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LETTER TO THE EDITOR

Self-organisation in the centre manifold of a dissipative system

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Abstract. We consider a far-from-equilibrium dissipative system sustaining a centre manifold. The decomposition in correlated subsystems inducing organisation by means of a nucleation process is analysed. The average lifetime of the organised subsystems determines the width of the strip of probability about the centre manifold in macrostate space.

Centre manifolds (CM) account for the stability and permanence of organisations far from equilibrium whenever the phase-space contraction which occurs beyond a dynamical instability is associated to a locally attractive and locally invariant region [1, 2]. The CM coordinates are collective modes with long lifetimes due to long-range cooperative behaviour and the collective fluctuations in the order parameter rate equations depend on the characteristic kinetic parameters of the unfolding via scaling laws. This universal picture relates the probability width about the CM in the space of macrostates with the phase-space exploration of accessible microstates responsible for the competition between the diffusive pressure about the CM and the slower deterministic drift towards the CM. The purpose of this letter is to obtain explicitly the time evolution of the probability distribution in a suitable coarse-grained phase space associated to every subsystem of the original dissipative open system [3, 4]. The ensemble of subsystems is not a device of virtual existence but it is obtained from the fluctuation-correlation scaling which holds at the onset of a CM. On the other hand, the coarse graining of phase space is defined by the space of realisations of the random source for collective fluctuations determined by the nature of the unfolding (cf [5]). Thus, throughout this work, those subsystems associated with macrostates lying in the strip about the CM will be regarded as information carriers or organised subsystems. Such subsystems can induce other subsystems to become organised by means of a nucleation process and, as information carriers lying in the CM, they have a finite lifetime which determines the diffusion pressure about the CM. Thus, the CM portion of phase space can be regarded as a free-energy source defined by the average lifetime of a phase trajectory, the temperature of the system and the amount of information gained by creating and sustaining the CM. Therefore, the total flux of free energy through the system is provided by the destruction of information carriers and by the dissipation corresponding to the free energy which is not absorbed from the external source during the process of organisation.

We shall focus on reductions of the macrostate space in which the order parameters are the CM coordinates subordinating the fast-relaxing degrees of freedom. Under such conditions, the intrinsic fluctuation correlations are determined by the Poincaré normal form of the system once the subordinated modes have been separated from the order parameters [4]. For example, in a dissipative spin system governed by a Ginzburg-Landau potential and coupled to a thermal reservoir one can show that a

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dynamic Kadanoff transformation is equivalent to a renormalisation determined by a centre manifold whose coordinates are the long-lifetime modes equal to the long-wavelength modes of the Kadanoff transformation [4, 6].

The spirit of the decomposition of the system of volume V into subsystems of volume W is the same as in the derivation of a virtual scaling factor L^{-1} for the fluctuation strength with [2]

$$W/V = L^{-1}. \tag{1}$$

The correlation between subsystems needs to be calculated in order to obtain the nucleation rates determining the rate of attraction of phase trajectories to the region of organised microstates. We shall be concerned only with those microstates whose corresponding macrostates belong to the CM but *not* to the attractor contained in the CM. The competition between induced organisation and destruction of information carriers is trivial on the attractor itself since the phase trajectories have infinite lifetime in the portion of phase space associated to the attractor (note that the attractor has measure zero with respect to the measure induced on the CM by the measure on the space of macrostates.)

We shall define an adequate multiplicity for macrostates not based on equally accessible microstates but based on cells of microstates in such a way that the coarse graining of the phase space is compatible with the ensemble of realisations of the random source term in the macroscopic rate equations. This random source denoted f corresponds to the intrinsic fluctuations in the system.

The coarse graning is defined by means of an equivalence relation '$\backsim$' such that the equivalence classes are the cells. The relation is defined as follows. Given a microstate A, consider all the microstates connected to A by a phase trajectory and having the same macrostate. Denote one such microstate by B. Then we have

$$A \backsim B \leftrightarrow \Delta f|_{A\to B} = 0 \leftrightarrow B \in c(A) \tag{2}$$

($c(A)$ = equivalence class containing element A) where the variation of the random source is associated with the displacement along the phase trajectory from A to B. Then, the coarse-grained space is the quotient space under the equivalence relation

$$\bar{\Sigma} = \Sigma/\backsim \tag{3}$$

where Σ denotes the phase space.

We shall define a probability distribution p on $\bar{\Sigma}$ whose behaviour in time must be determined from the probability distribution P about the CM in macrostate space. In order to carry this out we must determine P and its associated decomposition in subsystems. We shall concentrate upon the case of a hard-mode instability in an open system beyond which a time periodicity emerges. Other unfoldings are treated in a similar fashion (see e.g. [2]). It is not our aim to evaluate P for a generic case but to determine the organisation in coarse-grained space once P is given for the onset of a CM. The following derivation serves as an illustration for a particular unfolding but, given P and the CM decomposition, it can be extended to any unfolding *mutatis mutandis.*

The parameter L introduced in equation (1) is characteristic of the unfolding and will be used to display explicitly the scaling relations among the characteristic small parameters of the system. These are:

(1) the average Gaussian width of probability density about the CM, denoted $\bar{w}$;

(2) the unfolding or bifurcation parameter, denoted $b = q - q_c$;

(3) the scaling factor for the covariance matrix elements C_{ij}, for the internal fluctuations.

We shall assume, without loss of generality, that the system is already in Poincaré normal form [1, 2]. That is, the fast-relaxing enslaved modes, $\boldsymbol{X}_f$, and the enslaving modes, $\boldsymbol{X}_s$, have already been separated. In this $(\boldsymbol{X}_s, \boldsymbol{X}_f)$-representation, the explicit form of the covariance $\mathbf{C}$ is given by

$$C_{ij}(r, r', t, t') = \langle f_i(r, t) f_j(r', t') \rangle \tag{4}$$

where the angular brackets represent the thermal or statistical average, i.e. the average over a Gibbs ensemble of realisations of the random source terms, f_i (which represent the rate fluctuations). Thus, we have

$$C_{ij}(r, t, r, t) = L^{-1} \sum_{k=1}^{M} \sum_{n,m=1}^{N} \nu_{ki} \nu_{kj} b_{in} b_{jm} (v_k^+ + v_k^-). \tag{5}$$

Notice that we are only interested in the virtual volume that the fluctuations 'feel' and not in their macroscopic correlation length [2].

Here ν_{kj} represents the stoichiometric coefficient for the jth species in the kth elementary step; b_{ij} are the matrix elements of the transformation which reduces the Jacobian matrix to a Jordan normal form, i.e., it reduces the system to Poincaré normal form; ν_k^+ and ν_k^- are the forward and reverse rate for the kth elementary reaction step respectively.

In order to obtain a stochastic description of the highly cooperative long lifetime modes, $\boldsymbol{X}_s$, we must integrate the general Fokker-Planck (FP) equation for P with respect to the subordinated modes, along the CM, allowing for a continuous flow of probability about the CM. Then, the existence and structure of the collective modes involving the cooperative behaviour of a large number of particles is given by the smeared FP equation which is obtained from a CM reduction. In general, for S subordinating degrees of freedom and F subordinated variables, with $S+F=N$, we have the following general equation:

$$\int_{CM} \partial_t P(\boldsymbol{X}_s, \boldsymbol{X}_f, t)\, d\boldsymbol{X}_f$$

$$= \int_{CM} \Bigg(-\sum_{i=1}^{S} \partial_{X_{s,i}} \{[\dot{X}_{s,i} - (f)_{s,i}]P\} - \sum_{j=1}^{F} \partial_{X_{f,j}} \{[\dot{X}_{f,j} - (f)_{f,j}]P\}$$

$$+ \sum_{i,i'=1}^{S} \tfrac{1}{2} C_{ii'} \partial^2_{X_{s,i} X_{s,i'}} P + 2 \sum_{i=1}^{S} \sum_{j=1}^{F} \tfrac{1}{2} C_{ij} \partial^2_{X_{s,i} X_{f,j}} P + \sum_{j,j'=1}^{S} \tfrac{1}{2} C_{jj'} \partial^2_{X_{f,j} X_{f,j'}} P \Bigg) d\boldsymbol{X}_f. \tag{6}$$

In order to integrate this equation, we shall make use of the factorisation of the probability functional which gives the statistical subordination of fast variables

$$P(\boldsymbol{X}_s, \boldsymbol{X}_f, t) = \tilde{P}(\boldsymbol{X}_s, t) Q(\boldsymbol{X}_f | \boldsymbol{X}_s) \tag{7}$$

$$Q(\boldsymbol{X}_f | \boldsymbol{X}_s) = \prod_{j=1}^{F} (g_j/\pi)^{1/2} \exp\{-g_j [X_{f,j} - \tilde{F}_j(\boldsymbol{X}_s)]^2\}. \tag{8}$$

The centre manifold hypersurface in macrostate space need not be calculated here. For details, the reader may consult [1, 2, 4]. The CM is given by the equations

$$X_{f,j} = \tilde{F}_j(\boldsymbol{X}_s). \tag{9}$$

The Gaussian widths about the CM will be derived explicitly together with the scaling relations needed to obtain the smeared FP equation. In general they are given by the following relations:

$$g_j = \sum_{k=0}^{\infty} g_{jk}\left(\prod_{i_1+i_2+\ldots+i_s=k} X_{s,1}^{i_1} X_{s,2}^{i_2} \ldots X_{s,S}^{iS} \right) \qquad w_j = (2g_j)^{-1/2}. \tag{10}$$

We shall now adopt the following scaling relations in order to explicitly display the relative size of the terms resulting from the integration process:

$$C = L^{-1} \qquad X_{s,i} \simeq O(L^{-1/4}) \qquad \bar{w} = O(L^{-1/2}) \qquad b = O(L^{-1/2}) \tag{11}$$

where $\bar{w}$ is the width of the probability density averaged over the fast degrees of freedom.

For our case of interest, we have

$$\dot{X}_{s,1} - (f) = -wX_{s,2} + a_1 X_{s,1}^2 + b_1 X_{s,1} X_{s,2} + c_1 X_{s,2}^2 + O(L^{-3/4}) \tag{12}$$

$$\dot{X}_{s,2} - (f)_2 = wX_{s,1} + a_2 X_{s,1}^2 + b_2 X_{s,1} X_{s,2} + c_2 X_{s,2}^2 + O(L^{-3/4}) \tag{13}$$

$$\dot{X}_f - (f)_f = -\lambda X_f + a_{f1} X_{s,1}^3 + a_{f2} X_{s,2}^3 + O(L^{-1}). \tag{14}$$

Following the canonical procedure for a Hopf instability, we introduce the cylindrical coordinates

$$X_f = X_f \qquad X_{s,1} = r\cos\theta \qquad X_{s,2} = r\sin\theta. \tag{15}$$

Thus, we get the smeared FP equation

$$\begin{aligned}
\partial_t \tilde{P} = {} & -r^{-1}\partial_r\{[(q-q_c)L^{-1/2}r^2 + a_1 r^4]\tilde{P}\} - \partial_\theta[(w + b_1 r^2)\tilde{P}] \\
& + [(\tfrac{1}{2}\tilde{C}_{s,1;s,1})^{1/2}\cos\theta + (\tfrac{1}{2}\tilde{C}_{s,2;s,2})^{1/2}\sin\theta]^2 \partial_{rr}^2 \tilde{P} \\
& + [-\tfrac{1}{2}\tilde{C}_{s,1;s,1}\cos\theta\sin\theta + (\tilde{C}_{s,1;s,1}\tilde{C}_{s,2;s,2})^{1/2}\cos^2\theta \\
& + \tfrac{1}{2}\tilde{C}_{s,2;s,2}\sin\theta\cos\theta]\partial_r(r^{-1}\partial_\theta\tilde{P}) \\
& + r^{-1}[\tfrac{1}{2}\tilde{C}_{s,1;s,1}\sin^2\theta - (\tilde{C}_{s,1;s,1}\tilde{C}_{s,2;s,2})^{1/2}\cos\theta\sin\theta + \tfrac{1}{2}\tilde{C}_{s,2;s,2}\cos^2\theta]\partial_r\tilde{P} \\
& + r^{-2}[-\tilde{C}_{s,1;s,1}\sin\theta\cos\theta + 2(\tilde{C}_{s,1;s,1}\tilde{C}_{s,2;s,2})^{1/2}\sin^2\theta \\
& - \tilde{C}_{s,2;s,2}\cos\theta\sin\theta]\tfrac{1}{2}\partial_\theta\tilde{P}
\end{aligned} \tag{16}$$

where the tilde on top of the correlation matrix elements denotes restriction to the CM. This equation has been obtained making use of the first-order approximation

$$\bar{w} = N^{-1}\sum_{j=1}^{N}(2\tilde{C}_{jj}/\lambda_j)^{1/2}$$

where the λ_j are the damping constants for the $X_{f,j}$ and the subscript f has been dropped from the correlation elements.

Following a standard procedure, we shall get rid of the angular dependence by factorising P as follows:

$$\tilde{P}(r,\theta,t) = \tilde{\tilde{P}}(r,t)y(\theta|r). \tag{17}$$

This gives, to order $L^{-1/2}$, the equation of continuity for $\tilde{\tilde{P}}$ which ensures the continuous flow of probability about the CM and also verifies the validity of relations (11) and (16):

$$\partial_t \tilde{\tilde{P}}(r,t) = -\frac{1}{r}\partial_r\{[(q-q_c)L^{-1/2}r^2 + ar^4]\tilde{\tilde{P}}\} + \tfrac{1}{4}(\tilde{C}_{s,1;s,1} + \tilde{C}_{s,2;s,2})\partial_{rr}^2\tilde{\tilde{P}}. \tag{18}$$

The decomposition of the system in L interacting subsystems of volume W follows from equations (1), (5) and (11). All the subsystems have associated the same coarse-grained phase space defined by equations (2) and (3). Thus, the average over an ensemble of realisations of f is equal to the average over the ensemble of subsystems. Thus, our aim is to determine the time evolution p defined over $\bar{\Sigma}$. This distribution is made up of the following thermal averages:

$$p = \{p_A\}_{\text{all } c(A) \in \bar{\Sigma}} \qquad p_A = \langle \chi_A \rangle \tag{19}$$

where χ_A is the characteristic function for $c(A)$:

$$\chi_A = \begin{cases} 1 & \text{if the microstate of the subsystem belongs to } c(A) \\ 0 & \text{otherwise.} \end{cases} \tag{20}$$

We shall derive p making use of the information on P provided by the CM contraction in macrostate space.

Thus p_A is the probability that a subsystem is in cell $c(A)$ at a given time. Let Λ contained in $\bar{\Sigma}$ denote the set of cells whose macrostates realised the constraints given in (9) and do not belong to the limit cycle (attractor) emerging beyond the hard-mode instability. The subsystems of which Λ is made up are information carriers of finite lifetime.

Thus a measure of the degree of organisation is given by the fraction of organised subsystems

$$x = \sum_{c(B) \in \Lambda} \langle \chi_B \rangle. \tag{21}$$

At this point it must be emphasised that p and P are distributions defined on $\bar{\Sigma}$ and the macrostate space respectively.

The disorganised subsystems which do not lie on Λ are ergodic, thus, the amount of information $I = I(t)$ gained by sustaining the CM is given by

$$I = xL \ln(\bar{\mu}(\bar{\Sigma})/\bar{\mu}(\Lambda)) = xL \ln(m(\text{CM})) \tag{22}$$

where $\bar{\mu}$ is the measure induced on the quotient space by the Lebesgue measure μ on Σ and m is the normalised measure in macrostate space

$$m(\text{CM}) = \lim_{M \to \infty} \left[\int_M \mathrm{d}\boldsymbol{X}_s \int_{|\boldsymbol{X}_f - \bar{\boldsymbol{X}}_f| = 0}^{\infty} Q(\boldsymbol{X}_f | \boldsymbol{X}_s)\, \mathrm{d}\boldsymbol{X}_f \left(\int_M \mathrm{d}\boldsymbol{X} \right)^{-1} \right]. \tag{23}$$

The symbol $\int_M$ denotes integration restricted to the ball of radius M: $\{|\boldsymbol{X}| \leqslant M\}$.

Thus, the set of organised subsystems acts as a source of free energy since each information carrier has a finite lifetime given by the effective diffusion coefficient

$$D = N^{-1} \langle \|f\|^2 \rangle^{1/2}. \tag{24}$$

Therefore, the total flux F of free energy through the system is given by

$$F = N^{-1} \langle \|f\|^2 \rangle^{1/2} xLT \ln(m(\text{CM})) + F_{\text{dis}}. \tag{25}$$

The first term represents the contribution from the destruction of information carriers. The second term corresponds to the free energy which is dissipated without having been successfully used up in organising subsystems.

After a certain induction period or transient, the probability density P is confined to a strip about the CM. Thus, to describe the long-time behaviour of p, we need to derive the time evolution of the set of information carriers, i.e.

$$p_{\mathrm{CM}} = \{p_B\}_{c(B)\in\Lambda}. \tag{26}$$

The time evolution of p_{CM} depends on the cell correlations

$$S_{AB}(t) = \langle\langle \chi_A(\alpha)\chi_B(\beta)\rangle_\alpha\rangle_\beta \tag{27}$$

where α and β label subsystems in a generic sense. Thus, for an arbitrary $c(B)\in\Lambda$, we have

$$\langle\dot{\chi}_B\rangle = \left[\sum_{c(A)\in\Lambda}\left(\frac{\partial}{\partial t}S_{AB}\right)(1-x)\langle\chi_A\rangle\right] - N^{-1}\langle\|f\|^2\rangle^{1/2}\langle\chi_B\rangle. \tag{28}$$

This result requires further explanation. The first term in square brackets is made up of terms each of which represents the probability per unit time that a subsystem in a cell $c(A)$ which belongs to Λ induces a subsystem in any cell which does not belong to Λ to become organised, by evolving to $c(B)$. This statement can be readily verified by noting that the probability that a subsystem is in a disorganised cell is $(1-x)$.

Since we are interested in the distribution of subsystems in the CM, we must consider the normalised variables

$$y_A = p_A/x. \tag{29}$$

In this representation (26) becomes

$$\dot{y}_A = \sum_{c(B)\in\Lambda} M_{AB}y_B - y_A \sum_{c(C)}\sum_{c(B)\in\Lambda} M_{CB}y_B \tag{30}$$

where

$$M_{AB} = (1-x)(\partial/\partial t)S_{AB} - N^{-1}\langle\|f\|^2\rangle^{1/2}\delta_{\chi_A\chi_B}. \tag{31}$$

Equation (30) is isomorphic to the equation representing the selection process in a collection of self-reproducing macromolecular information carriers [7].

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