from a number of sources (Nitzan *et al* 1974, Gardiner *et al* 1976, Mou *et al* 1978). For this model our approach leads in a simple manner to the rather curious multiplicative noise suggested by Gardiner and Chaturvedi (1977) on the basis of a sophisticated treatment of the associated master equation. Analysing the scaling structure we find that the Schlögl model lies neither in the universality class of Reggeon theory as suggested by Grassberger and Sundermeyer (1978) nor that described by Goldhirsch and Procaccia (1981). Adopting our Langevin description a conventional dynamical renormalisation-group treatment (de Dominicis and Peliti 1978, Vvedensky *et al* 1983) may be employed, which unlike that of Goldhirsch and Procaccia is free of any *ad hoc* assumptions.

The Schlögl (1972) model for a chemical instability is defined by the coupled reactions

$$A + X \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 2X, \qquad B + X \underset{k_4}{\overset{k_3}{\rightleftharpoons}} C \tag{1}$$

where it is arranged for the concentrations of A, B, C to be held fixed (an open system) whilst the concentration of X, denoted by $[X] \equiv \psi(\boldsymbol{r}, t)$, is monitored. Phenomenologically we propose for the system a Langevin equation of the form

$$\partial\psi(\boldsymbol{r}, t)/\partial t = D\nabla^2\psi(\boldsymbol{r}, t) + [h + r\psi(\boldsymbol{r}, t) - \tfrac{1}{2}u\psi^2(\boldsymbol{r}, t)] + \eta(\boldsymbol{r}, t)g(\psi(\boldsymbol{r}, t)) \tag{2}$$

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with a gaussian noise $\eta(\boldsymbol{r}, t)$:

$$\langle \eta(\boldsymbol{r}, t) \rangle = 0, \qquad \langle \eta(\boldsymbol{r}, t)\eta(\boldsymbol{r}', t') \rangle = \delta(t-t')\delta(\boldsymbol{r}-\boldsymbol{r}'). \tag{3}$$

As one would expect the first term controls diffusion whilst the second represents the deterministic rate equation for the reaction (1); $h \equiv k_4[C]$, $r \equiv k_1[A] - k_3[B]$, $u \equiv 2k_2$. The novelty of our scheme lies in the function $g(\psi(\boldsymbol{r}, t))$ controlling the noise term which is to be specified below. Naturally for an equilibrium system $g(\psi)$ is specified directly by the fluctuation dissipation theorem associated with local stability of an equilibrium configuration, however for this *non-equilibrium* (open) system a new criterion must be sought. Seeking homogeneous steady-state solutions of (2), (3) the continuous phase transition is easily identified. We find for $h = 0$

$$\psi \equiv \begin{cases} 0, & r < 0 \\ 2r/u, & r > 0 \end{cases} \tag{4}$$

so that at $r = 0$ the system undergoes a continuous phase transition, closely resembling those seen in equilibrium systems with a divergent correlation length $\xi \sim r^{-1/2}$.

For $d > 4$ spatial dimensions it is well known (Mori and McNeil 1977) that the mean-field (or gaussian) approach to the Schlögl model is adequate even near the phase transition. One finds for example from the Master equation (Gardiner *et al* 1976) or Fokker–Planck (Nitzan *et al* 1974) techniques that the equal-time correlation function $C(\boldsymbol{q}, t)$ taken at momentum $\boldsymbol{q}$ is in the steady state for $h = 0$ of the form

$$C(\boldsymbol{q}, t) \sim \langle \psi \rangle / (Dq^2 + \tfrac{1}{2}u\langle \psi \rangle). \tag{5}$$

It is interesting to observe that as the critical point is approached from the ordered phase the zero momentum equal-time correlation function remains finite despite the divergence of the correlation length $\xi(h = 0)$, in sharp contrast to a more conventional phase transition.

On the other hand suppressing the fluctuation corrections (2) is easily solved by writing

$$\psi = \langle \psi \rangle + \delta\psi \tag{6}$$

where to leading order $\langle \psi \rangle$ satisfies for $h = 0$ the deterministic equation

$$r\langle \psi \rangle - \tfrac{1}{2}u\langle \psi \rangle^2 = 0. \tag{7}$$

The effective Langevin equation for $\delta\psi$ then leads directly to the expression

$$C(\boldsymbol{q}, t) \sim (g(\langle \psi \rangle))^2 / (Dq^2 + \tfrac{1}{2}u\langle \psi \rangle) \tag{8}$$

for the equal-time correlation function and whence by direct comparison of (5), (8) to the identification of the function $g(x)$

$$g(x) \sim x^{1/2} \tag{9}$$

at least at the mean-field level. We must now consider the possibility of fluctuation corrections to (9).

A useful framework within which to discuss the scaling and renormalisation-group structure associated with the Langevin equation (2) is the path integral formulation of classical statistical dynamics (de Dominicis and Peliti 1978). For the Langevin equation

(2), the generating function takes the form

$$Z(m, \hat{m}) = \int [\mathrm{d}\psi][\mathrm{d}\hat{\psi}] \exp\left(- \int \mathrm{d}\boldsymbol{x}\, \mathrm{d}t [L(\psi, \hat{\psi}) + m\psi + \hat{m}\hat{\psi}]\right) \tag{10}$$

where $L(\psi, \hat{\psi})$ is given by

$$L(\psi, \hat{\psi}) = \mathrm{i}\hat{\psi}(\boldsymbol{r}, t)[\partial\psi(\boldsymbol{r}, t)/\partial t - D\nabla^2\psi(\boldsymbol{r}, t) - h - r\psi(\boldsymbol{r}, t) + \tfrac{1}{2}u\psi^2(\boldsymbol{r}, t)] + \tfrac{1}{2}[\hat{\psi}(\boldsymbol{r}, t)g(\psi(\boldsymbol{r}, t))]^2 + \tfrac{1}{2}[r + u\psi(\boldsymbol{r}, t)]. \tag{11}$$

Here the first term arises directly from the deterministic equations of motion, the second from the noise and finally the third from the normalising Jacobian (Bausch *et al* 1976). As usual the correlation and response functions follow directly from $Z(m, \hat{m})$ via

$$\langle\psi(\boldsymbol{r}, t)\rangle = \partial Z(m, \hat{m})/\partial m(\boldsymbol{r}, t)\big|_{m=\hat{m}=0} \tag{12}$$

$$\langle\hat{\psi}(\boldsymbol{r}, t)\psi(\boldsymbol{r}', t')\rangle = (\partial/\partial h(\boldsymbol{r}, t))\langle\psi(\boldsymbol{r}', t')\rangle = \partial^2 Z(m, \hat{m})/\partial\hat{m}(\boldsymbol{r}, t)\partial m(\boldsymbol{r}', t')\big|_{m=\hat{m}=0} \tag{13}$$

and their natural generalisations.

To determine the relevance near the critical point of the non-linear terms appearing in (11) it is helpful to analyse the naive dimensions (Brezin *et al* 1973). In terms of a microscopic length l we may scale frequencies ω, momenta k and fields ψ, $\hat{\psi}$ as

$$r \sim \omega \sim k^2 \sim l^{-2}, \qquad \psi \sim \hat{\psi} \sim l^{-d/2} \tag{14}$$

so that we immediately conclude that the important non-linear coupling u scales as

$$u \sim l^{(d-4)/2} \tag{15}$$

and thus modifies the critical behaviour only for $d < 4$ spatial dimensions as expected. Additionally we observe from (9), (11) that it is natural to form a polynomial approximation for the squared function $g^2(x)$:

$$g^2(x) = vx + wx^2 + \cdots \tag{16}$$

where the parameters v, w scale as

$$v \sim l^{(d-4)/2}, \qquad w \sim l^{d-2}$$

and thus we deduce directly that the choice (9) will suffice to describe the phase transition for $d > 2$. Rescaling $\hat{\psi}$ we therefore arrive finally at the effective Lagrangian density

$$L(\psi, \hat{\psi}) = \mathrm{i}\hat{\psi}(\boldsymbol{r}, t)[\partial/\partial t - D\nabla^2 - r]\psi(\boldsymbol{r}, t) + \mathrm{i}\hat{\psi}(\boldsymbol{r}, t)h + \tfrac{1}{2}u[\mathrm{i}\hat{\psi}(\boldsymbol{r}, t)\psi^2(\boldsymbol{r}, t) + \hat{\psi}^2(\boldsymbol{r}, t)\psi(\boldsymbol{r}, t)] + \tfrac{1}{2}[r + u\psi(\boldsymbol{r}, t)]. \tag{17}$$

Our model is *not* equivalent to that proposed by Grassberger and Sundermeyer (1978). The Reggeon model (Abarbanel and Bronzan 1974) described by these authors is defined by the action

$$L(\phi, \phi^*) = \mathrm{i}\phi^*(\boldsymbol{r}, t)[\partial/\partial t - D\nabla^2 - r]\phi(\boldsymbol{r}, t) + \tfrac{1}{2}\mathrm{i}u[\phi^*(\boldsymbol{r}, t)\phi^2(\boldsymbol{r}, t) + (\phi^*)^2(\boldsymbol{r}, t)\phi(\boldsymbol{r}, t)] \tag{18}$$

where $\phi(\boldsymbol{r}, t)$ is a complex valued field. Taking $\phi = \psi + \mathrm{i}\hat{\psi}$ it seems clear that to identify (17), (18) we must append two new vertices: $z\hat{\psi}^3$, $y\psi^3$. For our Langevin approach

however the ψ^3 vertex would violate causality (see de Dominicis and Peliti 1978) whilst the $\hat{\psi}^3$ vertex would correspond to the introduction of a non-trivial third-order noise term ($\langle \eta^3 \rangle \neq 0$). Consequently the models (17), (18) are rather different. Indeed since these extra vertices are not dynamically generated by the renormalisation group they belong to different universality classes.

On the other hand Goldhirsch and Procaccia (1981) use a truncated form of (17) which includes no $\hat{\psi}^2\psi$ vertex. For such a model a conventional renormalisation-group treatment does not possess a non-trivial infrared stable fixed point so these authors were forced to propose a rather *ad hoc* scheme.

We have performed a complete renormalisation-group analysis of our model (17) (details to be reported elsewhere) which locates a non-trivial fixed point. The dynamical z and correlation length ν exponents are to leading order

$$z = 2 + \tfrac{3}{16}\varepsilon, \qquad \nu = \tfrac{1}{2} + \tfrac{1}{16}\varepsilon \tag{19}$$

which are indeed different from those of the Reggeon model at first order in $\varepsilon = 4 - d$ (Cardy and Sugar 1980). At an even more fundamental level it is clear that (17), (18) possesses entirely different ordered phases. For our model causality ensures $\langle \hat{\psi} \rangle = 0$ whilst in the Reggeon model $\langle \hat{\psi} \rangle \sim \langle \psi \rangle$.

To conclude we have proposed a simple method of deriving a non-equilibrium Langevin equation on the basis of the mean-field structure, which as in the Schlögl model is often known from a number of different sources (Master equation, Fokker–Planck, ...). For the Schlögl model a sophisticated analysis of the Master equation due to Gardiner and Chaturvedi (1977) leads basically to the same Langevin equation (including the curious multiplicative noise $g(x) \sim x^{1/2}$), however in most cases we are not so fortunate. We are currently studying the implications of our approach for the chemical Brusselator, the Bénard instability and the laser (Haken 1975).

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