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LETTER TO THE EDITOR

Correlation of subsystems for the transition to a convective pattern

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Abstract. We implement an evolutionary model of spatially coupled subsystems to clarify the cooperative effect causing the transition to a convective roll pattern in a Rayleigh-Bénard cell. This cell is swept through its threshold by means of a step in the heat input from the lower plate. The correlation of subsystems accounts for the amplification of fluctuations. The experimental transients for the onset of the convective pattern are shown to be theoretically reproducible.

Systematic mode reductions in fluid flow problems attempt at establishing hierarchies of equations essentially to capture the universality class for the order parameter equation (OPE) [1-3]. In spite of considerable progress in this direction, there are instances in which the cooperativity effects responsible for the stochastic source term in the OPE remain elusive [3, 4]. This is so when the OPE is obtained by truncating the underlying realistic equations.

The stochastic centre manifold (CM) theory provides a systematic renormalisation method by which this problem can be tackled [5, 6]. The CM is a locally attractive and locally invariant portion of phase space representing the statistical subordination of the fast-relaxing degrees of freedom. It is obtained essentially from a mean-field derivation with a free-energy potential containing higher-order terms coupling the fast-relaxing modes and the order parameters or dominant modes. The transition to a dissipative organisation can be viewed as the amplification and propagation of fluctuations along the CM. The point we would like to address in this paper can be formulated as follows: what is the nature of the cooperative effects involving subsystem correlation which is responsible for the collective fluctuations in the order parameter evolution? Specifically, we shall concentrate on a classical flow system on which this question remains open [4, 7]: the transition to a convective roll pattern in a Rayleigh-Bénard cell swept through its threshold by means of a step in the heat input at the lower plate. We are interested in the amplification of intrinsic fluctuations in the order parameters which results from the correlation of spatially coupled subsystems.

It should be noted that a CM reduction determines a canonical decomposition of the system in spatially coupled subsystems. Those subsystems whose microstate lies in the CM are regarded as 'organised' and thus the whole process of transition to the convective pattern can be then analysed in terms of the evolution of information carriers. Our analysis is cast in terms which bear a great similarity to novel calculational

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techniques involving cellular automata and lattice-gas approaches for hydrodynamics [2], especially in what pertains to the realm of the microscopic origin of cooperativity.

Following standard notation [4, 7], our problem is described by a vector field $\boldsymbol{V} = (\theta, \boldsymbol{u}, w)$, where $\boldsymbol{u} = (u, v)$ and (u, v, w) is the velocity field for the fluid and θ is the deviation of the temperature from the linear conduction profile between boundaries defined by $z = 0$ and $z = 1$. The evolution of the vector field is subject to the Boussinesq equations. The distance, time and temperature are scaled respectively by d, d^2/κ and $\kappa\nu/\alpha g d^3$, where d is the cell height, κ and ν are the thermal and viscous diffusivities and α is the thermal expansion coefficient. If $\boldsymbol{e}_{\boldsymbol{q}}^{(j)}$, $|\boldsymbol{q}| = q_0, j \geqslant 1$, are the eigenvectors for the linear self-adjoint Boussinesq operator, with $\boldsymbol{q}_0$ the critical horizontal wavevector for the onset, we get the generic canonical decomposition of the vector field into the subordinated component, $\boldsymbol{X}_{\mathrm{f}}$, and the CM mode vector, $\boldsymbol{X}_{\mathrm{s}}$:

$$\boldsymbol{X}_{\mathrm{f}} = \sum_{i \geqslant 2} \sum_{|\boldsymbol{q}| = q_0} V_{\boldsymbol{q}}^{(i)} \boldsymbol{e}_{\boldsymbol{q}}^{(i)} \tag{1}$$

$$\boldsymbol{X}_{\mathrm{s}} = \sum_{|\boldsymbol{q}| = q_0} V_{\boldsymbol{q}}^{(1)} \boldsymbol{e}_{\boldsymbol{q}}^{(1)}. \tag{2}$$

The inner product $\langle \boldsymbol{V}_1, \boldsymbol{V}_2 \rangle$ is defined by

$$\langle \boldsymbol{V}_1, \boldsymbol{V}_2 \rangle = \{\sigma\theta_1^* \theta_2 + R_{\mathrm{c}}(\boldsymbol{u}_1^* \cdot \boldsymbol{u}_2 + w_1^* w_2)\}_m \tag{3}$$

where the symbol $\{\ \}_m$ denotes the average over a column, i.e. along the vertical z coordinate. The critical Rayleigh number is $R = R_{\mathrm{c}}$ and σ denotes the Prandtl number. For free boundary conditions we have

$$(N-1)R/R_{\mathrm{c}} = c^2 \|\boldsymbol{X}_{\mathrm{s}}\|^2 \tag{4}$$

where N is the Nusselt number and c is a characteristic proportionality constant which depends on the critical number R_{c} and need not be specified here (the reader may consult [7] for details). The virtual volume W for fluctuations in the CM equation for $\boldsymbol{X}_{\mathrm{s}}$ scales with a power of the characteristic small parameter $L^{-1} = (R - R_{\mathrm{c}})/R_{\mathrm{c}}$. It is precisely this property which enables one to construct a decomposition of the system in spatially coupled subcells once the scaling factor for intrinsic fluctuations has been determined by dynamic renormalisation. The CM for this problem is determined by projection of the non-linear portion, $\boldsymbol{N}(\boldsymbol{V}_1, \boldsymbol{V}_2)$, of the Boussinesq operator [4]:

$$V_{\boldsymbol{q}}^{(j)} = |\lambda_{\boldsymbol{q}}^{(j)}|^{-1} \sum_{\boldsymbol{q}'} \sum_{\boldsymbol{q}''} \langle \boldsymbol{e}_{\boldsymbol{q}}^{(j)}, \boldsymbol{N}(\boldsymbol{e}_{\boldsymbol{q}'}^{(1)}, \boldsymbol{e}_{\boldsymbol{q}''}^{(1)}) \rangle V_{\boldsymbol{q}'}^{(1)} V_{\boldsymbol{q}''}^{(1)} = \langle\!\langle V_{\boldsymbol{q}}^{(j)} \rangle\!\rangle \tag{5}$$

where $\langle\!\langle\ \rangle\!\rangle$ denotes the thermal or statistical average and $|\lambda_{\boldsymbol{q}}^{(j)}|^{-1}$ is the lifetime of fast-relaxing mode $V_{\boldsymbol{q}}^{(j)}$. In order to renormalise, we consider the following factorisation for the probability density functional $P = P(\boldsymbol{X}_{\mathrm{s}}, \boldsymbol{X}_{\mathrm{f}}, t)$:

$$P = Q_{\mathrm{f}}(\{V_{\boldsymbol{q}'}^{(i)}\}_{\boldsymbol{q}', i}) Q_{\mathrm{s}}(\{V_{\boldsymbol{q}}^{(1)}\}_{\boldsymbol{q}}, t) \tag{6}$$

$$Q_{\mathrm{f}} = \prod_{|\boldsymbol{q}| = q_0} \prod_{i \geqslant 2} (g_{\boldsymbol{q}}^{(i)}/\pi)^{1/2} \exp[-g_{\boldsymbol{q}}^{(i)} (V_{\boldsymbol{q}}^{(i)} - \langle\!\langle V_{\boldsymbol{q}}^{(i)} \rangle\!\rangle)^2]. \tag{7}$$

It is precisely from the scaling laws to which the effective diffusion coefficients $d_{\boldsymbol{q}}^{(j)} = (2g_{\boldsymbol{q}}^{(j)})^{-1/2}$ are subject that we can obtain the decomposition of the system in information carriers. Let us decompose $d_{\boldsymbol{q}}^{(j)}$ in two factors: $d_{\boldsymbol{q}}^{(j)} = k\tilde{d}_{\boldsymbol{q}}^{(j)}$, with k to be scaled with L^{-1} and $\tilde{d}_{\boldsymbol{q}}^{(j)} = \mathrm{O}(1)$. Then the CM-reduced 'smeared' Fokker-Planck

equation is

$$\partial_t Q_s = -\sum_{|q|=q_0}\left(\partial_{V_q^{(1)}}(\langle\!\langle \dot V_q^{(1)}\rangle\!\rangle Q_s)+\langle\!\langle \dot V_q^{(1)}\rangle\!\rangle \sum_{j\geq 2}\sum_{q'}\frac{\partial_{V_q^{(1)}} g_{q'}^{(j)}}{2g_{q'}^{(j)}} Q_s\right)-\sum_{|q|=q_0}\sum_{j\geq 2}(\partial_{V_q^{(j)}}\langle\!\langle \dot V_q^{(j)}\rangle\!\rangle)Q_s$$
$$-\sum_{|q|=q_0}\sum_{j\geq 2}2k^2(\tilde d_q^{(j)})^2 g_q^{(j)} Q_s+\sum_{q,q'}\sum_{j\geq 2}4k^2\tilde d_q^{(1)}\tilde d_{q'}^{(j)} g_{q'}^{(j)}\partial_{V_q^{(1)}}(\langle\!\langle V_{q'}^{(j)}\rangle\!\rangle)Q_s$$
$$+k^2\sum_{q,q'}\tilde d_q^{(1)}\tilde d_{q'}^{(1)}\partial^2_{V_q^{(1)}V_{q'}^{(1)}}Q_s$$
$$+k^2\sum_{q,q',q''}\tilde d_q^{(1)}\tilde d_{q'}^{(1)}\sum_{j\geq 2}\left\{\frac{\partial_{V_q^{(1)}} g_{q''}^{(j)}}{g_{q''}^{(j)}}\partial_{V_q^{(1)}}Q_s+\left[\frac{\partial^2_{V_q^{(1)}V_{q'}^{(1)}} g_{q''}^{(j)}}{2g_{q''}^{(j)}}\right.\right.$$
$$\left.\left.-\left(\frac{\partial_{V_q^{(1)}} g_{q''}^{(j)}}{g_{q''}^{(j)}}\right)^2\frac{1}{4}-g_{q''}^{(j)}(\partial_{V_q^{(1)}}\langle\!\langle V_{q''}^{(j)}\rangle\!\rangle)^2\right]Q_s\right\}. \tag{8}$$

The fluctuations need to be renormalised so that (8) reduces to an equation which warrants a continuous flow of probability about the CM:

$$\partial_t Q_s = -\sum_q \partial_{V_q^{(1)}}\{\langle\!\langle \dot V_q^{(1)}\rangle\!\rangle Q_s\}+k^2\sum_{q,q'}\tilde d_q^{(1)}\tilde d_{q'}^{(1)}\partial^2_{V_q^{(1)}V_{q'}^{(1)}}Q_s. \tag{9}$$

Thus, to $O(L^{-1})$, we get

$$g_q^{(j)} = -\lambda_q^{(j)}/(k\tilde d_q^{(j)})^2 \tag{10}$$

$$g_q^{(j)} = \tilde g_q^{(j)}(L^{-1}\tau_0)^2 \tag{11}$$

where the average lifetime for the order parameter, Ψ, is given by

$$\tau_0^{-1} = \tfrac{3}{2}\pi^2\frac{\sigma}{\sigma+1} \tag{12}$$

where Ψ is given by

$$\Psi = c\sum_{|q|=q_0} V_q^{(1)}\exp(iq\cdot r). \tag{13}$$

Thus, intrinsic fluctuations scale with $W^{-1}=O(L)$, and therefore they grow boundlessly as we approach the critical point. The key point which emerges from this analysis is that we have associated to the onset of the CM a decomposition in subsystems of virtual volume W such that [3]

$$W/V = L^{-1} \tag{14}$$

where V is the thermodynamic volume.

The average lifetime of an information carrier depends on the distribution of probability about a strip along the CM, as determined by (7). Thus, the lifetime is extremely short as we approach criticality since

$$\tau \approx \frac{1}{\|f\|} \approx L^{-1} \tag{15}$$

where f is the stochastic source in the evolution of Ψ.

For convenience, we shall introduce the definition of 'organised subsystem' by which we mean a subsystem whose microstate lies in the CM excluding the attractor

(which in any case has measure zero relative to the measure induced in the CM). Microstates lying in the CM are given by mode vectors of the form:

$$(\{V_q^{(1)}\}_{\text{all } q}; \{\langle\langle V_q^{(j)}\rangle\rangle(\{V_q^{(1)}\}_{\text{all } q})\}_{\text{all } q;\, j\geq 2}). \tag{16}$$

We shall define an adequate multiplicity for macrostates not based on equally accessible microstates but based on cells of microstates so that the coarse-graining of phase space thus defined is compatible with the ensemble of realisations of the random source (denoted f). This procedure is carried out by introducing an equivalence relation '$\sim$' where the cells are the equivalence classes. The relation is defined as follows. Fixing arbitrarily a microstate A, all the microstates with the same macrostate as A and connected to A by a phase trajectory with $\Delta f = 0$ are equivalent to A. We denote one such microstate as B. Thus, we have

$$A \sim B \leftrightarrow B \in c(A) \tag{17}$$

where $c(A)$ is the cell containing A. The variation in the source term f is associated to the displacement along the phase trajectory. Thus, the coarse-grained phase space is the space of microstates modulo $\sim$, or the quotient space

$$\bar{\Sigma} = \Sigma / \sim \tag{18}$$

where Σ denotes the phase space. We need to describe the time evolution of a probability distribution p defined on $\bar{\Sigma}$ determined by the distribution P in the space of collective macroscopic modes. The distribution p is made up of the following thermal averages (the angular brackets represent this thermal average which is, in fact, the average over the ensemble of subsystems):

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

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

$$\chi_A = \begin{cases} 1 & \text{if the subsystem is in a microstate contained in } c(A) \\ 0 & \text{otherwise.} \end{cases} \tag{20}$$

Thus, p_A gives the probability that a subsystem is in cell $c(A)$ at a given time. Let Λ contained in $\bar{\Sigma}$ denote the collection of cells whose macrostates belong to the CM excluding the attractor emerging beyond a hard-mode instability. A measure of the degree of organisation is then given by the fraction of organised subsystems:

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

Thus, the CM acts as a transient source of free energy since each information carrier has a finite lifetime given by the reciprocal of the effective diffusion coefficient

$$D = S^{-1}\langle\langle \|f\|^2 \rangle\rangle^{1/2} \tag{22}$$

S being the dimension of the CM or the number of order parameters.

In order to describe the time behaviour of p, we need to derive the time evolution of the set of finite-lifetime information carriers, i.e. we restrict the density to

$$p_{\text{CM}} = \{p_B\}_{c(B)\in\Lambda}. \tag{23}$$

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

$$S_{AB}(t) = \langle\langle\langle \chi_A(\alpha)\chi_B(\beta)\rangle\rangle_\alpha\rangle\rangle_\beta \tag{24}$$

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

$$\langle\langle \dot{\chi}_B \rangle\rangle = \sum_{c(A)\in\Lambda} \left(\frac{\partial}{\partial t} S_{AB}\right)(1-x)\langle\langle \chi_A \rangle\rangle - \langle\langle \|f\|^2 \rangle\rangle^{1/2} \langle\langle \chi_B \rangle\rangle. \tag{25}$$

The terms proportional to $(1-x)$ give the probability per unit time that a subsystem in a cell $c(A) \in \Lambda$ induces a subsystem outside the CM to become organised by evolving to $c(B) \in \Lambda$. This is so since the probability that a subsystem is in a disorganised cell is $(1-x)$. The remaining term in (25) corresponds to the destruction of the information carrier. The variable $x(t)$ represents the level of self-organisation within the CM. Its behaviour depends implicitly on the kinetic parameters since the parameters L, D and S_{AB} are determined by the CM reduction. The induction period is given by the length of time which must elapse in order for the system to evolve along the CM until the microstates realising the attractor are reached by all the subsystems. In other words, the induction period is the time it takes the fluctuations to propagate along the CM. Thus, it is determined by the time evolution of x. The Perron number (the largest real positive eigenvalue), $\lambda_{\#}$, for the matrix $(\partial/\partial t\, S_{AB})$ coincides with the effective diffusion coefficient D since the final stationary state in the evolution of x is

$$x_{ss} = (1 - D/\lambda_{\#}) = 0. \tag{26}$$

This relation must hold in order for the attractor to be reached by all subsystems after the critical fluctuations have propagated and amplified through the CM. Figure 1 displays a numerical integration of equation (25). The induction period, T_{ind}, is given by

$$x(T_{ind}) = x_{ss} = 0. \tag{27}$$

In a simplified model we can impose the restriction of equal induction probabilities per unit time between any pair of microstate cells $c(A)$ and $c(B)$. Since L and D can be obtained from a stochastic CM treatment for a particular unfolding, the probability per unit time can be obtained from the fact that the Perron number is determined by equation (26).

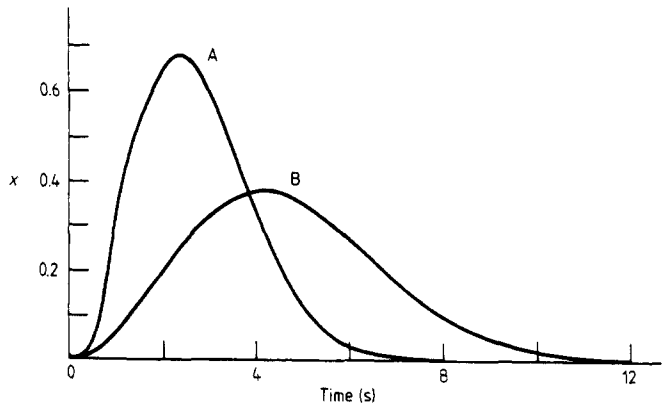

Figure 1. The induction period as a transient for the onset of a convective pattern. Time behaviour for the fraction, x, of organised subsystems as obtained by numerical integration of (25) with $x(0) = L^{-1}$. Curve A: $L^{-1} = 0.030 + \frac{8}{3}U^{-2}$. Curve B: $L^{-1} = 0.049 + \frac{8}{3}1.049\ U^{-2}$ (cf [7]). The other control parameters are specified in the text.

The transient for the onset of the convective pattern can thus be taken as T_{ind} and is displayed in figure 1 for realistic values of the control parameters. Curve A corresponds to $L^{-1} = (R - R_c)/R_c = 0.030 + \frac{8}{3}U^{-2}$ and curve B to $L^{-1} = 0.049 + 1.049\frac{8}{3}U^{-2}$. Here U is the radius of the cell under consideration: $U = 4.72$. The other parameters are: $\sigma = 0.78$; $q_0 d = \pi/\sqrt{2}$. Curve B gives a T_{ind} approximately equal to 12 s and is in very satisfactory agreement with the experimental results of [7].

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