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LETTER TO THE EDITOR

Constraints on the time-reversible Liouville equation in order to derive a stochastic order-parameter equation at the onset of a convective roll pattern

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Abstract. It is shown that an adequate Fokker-Planck equation for the transition to a convective roll pattern in a Rayleigh-Bénard cell can be derived by projecting the time-reversible Liouville equation onto the centre manifold for the onset and introducing the source of irreversibility on the initial conditions. Thus we elucidate the microscopic origin of the random source in the order-parameter evolution.

We shall be concerned with the microscopic origin of the random source in the order-parameter equation for the onset of a convective roll pattern in a Rayleigh-Bénard cell [1-4]. In a realistic experimental set-up, the cell is swept through its threshold by means of a controlled heat input. The temperature of the bottom plate is time dependent (and therefore so is the Rayleigh number) and there is a step in the heat input [3, 4]. At the level of macroscopic degrees of freedom, the Fokker-Planck (FP) equation associated with the transition can be conveniently derived by introducing a stochastic counterpart of the adiabatic following [4] of fast-relaxing degrees of freedom to the excited modes. In other words, the contraction in the space of macrovariables can be accounted for by means of the existence of a locally attractive locally invariant centre manifold (CM). The relevant macroscopic degrees of freedom are the Fourier components, denoted $V_{\boldsymbol{q}}^{(j)}$ ($j=1,2,\ldots$; $\boldsymbol{q}$ being a two-dimensional wavevector, as in the case of a smectic crystal) of a stochastic vector field $\boldsymbol{V}$ which comprises the velocity field $(\boldsymbol{u}, w)$ ($\boldsymbol{u}$ being the two-dimensional component) and the deviation of temperature from the linear conducting profile, denoted $\boldsymbol{\theta}$. Thus, near the threshold, the following decomposition holds:

$$\boldsymbol{V}=\boldsymbol{X}_{\mathrm{s}}+\boldsymbol{X}_{\mathrm{f}} \tag{1}$$

where

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

$$\boldsymbol{X}_{\mathrm{s}}=\sum_{|\boldsymbol{q}|=q_0} V_{\boldsymbol{q}}^{(1)}\boldsymbol{e}_{\boldsymbol{q}}^{(1)} \tag{3}$$

(q_0 = critical wavevector). The CM coordinates are the components of the vector $\boldsymbol{X}_{\mathrm{s}}$ and the subordinated modes are given by $\boldsymbol{X}_{\mathrm{f}}$. The vectors $\boldsymbol{e}_{\boldsymbol{q}}^{(j)}$ are the eigenvectors of the linear Boussinesq operator (see [3, 4] for details).

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In principle, the macrovariables $V_q^{(j)}$, $j=1, \ldots$, are functions of the position, q_m, and momenta, p_m, of all the particles of the fluid. Therefore, we can boldy state that it must be possible to derived a CM-smeared FP equation to be satisfied by the probability distribution $Q_s(\boldsymbol{X}_s, t)$ for the order parameters. Given that the Liouville equation for the microscopic distribution $p=p(\{p_m\}, \{q_m\}, t)$ is time reversible, it is intuitively clear that the irreversibility must be included in the process of smoothing the solution by averaging over the initial moments of time [5, 6]. In doing so, we get rid of the unphysical dependence of p on the initial moment t_0. At that moment, p coincides with a microscopic CM distribution β, to be determined. This is done by taking into account that the thermal average of $\delta(\boldsymbol{X}'_s - \boldsymbol{X}_s)$ which is equal to Q_s must be the same as the average obtained making use of β:

$$\langle\langle \delta(\boldsymbol{X}'_s - \boldsymbol{X}_s)\rangle\rangle_\beta = \langle\langle \delta(\boldsymbol{X}'_s - \boldsymbol{X}_s)\rangle\rangle. \tag{4}$$

The symbol $\langle\langle\ \rangle\rangle$ denotes a thermal or statistical average and $\boldsymbol{X}'_s$ is the order-parameter vector, dependent on p_m and q_m (m labels each particle).

Thus, the basic strategy is to introduce a Mori-type [5, 6] projector formalism to reduce the Liouville equation to the CM. In order to make this clear, we shall first give the basic tenets of the CM approach.

(i) Let $\lambda_q^{(j)} \ll 0$ denote the damping constant for the fast-relaxing degree of freedom $V_q^{(j)}$, $j \geqslant 2$. Then, after a relaxation time T_{CM} given by

$$T_{\mathrm{CM}} = \mathrm{O}\left(\sup_j\{|\lambda^{(j)}|^{-1}\}\right) \tag{5}$$

the probability density functional $P=P(\boldsymbol{X}_s, \boldsymbol{X}_f, t)$ is constrained to a narrow strip about the CM such that

$$\langle\langle \boldsymbol{X}_f \rangle\rangle = \langle\langle \tilde{\boldsymbol{X}}_f(\boldsymbol{X}_s)\rangle\rangle. \tag{6}$$

(ii) The following ansatz is valid:

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

where Q_f represents a conditional probability which describes the statistical enslavement of the fast-relaxing variables to the order parameters. In order to allow for a continuous flow of probability about the CM, Q_f takes the form of a Gaussian peaked at the CM:

$$Q_f = \prod_{|\boldsymbol{q}|=q_0} \prod_{i \geqslant 2} (g_q^{(i)}/\pi)^{1/2} \exp[-g_q^{(i)}(V_q^{(i)} - \langle\langle V_q^{(i)}\rangle\rangle)^2] \tag{8}$$

where the Gaussian widths $w_q^{(i)} = (2g_q^{(i)})^{-1}$ must be determined from the condition that the integration of the general FP equation for P along the CM, i.e. with respect to the fast variables, should yield the appropriate FP equation for Q_s [1, 2]. This procedure accounts for the effect of fast hydrodynamic modes which have been projected out in the derivation of the FP equation for the transition to the convective pattern.

Thus, the microscopic distribution β has the general form

$$\beta(t) = \int (I(\delta(\boldsymbol{X}'_s - \boldsymbol{X}_s)))^{-1} Q(\boldsymbol{X}_s, t)\delta(\boldsymbol{X}'_s - \boldsymbol{X}_s)\mathrm{d}\boldsymbol{X}_s \tag{9}$$

where $I(\ )$ denotes integration over the coordinates and momenta of all the particles normalised by the factor $1/(h^{3N}N!)$.

We shall show that the source of irreversibility in the procedure of derivation of a smeared FP equation for the order parameters does not come from the Liouville equation but from the causal character of the boundary conditions imposed. The starting point is the Liouville equation for $p(t)$:

$$\frac{\partial}{\partial t} p(t) + \mathrm{i}Lp(t) = 0 \tag{10}$$

where L is the Liouville operator $\mathrm{i}Lp = \{H, p\}$, with H being the Hamiltonian of the system.

The source of irreversibility is introduced by assuming that, in agreement with the CM reduction, the solution of (10) coincides with the CM microstate distribution at the instant t_0 in the remote past:

$$p(t) = \exp(-\mathrm{i}L(t-t_0))\beta(t_0). \tag{11}$$

In order to get rid of this unphysical dependence on the initial moment t_0, we introduce a smoothing procedure by averaging over all initial moments t_0' between t_0 and t:

$$p(t) = T^{-1}\int_{t_0}^{t} \exp[-\mathrm{i}L(t-t_0')]\beta(t_0')\,\mathrm{d}t_0' \qquad T = t - t_0 \tag{12}$$

i.e. over the length of time T which is very near the thermodynamic limit $T\to\infty$ (cf [5]).

However, this procedure leads to a breakdown of the time-reversal symmetry since the function given by (12) is a solution, not of the Liouville equation in its original form, but of a new equation containing an infinitesimal source describing the relaxation of $p(t)$ to the CM:

$$\frac{\partial}{\partial t} p + \mathrm{i}Lp = -T^{-1}(p(t) - \beta(t)). \tag{13}$$

This relaxation to the CM has an extremely slow mean time if we operate near the thermodynamic limit. Therefore, the source of irreversibility due to 'contamination' with the phenomenological CM contraction can be made arbitrarily small.

In the spirit of Mori's projection operator formalism [6], we shall define a projector in order to restrict the system to the CM, i.e. we transform a microstate distribution A into an order parameter distribution UA:

$$UA = \int (I(\delta(\boldsymbol{X}_s' - \boldsymbol{X}_s)))^{-1} I(A\delta(\boldsymbol{X}_s' - \boldsymbol{X}_s))\delta(\boldsymbol{X}_s' - \boldsymbol{X}_s)\,\mathrm{d}\boldsymbol{X}_s \tag{14}$$

$$UA = UA(\boldsymbol{X}_s', t). \tag{15}$$

It can be readily verified that this operator is a projection operator and that it has the additional properties

$$Up = \beta \tag{16}$$

$$U\beta = \beta. \tag{17}$$

Therefore, we can write an equation for β in the compact form

$$\frac{\partial}{\partial t}\beta = U\dot{p} = -U\mathrm{i}L(p-\beta) - U\mathrm{i}L\beta. \tag{18}$$

Making use of this formalism we can now derive the generalised force, $M(\boldsymbol{X}_s)$, responsible for the diffusive pressure produced by the far-from-equilibrium fluctuations. This diffusive pressure competes with the deterministic fast drift towards the CM determined by the separation of relaxation timescales. Therefore, the generalised forces determine the Gaussian width of the probability density Q_f about the CM. In other words, these forces are orthogonal to the CM:

$$M(\boldsymbol{X}_s) = (1-U)\delta(\boldsymbol{X}_s' - \boldsymbol{X}_s)\mathrm{i}L\boldsymbol{X}_s'. \tag{19}$$

The conjugated fluxes orthogonal to the CM are

$$J(\boldsymbol{X}_s) = -\frac{\partial}{\partial \boldsymbol{X}_s} M(\boldsymbol{X}_s) = (1-U)\mathrm{i}L\delta(\boldsymbol{X}_s' - \boldsymbol{X}_s). \tag{20}$$

The thermal average of the fluxes is therefore given by

$$\langle\!\langle J(\boldsymbol{X}_s)\rangle\!\rangle = \frac{\partial}{\partial \boldsymbol{X}_s}\int \mathrm{d}\boldsymbol{X}_s' \int_{-\infty}^{t} \mathrm{d}t' \exp[T^{-1}(t'-t)]K(\boldsymbol{X}_s', \boldsymbol{X}_s, t-t')V(\boldsymbol{X}_s', t') \tag{21}$$

where the kernel K is given by

$$K(\boldsymbol{X}_s', \boldsymbol{X}_s, t) = I(M(\boldsymbol{X}_s)\exp[(1-U)\mathrm{i}tL]M(\boldsymbol{X}_s')) \tag{22}$$

and

$$V(\boldsymbol{X}_s', t) = \frac{\partial}{\partial \boldsymbol{X}_s'}(Q_s(\boldsymbol{X}_s', t')/L(\boldsymbol{X}_s')) \tag{23}$$

where

$$L(\boldsymbol{X}_s) = I(\delta(\boldsymbol{X}_s' - \boldsymbol{X}_s)). \tag{24}$$

Finally, the speed of the order parameters is given by

$$W(\boldsymbol{X}_s) = I(\delta(\boldsymbol{X}_s' - \boldsymbol{X}_s)\mathrm{i}L\boldsymbol{X}_s')/L(\boldsymbol{X}_s) = (\langle\!\langle \dot{V}_{\boldsymbol{q}}^{(1)}\rangle\!\rangle)_{\boldsymbol{q}}. \tag{25}$$

Thus, we arrive at the retarded FP equation for Q_s:

$$\frac{\partial}{\partial \boldsymbol{X}_s} Q_s(\boldsymbol{X}_s, t) = -\frac{\partial}{\partial \boldsymbol{X}_s} W(\boldsymbol{X}_s)Q_s(\boldsymbol{X}_s, t) + \langle\!\langle J(\boldsymbol{X}_s)\rangle\!\rangle. \tag{26}$$

In order to explicitly evaluate the averaged flow, we must make use of the following additional property of the projector:

$$(1-U)p = \tilde{\beta} \tag{27}$$

where $\tilde{\beta}$ is the microscopic distribution induced by Q_f. The definition of $\tilde{\beta}$ is completely analogous to that of β. In addition, the calculation requires the explicit equation for the CM. This is given by [1]

$$V_{\boldsymbol{q}}^{(j)} = |\lambda_{\boldsymbol{q}}^{(j)}|^{-1} \sum_{\boldsymbol{q}', \boldsymbol{q}''} \langle \boldsymbol{e}_{\boldsymbol{q}}^{(j)}, N(\boldsymbol{e}_{\boldsymbol{q}'}^{(1)}, \boldsymbol{e}_{\boldsymbol{q}''}^{(1)})\rangle V_{\boldsymbol{q}'}^{(1)} V_{\boldsymbol{q}''}^{(1)} \tag{28}$$

where the inner product $\langle \boldsymbol{V}_1, \boldsymbol{V}_2\rangle$ is given by

$$\langle \boldsymbol{V}_1, \boldsymbol{V}_2\rangle = [\sigma\theta_1^*\theta_2 + R_c(\boldsymbol{u}_1^* \cdot \boldsymbol{u}_2 + w_1^* w_2)]_m. \tag{29}$$

The symbol $[\ ]_m$ denotes an average over a layer, i.e. along the coordinate orthogonal to the $\boldsymbol{q}$ space. The bilinear operator $N(\boldsymbol{V}_1, \boldsymbol{V}_2)$ is the non-linear part of the Boussinesq operator [3, 4].

In order to make use of equation (27), we need the explicit form of the $g_{\boldsymbol{q}}^{(j)}$ which give the competition between the fast drift towards the CM and the effect of the diffusive pressure:

$$g_{\boldsymbol{q}}^{(j)} = -\lambda_{\boldsymbol{q}}^{(j)} / (d_{\boldsymbol{q}}^{(j)})^2 \tag{30}$$

where the $d_{\boldsymbol{q}}^{(j)}$ are the effective diffusion coefficients [1]. In order to properly scale these coefficients, we factorise them as $d_{\boldsymbol{q}}^{(j)} = k\tilde{d}_{\boldsymbol{q}}^{(j)}$ where k is a small parameter which in the phenomenological derivation is scaled with the small control parameters and $\tilde{d}_{\boldsymbol{q}}^{(j)} = \mathrm{O}(1)$.

Making use of (21) and (27)-(30), we obtain the following equation:

$$\begin{aligned}
\langle\!\langle J(\boldsymbol{X}_{\mathrm{s}})\rangle\!\rangle = &- \sum_{|\boldsymbol{q}|=q_0} \left(\langle\!\langle \dot{V}_{\boldsymbol{q}}^{(1)} \rangle\!\rangle \sum_{j\geqslant 2} \sum_{\boldsymbol{q}'} \frac{\partial_{V_{\boldsymbol{q}}^{(1)}} g_{\boldsymbol{q}'}^{(j)}}{2 g_{\boldsymbol{q}'}^{(j)}} Q_{\mathrm{s}} \right) - \sum_{|\boldsymbol{q}|=q_0} \sum_{j\geqslant 2} (\partial_{V_{\boldsymbol{q}}^{(j)}} \langle\!\langle \dot{V}_{\boldsymbol{q}}^{(j)} \rangle\!\rangle) Q_{\mathrm{s}} \\
&- \sum_{|\boldsymbol{q}|=q_0} \sum_{j\geqslant 2} 2k^2 (\tilde{d}_{\boldsymbol{q}}^{(j)})^2 g_{\boldsymbol{q}}^{(j)} Q_{\mathrm{s}} + \sum_{\boldsymbol{q},\boldsymbol{q}'} \sum_{j\geqslant 2} 4k^2 \tilde{d}_{\boldsymbol{q}}^{(1)} \tilde{d}_{\boldsymbol{q}'}^{(j)} \partial_{V_{\boldsymbol{q}}^{(1)}} (\langle\!\langle V_{\boldsymbol{q}'}^{(j)} \rangle\!\rangle) Q_{\mathrm{s}} \\
&+ k^2 \sum_{\boldsymbol{q},\boldsymbol{q}'} \tilde{d}_{\boldsymbol{q}}^{(1)} \tilde{d}_{\boldsymbol{q}'}^{(1)} \partial^2_{V_{\boldsymbol{q}}^{(1)} V_{\boldsymbol{q}'}^{(1)}} Q_{\mathrm{s}} + k^2 \sum_{\boldsymbol{q},\boldsymbol{q}',\boldsymbol{q}''} \tilde{d}_{\boldsymbol{q}}^{(1)} \tilde{d}_{\boldsymbol{q}'}^{(1)} \sum_{j\geqslant 2} \left(\frac{\partial_{V_{\boldsymbol{q}}^{(1)}} g_{\boldsymbol{q}''}^{(j)}}{g_{\boldsymbol{q}''}^{(j)}} \partial_{V_{\boldsymbol{q}}^{(1)}} Q_{\mathrm{s}} \right. \\
&\left. + \left[\frac{\partial^2_{V_{\boldsymbol{q}}^{(1)} V_{\boldsymbol{q}'}^{(1)}} g_{\boldsymbol{q}''}^{(j)}}{2 g_{\boldsymbol{q}''}^{(j)}} - \frac{1}{4} \left(\frac{\partial_{V_{\boldsymbol{q}}^{(1)}} g_{\boldsymbol{q}''}^{(j)}}{g_{\boldsymbol{q}''}^{(j)}} \right)^2 - 2 g_{\boldsymbol{q}''}^{(j)} (\partial_{V_{\boldsymbol{q}}^{(1)}} \langle\!\langle V_{\boldsymbol{q}''}^{(j)} \rangle\!\rangle)^2 \right] Q_{\mathrm{s}} \right\}
\end{aligned} \tag{31}$$

where the speed of the fast-relaxing degrees of freedom is determined by an equation analogous to (25):

$$(\langle\!\langle \dot{V}_{\boldsymbol{q}}^{(j)} \rangle\!\rangle)_{\boldsymbol{q},j} = W(\boldsymbol{X}_{\mathrm{f}}) = (I(\delta(\boldsymbol{X}_{\mathrm{f}}' - \boldsymbol{X}_{\mathrm{f}}) \mathrm{i} L \boldsymbol{X}_{\mathrm{f}}') / L(\boldsymbol{X}_{\mathrm{f}}). \tag{32}$$

It is clear that equation (26) with the averaged flow orthogonal to the CM as given by equation (31) is identical to the results given previously in [1] where a restriction of the Navier–Stokes equation to the CM was performed.

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