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Abstract. From the reaction-diffusion master equation formulation of the Schlögl model we develop a comprehensive description of the non-equilibrium dynamics. Using the Poisson transformation and the dynamical renormalisation group we firstly show how the equilibrium limit is recovered, and secondly describe the low-frequency, low-momenta scaling behaviour of the concentration fluctuations. Our approach extends, simplifies or corrects previous studies and is easily generalised to treat more complicated systems.

1. Introduction

In recent years non-equilibrium phase transitions have been described by many authors (Haken 1975, Nicolis and Prigogine 1977). Simple reaction-diffusion models (Gardiner 1982) for example show an exciting array of critical phenomena, ranging from the continuous transitions reminiscent of equilibrium systems to the spectacular chemical oscillators. In direct contrast to equilibrium studies, however, scaling and renormalisation group ideas (Wilson and Kogut 1974, Hohenberg and Halperin 1977) have not yet been systematically applied. Broadly this can be attributed to the absence of a realistic dynamical Landau-Ginzburg description for the critical fluctuations. Quite generally for these non-equilibrium systems both the stationary distribution functions and the associated fluctuation dissipation theorems are unknown. It is therefore difficult to motivate simple phenomenological dynamical equations (Nitzan *et al* 1974, Keizer 1976, Vvedensky *et al* 1984), again in direct contrast to equilibrium studies (Ma and Mazenko 1975). An alternative approach to these reaction-diffusion systems is provided by the stochastic master equations of Gardiner *et al* (1976), van Kampen (1976), Nicolis and Prigogine (1977), which are readily solved at the mean field level of approximation. Such analyses indicate that the underlying Langevin description must possess several curious features, such as the dominance of multiplicative noise (Schenzle and Brand 1979) or the absence of a potential (Szépfalusy and Tél 1982).

In the search for a dynamical Landau-Ginzburg description a significant advance was made by Gardiner and Chaturvedi (1977, hereafter refered to as GC), who introduced the 'Poisson transform' (Gardiner 1983) via which simple *exact* Langevin or Fokker-Planck equations could be developed from the stochastic master equation approach. Unhappily, however, further progress was seriously hampered by the absence of a simple multi-time relation between the 'Poissonian' fluctuations and those of the original chemical master equation. This has very recently been remedied (Elderfield 1985), so for the first time a complete 'first principles' dynamical description

for these reaction–diffusion systems is now available based on powerful scaling and renormalisation group techniques. In this communication we study the simplest of these non-equilibrium transitions. Described originally by Schlögl (1972), the model reaction system

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

where it is arranged for the concentrations of A, B, C to be held fixed (an open system), whilst the concentration of X is monitored, undergoes a continuous transition reminiscent of those seen in equilibrium studies. Using the Poisson transform to factor out the critical fluctuations, we shall employ the renormalisation group to provide for the first time a complete dynamical scaling description. Our computation corrects, simplifies and extends the previous studies (Mori and McNeil 1977, Dewel *et al* 1977, Grassberger and Sundermeyer 1978, Janssen 1981, Goldhirsch and Procaccia 1981, Vvedensky *et al* 1984, Nicolis and Malek-Mansour 1984). In particular we show how in the equilibrium limit one recovers *precisely* the statistical mechanics result.

2. The Poisson representation for multi-time correlation and response functions

Phenomenologically for the Schlögl model (1) the reaction–diffusion master equation is defined (GC) by the following spatially discrete form:

$$\frac{\partial}{\partial t} P(\{x_i\}, t) = \sum_{i,j=1}^{N} D_{ij}[(x_i + 1) P(x_1, \ldots, x_i + 1, \ldots, x_j - 1, \ldots, x_N, t) - x_i P(\{x_i\}, t)]$$

$$+ \sum_{i=1}^{N} \{(k_1 B + k_4 x_i)(x_i + 1) P(x_1, \ldots, x_i + 1, \ldots, x_N, t)$$

$$+ [k_3 C + k_2 A(x_i - 1)] P(x_1, \ldots, x_i - 1, \ldots, x_N, t)$$

$$- [k_1 B x_i + k_3 C + k_2 A x_i + k_4 x_i(x_i - 1)] P(\{x_i\}, t)\}. \tag{2}$$

Here x_i is the number of X molecules in the ith cell, the non-local term represents cell to cell diffusion and the local term specifies the chemical reaction (1). To solve (2) GC proposed writing P as a superposition of Poissonians

$$P(\{x_i\}, t) = \int_{\mathscr{D}} \prod_{i=1}^{N} \left(d\mu(\alpha_i) \frac{e^{-\alpha_i}}{(x_i)!} (\alpha_i)^{x_i} \right) f(\{\alpha_i\}, t). \tag{3}$$

For our purposes it will be sufficient to consider only the real Poisson transform $(d\mu(\alpha) = d\alpha, \ \mathscr{D} \subset \mathbb{R})$; however we should remark that for this case f need not be positive definite, so it is best viewed as a Markovian quasi-probability (Gardiner 1982). Using (3) in (2), one deduces (GC) that the Poissonian fluctuations are described exactly by the Langevin equation (no *ad hoc* truncations)

$$\frac{d\alpha_i}{dt} = \sum_{j=1}^{N} D_{ij}\alpha_j + [k_3 C + (k_2 A - k_1 B)\alpha_i - k_4 \alpha_i^2] + [2\alpha_i(k_2 A - k_4 \alpha_i)]^{1/2} \xi_i(t)$$

$$\langle \xi_i(t) \xi(t') \rangle = \delta_{ij} \delta(t - t') \tag{4}$$

where the Itô prescription for the noise is to be understood. Adopting (3) on the

associated Fokker–Planck equation, we thus have a very flexible framework for computing Poissonian dynamics; however, as noted above, there is a serious drawback. Let us consider for a moment the relation between concentration and Poissonian fluctuations. For *equal* time correlations it follows directly from (3) that

$$\left\langle\!\!\!\left\langle \frac{(x_i)!}{(x_i-p)!}\frac{(x_j)!}{(x_j-k)!}\cdots \right\rangle\!\!\!\right\rangle^{i\neq j\neq} = \langle(\alpha_i)^p(\alpha_j)^k\ldots\rangle \tag{5}$$

or more explicitly

$$\langle\!\langle x_i\rangle\!\rangle = \langle\alpha_i\rangle$$
$$\langle\!\langle x_i x_j\rangle\!\rangle = \langle\alpha_i\alpha_j\rangle + \delta_{ij}\langle\alpha_j\rangle \tag{6}$$
$$\vdots \qquad \vdots$$

To obtain multi-time information is far more difficult; however this has recently been accomplished (Elderfield 1985).

Recasting (4) in terms of functional integrals using a variant of the Martin–Siggia–Rose formalism (de Dominicis and Peliti 1978) one can show (Elderfield 1985) that the response/correlation functions are generated by a functional $Z(\hat{l}, l)$ defined as follows

$$Z(\hat{l}, l) = \int [\mathrm{d}\alpha]\int[\mathrm{d}\hat{\alpha}]\exp\!\left(\int \mathrm{d}t\, L + \hat{l}\hat{\alpha} + l\alpha\right) \tag{7}$$

where the Lagrangian L takes the continuum form

$$L = \int \mathrm{d}r^d\{\mathrm{i}\hat{\alpha}(r,t)[(-D\nabla^2+\partial/\partial t+r)\alpha(r,t)+u\alpha^2(r,t)]-\hat{\alpha}^2(r,t)(v\alpha(r,t)-u\alpha^2(r,t))$$
$$-\mathrm{i}\hat{\alpha}(r,t)h\}. \tag{8}$$

As usual one has

$$\langle\alpha(r,t)\rangle = \partial Z(\hat{l},l)/\partial l(r,t)|_{l=\hat{l}=0}$$
$$\langle\hat{\alpha}(r,t)\alpha(r',t')\rangle = \mathrm{i}\frac{\partial}{\partial h(r,t)}\langle\alpha(r',t)\rangle = \frac{\partial^2 Z(\hat{l},l)}{\partial\hat{l}(r,t)\,\partial l(r',t')}\bigg|_{l=\hat{l}=0} \tag{9}$$

with their natural generalisations. Here the continuum couplings D, r, u, v and h are related to the original reaction/diffusion constants (2) as follows

$$r = (k_1 B - k_2 A) \qquad u = k_4\Lambda^{-d} \qquad v = k_2 A$$
$$h = k_3 C\Lambda^d \qquad D\nabla^2 \sim D_{ij} \tag{10}$$

through the continuum limit $\Lambda\to\infty$ at fixed densities $\rho(r,t)\equiv x_i\Lambda^d$, $\alpha(r,t)\equiv\alpha_i\Lambda^d$ with $\hat{\alpha}(r,t)\equiv\alpha_i$ in d spatial dimensions. In this framework the connection formula relating Poissonian and concentration fluctuations takes, for the two-point function, the form

$$\langle\!\langle\rho(r,t)\rho(r',t')\rangle\!\rangle^{t>t'} = (1+\partial/\partial h(r',t'))\langle\alpha(r,t)\alpha(r',t')\rangle \tag{11}$$

or equivalently

$$\langle\!\langle\rho(r,t)\rho(r',t')\rangle\!\rangle^{t>t'} = \langle\alpha(r,t)\alpha(r',t')\rangle + (\partial/\partial r(r',t'))\langle\alpha(r,t)\rangle \tag{12}$$

where the couplings $h(r,t)$, $r(r,t)$ (see (8) and (10)) have been used as sources. In

the equal time limit $t - t' \to 0^{+}$, (11), (12) reduce smoothly to the known equal time expression (GC)

$$\langle\!\langle\rho(\mathbf{r}, t)\rho(\mathbf{r}', t)\rangle\!\rangle = \langle\alpha(\mathbf{r}, t)\alpha(\mathbf{r}', t)\rangle + \delta(\mathbf{r} - \mathbf{r}')\langle\alpha(\mathbf{r}, t)\rangle \tag{13}$$

which is simply the continuum version of (6). We refer to Elderfield (1985) for a treatment of the higher-order correlation functions. Connection formulae for response functions follow by direct functional differentiation, using the identities (10). As an example, consider the general relation (6)

$$\langle\!\langle\rho(\mathbf{r}, t)\rangle\!\rangle = \langle\alpha(\mathbf{r}, t)\rangle \tag{14}$$

which implies directly that

$$\chi \equiv (\partial/\partial c(\mathbf{r}, t))\langle\!\langle\rho(\mathbf{r}', t')\rangle\!\rangle = (\partial/\partial c(\mathbf{r}, t))\langle\alpha(\mathbf{r}', t')\rangle \tag{15}$$

where the concentration of $c \equiv c(\mathbf{r}, t)$ is used as a probe. On a technical level, readers familiar with the MSR formalism will observe that our Lagrangian contains no 'Jacobian' factor, so that the equal time mixed correlation/response functions satisfy

$$\langle(\hat{\alpha}(t))^{p}(\alpha(t))^{q}\rangle = 0 \tag{16}$$

for $p \geq 1$ and any q. Of course response functions are naturally discontinuous at equal time, so we are free to make any choice, providing the connection formula (11) is modified consistently (see Elderfield 1985). For Langevin equations with multiplicative noises this is a serious concern for an inappropriate choice (e.g. see Phythian 1977) can seriously complicate the associated diagrammatics.

3. Scaling, mean field theory and the equilibrium limit

Given (8) and the appropriate connection formulae (11), (12) and (15), it is now a simple matter to reproduce the known mean field behaviour (Gardiner *et al* 1975, Gardiner 1982), using a conventional loop expansion (de Dominicis and Peliti 1975).

Assuming the system is in *a stationary state* for which

$$\langle\rho(\mathbf{r}, t)\rangle = M, \tag{17}$$

then within the mean field (or tree level) approximation the two-point correlation/response functions take the form

$$G(\mathbf{q}, \omega) \equiv \frac{\partial}{\partial h(\mathbf{q}, \omega)}\langle\!\langle\rho(\mathbf{q}', \omega')\rangle\!\rangle = \delta(\mathbf{q} + \mathbf{q}')\delta(\omega + \omega')\left(\frac{1}{D(q^2 + \xi^{-2}) + \mathrm{i}\omega}\right) \tag{18}$$

$$C(\mathbf{q}, \omega) \equiv \langle\!\langle\rho(\mathbf{q}, \omega)\rho(\mathbf{q}', \omega')\rangle\!\rangle$$

$$= \delta(\mathbf{q} - \mathbf{q}')\delta(\omega - \omega')\left[\frac{2(vM - uM^2)}{[D(q^2 + \xi^{-2})]^2 + \omega^2} + M\left(\frac{1}{D(q^2 + \xi^{-2}) + \mathrm{i}\omega} + \mathrm{CC}\right)\right.$$

$$\left. + (2\pi)^{d+1}M^2\delta(\mathbf{q})\delta(\omega)\right] \tag{19}$$

where M satisfies the deterministic equation

$$-h + rM + uM^2 = 0 \tag{20}$$

and we have introduced the correlation length

$$\xi = [(h + uM^2)/MD]^{-1/2}.$$ (21)

Qualitatively, therefore, for $h = 0$ as r passes through zero the system undergoes a continuous phase transition closely resembling those seen in equilibrium. Briefly as $r \to 0^+$ the correlation length ξ diverges in the classical manner, with the onset of long range order giving rise to a spontaneous 'magnetisation' M. As emphasised by Gardiner and Walls (1978), Nicolis and Malek-Mansour (1984), there are, however, important differences. Consider, for example, the time resolved two-point correlation function $C(q, t)$ which from (19) takes the form

$$C(q, t) \stackrel{t>0}{=} \delta(q - q') \left[\exp(-D(q^2 + \xi^{-2})t) \left(\frac{(vM - uM^2)}{D(q^2 + \xi^{-2})} + M \right) + (2\pi)^d M^2 \delta(q) \right].$$ (22)

In the *equilibrium* limit when the reactions (1) balance independently (Gardiner 1983), one must replace (20) by

$$vM - uM^2 = 0 = -h + (r + v)M$$ (23)

so that one obtains

$$C_{eq}(q, t) \stackrel{t>0}{=} \delta(q - q')[M \exp(-D(q^2 + \xi^{-2})t) + (2\pi)^d \delta(q)M^2]$$ (24)

or equivalently

$$\langle\!\langle (\rho(r, t) - M)(\rho(r', 0) - M) \rangle\!\rangle_{eq} \stackrel{t>0}{=} M \left(\frac{1}{4\pi Dt} \right)^{d/2}$$

$$\times \exp\left(-\left(\frac{(r - r')^2}{4Dt} + \frac{Dt}{\xi^2} \right) \right) \stackrel{t\to 0}{\longrightarrow} \delta(r - r')M$$ (25)

so that at short times correlations are intrinsically short range. On the other hand, for non-equilibrium steady states, characterised by the lack of detailed balance (or fluxes of A, B, C), then there are long range correlations even at short times. For $d = 3$ spatial dimensions (22) reduces at equal time to

$$\langle\!\langle (\rho(r, t) - M)(\rho(r', t) - M) \rangle\!\rangle = \frac{(vM - uM^2)}{4\pi D(|r - r'|)} \exp\left(\frac{-|r - r'|}{\xi} \right) + \delta(r - r')M$$ (26)

in agreement at large distances with the work of Nicolis and Malek-Mansour (1984). The relation (25) is of course not entirely surprising for one would surely hope to recover the Poissonian statistics of equilibrium statistical mechanics (Gardiner *et al* 1976) in the equal time limit $(t - t' \to 0^+)$ for this special case. Using the Poisson transform, it is quite simple to prove that this is a general feature. Shifting the field $\alpha(r, t)$

$$\alpha(r, t) = \tilde{\alpha}(r, t) + M$$ (27)

leads to a Lagrangian $L(\hat{\alpha}, \tilde{\alpha})$ of the form

$$L = \int dr^d \{ i\hat{\alpha}(-h + rM + uM^2) - \hat{\alpha}^2(vM - uM^2) $$

$$+ i\hat{\alpha}[(-D\nabla^2 + \partial/\partial t + r + 2uM]\tilde{\alpha} + u\tilde{\alpha}^2) - \hat{\alpha}^2[(v - 2uM)\tilde{\alpha} - u\tilde{\alpha}^2] \}.$$ (28)

Now, choosing M to satisfy the deterministic equation (20), one finds in equilibrium (23) that (28) possesses the symmetry

$$i\hat{\alpha}(t) \rightleftharpoons [u/(v - 2uM)]\tilde{\alpha}(-t)$$ (29)

and therefore all the connected correlation functions vanish

$$\langle \tilde{\alpha}(r_1, t_1)\tilde{\alpha}(r_2, t_2) \ldots \tilde{\alpha}(r_k, t_k)\rangle_{eq} = 0 \tag{30}$$

since trivially pure response functions are identically zero, whence the equilibrium steady state distribution agrees with the statistical mechanics approach.

More generally, our formalism provides a flexible description of non-stationary or spatially inhomogeneous states $\langle \alpha(r, t)\rangle \equiv M(r, t)$, closely akin to a dynamical Landau-Ginzburg description. Introducing the 'generalised thermodynamical potential'

$$\Gamma(\{\hat{M}, M\}) \equiv \ln(Z(\{\hat{l}, l\})) - \int dr^d \, dt(\hat{l}\hat{M} + lM) \tag{31}$$

which for the Schlögl model in mean field theory takes the form

$$\Gamma(\{\hat{M}, M\}) = \int dr^d \{i\hat{M}(r, t)[(-D\nabla^2 + \partial/\partial t + r)M(r, t) + uM^2(r, t)] \tag{32}$$

$$-\hat{M}(r, t)^2(vM(r, t) - uM^2(r, t)) - ih\hat{M}(r, t)\}$$

one has a complete description through the extremal relations

$$\partial\Gamma/\partial M(r, t) = 0 = \partial\Gamma/\partial\hat{M}(r, t) \tag{33}$$

in association with the familiar correlation/response equations (de Dominicis and Peliti 1978)

$$\int dr'^d \int dt' \begin{bmatrix} 0 & \dfrac{\partial\langle\alpha(r', t')\rangle}{\partial h(r, t)} \\[2ex] \dfrac{\partial\langle\alpha(r, t)\rangle}{\partial h(r', t')} & \langle(\alpha(r, t) - \langle\alpha(r, t)\rangle)(\alpha(r', t') - \langle\alpha(r', t')\rangle\rangle \end{bmatrix}$$

$$\times \begin{bmatrix} \dfrac{\partial^2\Gamma}{\partial\hat{M}(r', t')\partial\hat{M}(r'', t'')} & \dfrac{\partial^2\Gamma}{\partial\hat{M}(r', t')\partial M(r'', t'')} \\[2ex] \dfrac{\partial^2\Gamma}{\partial M(r', t')\partial\hat{M}(r'', t'')} & 0 \end{bmatrix}$$

$$= \delta(r - r'')\delta(t - t''). \tag{34}$$

Using the connection formulae (6), (11), (12) and (15), predictions for the reaction-diffusion problem then follow in a controllable way. In the *mean field approximation*, for example, the two-point correlation function is given by

$$\langle \rho(r, t)\rho(r', t')\rangle \overset{t>t'}{=} \langle\alpha(r, t)\alpha(r', t')\rangle + \langle\alpha(r', t')\rangle \frac{\partial}{\partial h(r',t')}\langle\alpha(r, t)\rangle \tag{35}$$

which reduces for stationary and homogeneous states (17), to the previous expression.

4. Scaling and the renormalisation group

In the vicinity of the phase transition of course the mean field approximation ((17) *et seq*) is rather poor, for the corrections diverge through the dimensionless coupling

$$g \equiv (uv/D^2)(\xi)^{(4-d)} \tag{36}$$

in $d < 4$ spatial dimensions (Mori and McNeil 1977). In our formalism this feature is very clear. Rescaling the fields $\hat{\alpha}$, α we may write in the form

$$L = \int \mathrm{d}r^d \{\mathrm{i}\hat{\beta}(r, t)[(-D\nabla^2 + \partial/\partial t + r)\alpha(r, t) - s]$$

$$+ w(\mathrm{i}\hat{\beta}(r, t)\beta^2(r, t) - \hat{\beta}^2(r, t)\beta(r, t)) + u(\hat{\beta}(r, t)\beta(r, t))^2\} \tag{37}$$

where

$$\beta = \alpha(u/v)^{1/2}, \qquad \hat{\beta} = \hat{\alpha}(v/u)^{1/2}, \qquad s = h(u/v)^{1/2} \tag{38}$$

and the dominant nonlinear coupling w is given by the relation

$$w = (uv)^{1/2}. \tag{39}$$

To determine the relevance near the critical point of the various non-linear couplings in (37) we now follow Brezin *et al* (1973) and analyse their naive dimensions. In terms of the microscopic length l (or time $\tau \equiv l^2/D$) we can scale frequencies ω, momenta k and fields $\hat{\beta}$, β as

$$\omega \sim k^2 \sim l^{-2}, \qquad \hat{\beta} \sim \beta \sim l^{-d/2} \tag{40}$$

and so immediately conclude that the nonlinear couplings (37) satisfy

$$w \sim l^{(d-4)/2}, \qquad u \sim l^{(d-2)} \tag{41}$$

leading directly to the identification of w as the dominant coupling, and whence to (36). Of course, as one would expect, we can control the divergent corrections to mean field theory using the dynamical renormalisation group (de Dominicis and Peliti 1978); however, let us first compare (37) with the phenomenological Lagrangians of Vvedensky *et al* (1984) and Janssen (1981):

$$L_V \equiv \int \mathrm{d}r^d \{\mathrm{i}\hat{\rho}(r, t)[(-D\nabla^2 + \partial/\partial t + r)\rho(r, t) - s] + w(\mathrm{i}\hat{\rho}(r, t)\rho^2(r, t) - \hat{\rho}^2(r, t)\rho(r, t))\} \tag{42}$$

$$L_J \equiv L_V + \int \mathrm{d}r^d[\tfrac{1}{2}s\hat{\rho}^2(r, t) - D\rho(r, t)(\nabla\hat{\rho}(r, t))^2]. \tag{43}$$

As u (41) is an irrelevant coupling we see that the low frequency/momentum properties of L and L_V are identical. If the Poissonian and concentration fluctuations are effectively indistinguishable at such scales, the phenomenological approach of Vvedensky *et al* (1984) is therefore vindicated. This is indeed the case, for analysing the connection formula ((11), (12)) perturbatively, we observe that the Poisson correlations satisfy

$$\langle\beta\beta\rangle = \tag{44}$$

whilst the concentration fluctuations obey

$$(u/v)(\langle\rho\rho\rangle - \langle\rho\rangle) - \langle\beta\beta\rangle = \tag{45}$$

and thus the dominant terms at low frequencies and momenta are common to both systems. Here ——— are correlation, whilst —⋀⋀ are response lines. In sharp contrast the scaling properties of L_J are rather different. Janssen (1981), in attempting to describe both local and non-local correlations (see (22) *et seq*), loses both control over

the equilibrium limit and seriously complicates the scaling properties. For $s \neq 0$ (43) is a model with tricritical scaling rather than the Reggeon-like scaling expected (Grassberger and Sundermeyer 1978).

Now for polynomial field theories such as (37), the dynamical renormalisation group technique is well established (Brezin *et al* 1973, de Dominicis and Peliti 1978). Focusing on the function $\Gamma[\hat{M}, M]$ (31), it is straightforward to show

$$
\left(-\tau \frac{\partial}{\partial \tau} + \beta(\bar{w}) \frac{\partial}{\partial \bar{w}} + \theta(\bar{w}) D \frac{\partial}{\partial D} + \phi(\bar{w}) r \frac{\partial}{\partial r} \right) \Gamma(\{\hat{M}, M\}, \bar{w}, D, \tau)
$$

$$
= \tfrac{1}{2} \eta(\bar{w}) \int_{Dq^2, \omega \ll \tau^{-1}} dq^d \int d\omega \left(\hat{M}(q, \omega) \frac{\partial}{\partial \hat{M}(q, \omega)} \right.
$$

$$
\left. + M(q, \omega) \frac{\partial}{\partial M(q, \omega)} \right) \Gamma(\{\hat{M}, M\}, \bar{w}, D, t, \tau) \tag{46}
$$

where τ is the microscopic timescale $(\tau \equiv l^2/D)$ and the dimensionless coupling $\bar{w}$ is defined by

$$
\bar{w} = w\tau(D\tau)^{-d/4}. \tag{47}
$$

The functions $\beta(\bar{w})$, $\theta(\bar{w})$, $\phi(\bar{w})$ are identical (up to a finite irrelevant renormalisation) to those of the Reggeon model (Abarbanel *et al* 1976), so that the Schlögl model is in the same universality class since therefore the critical exponents are identical (Brezin *et al* 1973). This feature can be traced to the common symmetry

$$
i\hat{\beta}(r, t) \rightleftharpoons \beta(r, -t) \tag{48}
$$

which in the Schlögl model is essential if the appropriate equilibrium limit is to be found (see (29)). At the transition this symmetry of course breaks unless equilibrium conditions prevail, in which case the system trivialises. Legendre transforming (46), one finds directly

$$
\left(-\tau \frac{\partial}{\partial \tau} + \beta(\bar{w}) \frac{\partial}{\partial \bar{w}} + \theta(\bar{w}) D \frac{\partial}{\partial D} + \phi(\bar{w}) r \frac{\partial}{\partial r} \right) \ln(Z(\{l, \hat{l}\}, w, D, r, \tau))
$$

$$
= -\tfrac{1}{2} \eta(\bar{w}) \int_{Dq^2, \omega \ll \tau^{-1}} dq^d \int d\omega \left[\hat{l}(q, \omega) \frac{\partial}{\partial \hat{l}(q, \omega)} \right.
$$

$$
\left. + l(q, \omega) \frac{\partial}{\partial l(q, \omega)} \right] \ln(Z(\{\hat{l}, l\}, w, D, r, \tau)) \tag{49}
$$

which on functional differentiation yield the renormalisation group equations

$$
\left[-\tau \frac{\partial}{\partial \tau} + \beta(\bar{w}) \frac{\partial}{\partial \bar{w}} + \theta(\bar{w}) r \frac{\partial}{\partial r} + \tfrac{1}{2} \eta(\bar{w}) \left(h \frac{\partial}{\partial h} + 1 \right) \right] \langle \rho \rangle = 0 \tag{50}
$$

$$
\left[-\tau \frac{\partial}{\partial \tau} + \beta(\bar{w}) \frac{\partial}{\partial \bar{w}} + \theta(\bar{w}) r \frac{\partial}{\partial r} + \tfrac{1}{2} \eta(\bar{w}) \left(h \frac{\partial}{\partial h} + 2 \right) \right] \langle \rho(q, w)\rho(q', \omega') \rangle = 0 \tag{51}
$$

for the concentration $\langle \rho \rangle$ $(= \langle \alpha \rangle$ see (14)) and the two-point correlation function. We

have employed the familiar relations (see (9))

$$\langle \alpha \rangle = \partial Z\{\hat{l}, l\})/\partial l|_{l=\hat{l}=0} \tag{52}$$

$$\langle \alpha(q, \omega)\alpha(q', \omega') \rangle = \partial^2 Z(\{\hat{l}, l\})/\partial l(q, \omega)\partial l(q', \omega')|_{l=\hat{l}=0} \tag{53}$$

and on the basis of our discussion ((44) *et seq*) equated the Poisson and chemical correlation functions in the low frequency/momentum domain of interest. The solution of the renormalisation group equations (50) and (51) is now standard (Brezin *et al* 1973). In the vicinity of the phase transition the coupling $\bar{w}$ takes its fixed point value $\bar{w}^* \simeq [\frac{1}{3} S_4 \varepsilon (2\pi)^{-4}]^{1/2}$ leading to the scaling forms

$$\langle \rho \rangle = (v/uD^{d/2})^{1/2}|r|^{\nu(d+z\eta)/2}f(h(uD^{d/2}/v)^{1/2}/|r|^{\nu(d+(2-\eta)z)/2})$$

$$\langle \rho(q, \omega)\rho(q', \omega') \rangle = \delta(q-q')\delta(\omega-\omega')((v/u)|r|^{-Vz(1-\eta)}$$

$$\times g(\omega/|r|^{\nu z}, Dq^2/r^{2\nu}, h(uD^{d/2}/v)^{1/2}/|r|^{\nu(d+(2-\eta)z)/2})$$

$$+ (2\pi)^{d+1}\langle \rho \rangle^2 \delta(q)\delta(\omega)) \tag{54}$$

in which the critical exponents $z \equiv 2/(1 - \theta(\bar{w}^*))$, $\nu = \frac{1}{2}(1 - \theta(\bar{w}^*))/(1 - \phi(\bar{w}^*))$, $\eta = \eta(\bar{w}^*)$ are identified. The functions f, g are universal. At leading order in $\varepsilon = 4 - d$ we find

$$f\left(\frac{r}{|r|} + \bar{w}^*f\right) = h\left(\frac{uD^{d/2}}{r}\right)^{1/2} \Big/ |r|^{\frac{1}{2}\nu(d+(2-\eta)z)}$$

$$g = \frac{2\bar{w}^*f}{(Dq^2/|r|^{2\nu} + r/|r| + 2\bar{w}^*f)^2 + (\omega/|r|^{\nu z})^2} \tag{55}$$

so for the first time the scaling behaviour of the Schlögl model is characterised in the vicinity of the phase transition for all values of the scaling parameter $h/|r|^{\nu(d+(2-\eta)z)/2}$. To the first non-trivial order the critical exponents are given by

$$z \equiv 2/(1 - \theta(\bar{w}^*)) = 2 - \frac{1}{12}\varepsilon + o(\varepsilon^2)$$

$$\nu \equiv \frac{1}{2}(1 - \theta(\bar{w}^*))/(1 - \phi(\bar{w}^*)) = \frac{1}{2} + \frac{1}{16}\varepsilon + o(\varepsilon^2) \tag{56}$$

$$\eta \equiv \eta(\bar{w}^*) = -\frac{1}{12}\varepsilon + o(\varepsilon^2)$$

although they are known already to $O(\varepsilon^2)$ from the Reggeon model (Abarbanel *et al* 1976). We thus correct the previous work of Goldhirsch and Procaccia (1981) and Vvedensky *et al* (1984). It is also important to observe that, although the critical exponents of the Reggeon and Schlögl models are the same (see (46) and (47)), the ordered phases are rather different. In the Schlögl model there is a stationary state, whilst in the Reggeon system one obtains the 'expanding cone', Amati *et al* (1976) solutions familiar from a directed percolation analogy (Cardy and Sugar 1980). Using our formalism we have, therefore, a comprehensive description of the low-frequency, low-momenta structure of the Schlögl model; however, we would emphasise that to obtain the equal (or short) time behaviour is rather more difficult. For the Schlögl model in the presence of diffusion there are no 'potential' solutions (Haken 1975, Gardiner 1983), so it is intrinsically very difficult to identify the fluctuation dissipation theorems (Risken 1984), via which the equal time correlation functions can be inferred directly from the low-frequency response functions described above. At present the

best we can do is naively integrate the scaling form (55) and (56) obtaining

$$\langle \rho(\boldsymbol{q}, t)\rho(\boldsymbol{q}', t')\rangle = \delta(\boldsymbol{q} - \boldsymbol{q}')\left(\bar{w}^*\left(\frac{v}{u}\right)\frac{|r|^\eta \exp[-(Dq^2/|r|^{2\nu} + 1 + 2\bar{w}^* f)|t - t'|r|^{\nu z}]}{(Dq^2/|r|^{2\nu} + r/|r| + 2\bar{w}^* f)}\right.$$

$$\left. + (2\pi)^d \langle \rho \rangle^2 \delta(\boldsymbol{q})\right). \tag{57}$$

5. Summary

We have demonstrated how the Poisson transform of Gardiner and Chaturvedi (1977) with the connection formulae developed by Elderfield (1985) can give a comprehensive description of Schlögl model (1). Our computation corrects, simplifies and extends the many previous studies. We would emphasise that we have demonstrated for the first time how in the equilibrium limit one regains *precisely* the steady state distribution suggested by statistical mechanics (Gardiner *et al* 1976, Nicolis and Malek-Mansour 1984); a result which hints at the power of the Poisson transform. Close to the critical point we have shown the Schlögl and Reggeon models belong to the same universality class in that they share common critical exponents. The ordered phases (stationary state against expanding cone) are of course decidedly different. We would finally note that the characterisation of the stationary distribution function remains, beyond mean field theory, an interesting but essentially unsolved problem.

Acknowledgments

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