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Amplification of Molecular Fluctuations into Macroscopic Vortices by Convective Instabilities.

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Abstract. – The statistical dynamics of fluctuating Taylor vortex flow (TVF) and Rayleigh-Bénard convection (RBC) in the presence of externally imposed throughflow is studied in the convectively unstable regime in the presence of thermal noise. A relation between thermal fluctuations at the inlet and downstream vortex flow is derived by coarse-graining appropriate microscopic fields. The downstream growth of macroscopic vortices out of molecular fluctuations is investigated and relevant fluctuation spectra are evaluated.

The old question of the effect of molecular fluctuations on coarse-grained macroscopic hydrodynamic fields [1] has recently attracted new interest [2]. There have been several new experimental investigations on the possible influence of thermal fluctuations on vortex flow arising near the primary instability in the Rayleigh-Bénard (RB) system [3, 4], the Taylor-Couette (CT) system [5, 6], and electroconvection [7]. Early theoretical results [8, 9] show (cf. further below) that measuring the effect of thermal noise, say in water, on vortices in a closed RB or TC system is difficult with the current resolution (the situation in gases being more favourable [10]). However, in the presence of an externally imposed throughflow [5, 6, 11] the observation of the amplification of thermal fluctuations into a fluctuating macroscopic field should be simpler. Above the instability for onset of vortex flow in the convectively unstable range these open-flow systems act as selective amplifiers [12] where the growth of vortices is spatially deconvoluted and spread in downstream direction by advection. With experimental boundary conditions that suppress vortices at the inlet one can then observe the downstream growth of the vortex structure with a continuously progressing throughflow-enforced spatial displacement reflecting the temporal growth. The amplification occurs only in a narrow spectral band. Only those modes of the macroscopic velocity field $\boldsymbol{u}(\boldsymbol{r}, t)$ that lie in the spectral vicinity of the critical one grow.

In analogy to work [13] on the fluctuation-induced decay of an unstable state we treat the growth of macroscopic fields out of molecular fluctuations as an effective initial/boundary-value problem. The known [14, 15] fluctuations around thermal equilibrium (changes due to the applied temperature gradient or shear [16] are irrelevant to our problem) provide the initial/boundary conditions for the near-critical macroscopic modes. Here we investigate the *deterministic* hydrodynamics of $\boldsymbol{u}(\boldsymbol{r}, t)$ subject to the boundary condition of thermal momentum density fluctuations at the inlet, $x = 0$, thus ignoring the effect of, *e.g.*, phenomenological fluctuating forces [1, 8, 9] coupling additively to the macroscopic fields throughout the system. The motivation for this approximation is that the hydrodynamic fields are only initially—when their amplitudes are still infinitesimally small—susceptible to molecular fluctuations. After the vortex amplitudes have outgrown the thermal background the deterministic forces in the field equations are much larger than the fluctuating forces of the thermal noise. Furthermore, our approach reflects the fact [17] that in the convectively unstable regime the fields at any downstream position x are caused *only* by upstream perturbations. Hence the fields are dominated by those fluctuations that had the longest time/distance to grow out of the thermal bath, *i.e.* one observes at x predominantly field fluctuations that have grown out of molecular fluctuations at the inlet $x \simeq 0$.

We consider the fluid as a system of N interacting classical point particles of mass m in a volume V [14, 15]. We denote microscopic quantities with a caret, *e.g.*, the momentum density $\hat{\boldsymbol{j}}(\boldsymbol{r}, t) = m \sum_n \hat{\boldsymbol{v}}_n(t) \delta(\boldsymbol{r} - \hat{\boldsymbol{r}}_n(t))$. Here $\hat{\boldsymbol{r}}_n(t)$ and $\hat{\boldsymbol{v}}_n(t)$ are the position and velocity, respectively, of particle n. Macroscopic fields $f(\boldsymbol{r}, t)$ are introduced by coarse-graining microscopic fields $\hat{f}(\boldsymbol{r}, t)$ isotropically, *e.g.*, with a Gaussian of width l so that in Fourier space $f(\boldsymbol{q}, t) = \hat{f}(\boldsymbol{q}, t) \exp[-q^2 l^2/2]$. Hence we do not need divergence avoiding large-q cut-offs. Here l is large compared to interatomic distances but smaller than the macroscopic vortex scales. For later use we list some averages, denoted by $\langle ... \rangle$, of fluctuations around thermal equilibrium

$$\langle \rho(\boldsymbol{r}, t) \rangle = \rho_0 = mN/V; \qquad \langle \boldsymbol{j}(\boldsymbol{r}, t) \rangle = 0; \qquad \langle [j_\alpha(\boldsymbol{r}, t)]^2 \rangle = \rho_0 k_B T / V_l . \tag{1}$$

The last one follows from $\langle [\hat{j}_\alpha(\boldsymbol{r}, t) \hat{j}_\beta(\boldsymbol{r}', t) \rangle = \rho_0 k_B T \delta_{\alpha\beta} \delta(\boldsymbol{r} - \boldsymbol{r}')$ [15], and $V_l = 8\pi^{3/2} l^3$ is the coarse-graining volume. Note that averages depend—to a varying degree—on l which does not always seem to have been considered appropriately in the literature. Defining the macroscopic velocity field by $\boldsymbol{u}(\boldsymbol{r}, t) = \boldsymbol{j}(\boldsymbol{r}, t)/\rho_0$ eq. (1) shows that its thermal fluctuations, $\langle (u_\alpha(\boldsymbol{r}, t))^2 \rangle = (k_B T/m)(1/N_l)$, are reduced relative to microscopic velocity fluctuations of a single particle by the inverse of the number $N_l = NV_l/V$ of particles in the coarse-graining volume V_l. Thus, for devices measuring macroscopic fields by an effective coarse graining the spatial resolution should be high to better see effects of molecular fluctuations.

It is instructive to compare $\langle u_\alpha^2 \rangle$ with vortex flow intensities obtained from the deterministic field equations [18]. Let w be the vertical (axial) velocity field of RBC (TVF). Its intensity grows shortly above onset linearly, $w^2 \sim \mu v_d^2$, with the control parameters $\mu = \Delta T/\Delta T_c - 1$ or $\mu = \Omega^2/\Omega_c^2 - 1$. Here ΔT is the temperature difference across the fluid layer of the RB set-up and Ω is the rotation rate of the inner cylinder in the TC system. The subscript c denotes the respective critical value for onset of vortex flow. Its characteristic velocity scale is $v_d = d/\tau_d$, where d is the thickness of the fluid layer and $\tau_d = d^2/\kappa$ ($\tau_d = d^2/\nu$) is the characteristic time for diffusing heat (momentum) across it in the RB (TC) set-up with κ being the heat diffusivity and ν the kinematic viscosity. The mean-square thermal fluctuations are

$$\langle u_\alpha^2 \rangle \simeq \frac{E_{\text{th}}}{(l/d)^3} v_d^2 , \qquad E_{\text{th}} = \frac{k_B T}{\rho_0 d^3 v_d^2} . \tag{2}$$

Here E_{th} is the thermal energy measured in characteristic units of the macroscopic fields. For a typical TC set-up $E_{\text{th}} \simeq 10^{-10}$ [5], while $w^2 \simeq 250 \mu v_d^2$ [18]. Thus, measuring the velocity field in the standard closed set-up with a coarse-graining resolution of, say, $l/d \simeq 1/10$ would require a resolution in μ of the order of $4 \cdot 10^{-10}$ to see microscopic fluctuations $\langle u_\alpha^2 \rangle$ (2) of the order of w^2 (1).

We consider open RB (TC) set-ups with imposed horizontal (axial) mean flow through a not too wide rectangular convective channel (annulus between the concentric cylinders). In both cases the critical wave vector is oriented along the flow direction for not too large throughflow Reynolds numbers Re. We decompose wave vectors $\boldsymbol{q} = k\boldsymbol{e}_x + \boldsymbol{q}_\perp$ and positions $\boldsymbol{r} = x\boldsymbol{e}_x + \boldsymbol{r}_\perp$ into components along the throughflow (k and x, respectively) and into vectors perpendicular to it. For small supercritical control parameters, $\mu \ll 1$, the evolution dynamics is governed by a narrow band of near critical modes. Thus one does not have to integrate the full hydrodynamic field equations but can rather use the Ginzburg-Landau (GL) amplitude equation approximation

$$w(\boldsymbol{r}, t) = A(x, t) \exp[i(k_c x - \omega_c t)] \varphi_c(\boldsymbol{r}_\perp) + \text{c.c.}, \tag{3a}$$

$$\tau_0(\partial_t + v_g \partial_x) A = [\mu(1 + ic_0) + \xi_0^2(1 + ic_1)\partial_x^2 - \gamma(1 + ic_2)|A|^2]A. \tag{3b}$$

All quantities entering (3) including the critical eigenfunction $\varphi_c(\boldsymbol{r}_\perp)$ are known from linear [11, 5, 19] and non-linear [11, 19] analyses of the deterministic field equations. For small throughflow the coefficients c_0, c_1, c_2 are very small, the group velocity v_g and ω_c grows linearly with Re while k_c, τ_0, ξ_0, γ have small quadratic corrections to their $Re = 0$ values. Above the stability threshold, $\mu = 0$, the secondary field (3*a*) can grow. However, in the convectively unstable range [17]

$$\mu < \mu_{\text{conv}}^c = \frac{\tau_0^2 v_g^2}{4\xi_0^2(1 + c_1^2)} \tag{4}$$

a permanent upstream source of perturbations is necessary [12] to sustain a finite field w at a downstream position x. Moreover the field is influenced only by upstream but not downstream perturbations. By switching off their forcing, the vortex structure is convected away by the throughflow and the system returns to the basic homogeneous state. For $\mu > \mu_{\text{conv}}^c$, in the absolutely unstable regime, however, the deterministic forcing in (3*b*) is sufficiently large to sustain the dissipative structure and the latter is almost insensitive to noise.

We shall discuss the growth dynamics (3) of w resulting from fluctuations of the complex amplitude A that are caused by transversal-momentum density fluctuations close to the inlet. The macroscopic flow is incompressible, so we ignore longitudinal momentum and mass density fluctuations. We neglect energy density fluctuations since their effect is small [9]. Assuming that the molecular fluctuations do not favour a particular phase relations of A, the probability distributions of $A_r = \text{Re}\,A$ and of $A_i = \text{Im}\,A$ are the same at $x = 0$ and the former are statistically independent of the latter. Thus the fluctuations of $A(x = 0, t)$ are characterized up to the two-point level by

$$\langle A(x = 0, t) \rangle = 0; \qquad \langle A(x = 0, t) A^*(x = 0, t') \rangle = D(t - t'). \tag{5}$$

The dimensionless even, real correlation function D is determined by projecting thermal momentum density fluctuations in the direction of w onto the amplitude of the critical mode of

(1) It would be interesting to see whether the commonly used Laser-Doppler velocimeters allow measuring the thermally induced Brownian motion of the macroscopic particles that are added to the fluid in order to infer the local macroscopic velocity field from their Lagrangian velocity .

the velocity field $w = j_w/\rho_0$:

$$D(t-t') = \frac{\int_{S_\perp} d^2r_\perp \int_{S_\perp} d^2r'_\perp \langle j_w(x=0, \boldsymbol{r}_\perp; t) j_w(x=0, \boldsymbol{r}'_\perp; t')\rangle \exp[i\omega_c(t-t')]\,\varphi_c^*(\boldsymbol{r}_\perp)\varphi_c(\boldsymbol{r}'_\perp)}{2\rho_0^2(S_\perp v_d^2)^2} + \text{c.c.} \quad (6)$$

More precisely, we relate the correlations—not the fluctuations—of $A\exp[i(k_c x - \omega_c t)]$ to those of $\int_{S_\perp} d^2r_\perp\, w(\boldsymbol{r}, t)\varphi_c^*(\boldsymbol{r}_\perp) / \int_{S_\perp} d^2r_\perp\, |\varphi_c(\boldsymbol{r}_\perp)|^2$. We use the normalization $\int_{S_\perp} d^2r_\perp\, |\varphi_c(\boldsymbol{r}_\perp)|^2 = v_d^2 S_\perp$, where $S_\perp$ is the area of the system perpendicular to the flow. Ignoring longitudinal current fluctuations, $\boldsymbol{q}\cdot\boldsymbol{j}(\boldsymbol{q}, t) = 0$, one has

$$\langle j_w(\boldsymbol{r}, t) j_w(\boldsymbol{r}', t')\rangle = \rho_0 k_B T \int \frac{d^3q}{(2\pi)^3}\left(1 - \frac{q_w^2}{q^2}\right)\exp[-\nu q^2|t-t'| - q^2 l^2 + i\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}')]. \quad (7)$$

Since the coarse graining eliminates fluctuations on length scales less than l, we use the «hydrodynamic limit» [14, 15] of the transverse-current correlation function. The evaluation of $D(t)$ is more convenient in Fourier space. Using (7) in (6), one obtains for the amplitude correlation function

$$D(t) = E_{\text{th}} d^3 \int \frac{d^3q}{(2\pi)^3}\left(1 - \frac{q_w^2}{q^2}\right)\exp[-(\nu|t| + l^2)q^2]\left|\frac{\varphi_c(\boldsymbol{q}_\perp)}{S_\perp v_d}\right|^2 \cos(\omega_c t), \quad (8)$$

where $\varphi_c(\boldsymbol{q}_\perp) = \int_{S_\perp} d^2r_\perp\, \varphi_c(\boldsymbol{r}_\perp)\exp[-i\boldsymbol{q}_\perp\cdot\boldsymbol{r}_\perp]$. The integrals in (7), (8) extend over the whole $\boldsymbol{q}$-space.

Note that the downstream velocity fluctuations are related via (3) to those of $A(x=0, t)$. The frequency spectrum, $D(\omega)$, of the latter (cf. fig. 1) is not white. Its total spectral power is

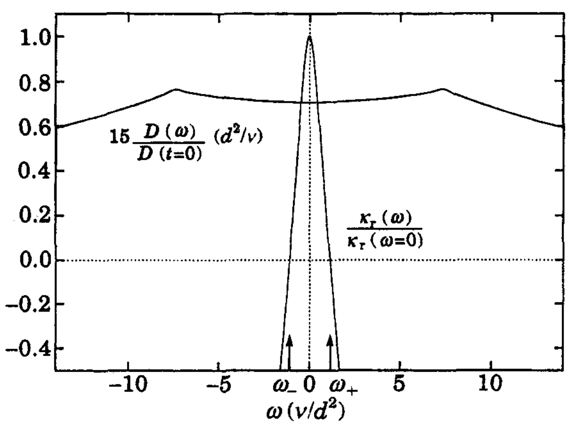

Fig. 1. – Normalized frequency spectrum of the correlations $D(t)$ (8) of inlet amplitude fluctuations and real part $\kappa_r(\omega)$ of the complex spatial growth rate (10) for a TC set-up with $\eta = 0.75$, $Re = 2$, $\mu = \mu_{\text{conv}}^c/2 = 0.03$, $\omega_c = 7.35\nu/d^2$, $l/d = 0.1$. Here $\kappa_r(\omega = 0) = 0.19/d$ and $D(t=0) = 0.073 E_{\text{th}}$, where $1 - q_w^2/q^2$ was approximated in (8) by 2/3.

quickly estimated to be $D(t = 0) \simeq E_{\rm th}/(\Gamma_\perp l/d)$, where $\Gamma_\perp = S_\perp/d^2$ is the systems cross-section in units of d^2. For a rotating TC system $\Gamma_\perp = \pi(1 + \eta)/(1 - \eta) = 7\pi$ if the radius ratio is $\eta = 0.75$. For typical convection cells $\Gamma_\perp \simeq 4$. The above estimate follows when $q_\perp |\varphi_c(\boldsymbol{q}_\perp)|^2$ drops to zero faster than $\exp[-q_\perp^2 l^2]$, *i.e.* for $l \ll d$. Then one can approximate in the $\boldsymbol{q}_\perp$-integral $\exp[-q_\perp^2 l^2] \simeq 1$. The intensity, $D(t = 0)$, of thermally driven amplitude fluctuations of the critical mode at $x = 0$ decreases with increasing area $S_\perp$: the critical mode loses weight to non-critical modes whose number increases with $S_\perp$, while the total spectral weight of velocity field fluctuations is limited by (2). Thus thermal fluctuations optimally drive the critical mode in systems with small $\Gamma_\perp$—noise initiates axisymmetric Taylor vortices (straight convection rolls) more likely when the transversal homogeneity required by criticality has to extend only over a short circumference (length). This result is best tested experimentally by comparing two TC set-ups that have different radius ratios η but the same $E_{\rm th}$ or gap width d.

Now we shall investigate the noise-sustained velocity fluctuations in the convectively unstable region $0 < \mu < \mu^{\rm c}_{\rm conv}$. In order to do that analytically, we restrict ourselves here to the downstream range in which the modulus of $A = R \exp[i\phi]$ is still small compared to $\sqrt{\mu/\gamma}$ so that the dynamics is still linear. In this range the appropriate solution of the (linear) GL equation is [11, 12]

$$A(x, t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \exp[-i\omega t] \exp[\kappa(\omega) x] A(x = 0, \omega), \tag{9}$$

where $A(x = 0, \omega)$ is the Fourier transformed noise source. The complex spatial growth rate $\kappa(\omega)$ is given by the eigenvalue that develops for $\mu < 0$ a negative real part

$$\xi_0 \left[\frac{1 + ic_1}{1 - ic_1}\right]^{1/2} \kappa(\omega) = (\mu^{\rm c}_{\rm conv})^{1/2} - \left[\mu^{\rm c}_{\rm conv} - \frac{\mu(1 + ic_0) + i\omega\tau_0}{1 - ic_1}\right]^{1/2}. \tag{10}$$

Thus fluctuations with frequencies $\omega_- < \omega < \omega_+$ for which $\kappa_{\rm r} = {\rm Re}\,\kappa$ is positive (negative) are exponentially amplified (damped) in drownstream direction and $\tau_0 \omega_\pm = \pm 2[\mu\mu^{\rm c}_{\rm conv}(1 + c_1^2)]^{1/2} + \mu(c_1 - c_0)$. Figure 1 shows $\kappa_{\rm r}(\omega)/\kappa_{\rm r}(\omega = 0)$ for the TC set-up.

We shall discuss here correlation functions

$$\langle f(\boldsymbol{r}, t) f^*(\boldsymbol{r}, t')\rangle = C_{ff}(\boldsymbol{r}; t - t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} C_{ff}(\boldsymbol{r}; \omega) \exp[-i\omega(t - t')] \tag{11}$$

and their frequency spectra, $C_{ff}(\boldsymbol{r}; \omega)$, in the linear regime at a common, fixed position $\boldsymbol{r}$ or x for $f = w$ and A. Correlations of R, ϕ, the wave number $\partial_x \phi$, and the frequency $\partial_t \phi$ involving higher-order correlations of the noise-source $A(x = 0, t)$ will not be discussed here. For a statistically stationary noise source all correlations are invariant under time translation but due to the inlet boundary they are not invariant under spatial translation. The fluctuation spectra

$$C_{AA}(x; \omega) = \exp[2\kappa_{\rm r}(\omega) x] D(\omega), \tag{12}$$

$$C_{ww}(\boldsymbol{r}; \omega) = [C_{AA}(x; \omega - \omega_c) + C_{AA}(x; -\omega - \omega_c)] |\varphi_c(\boldsymbol{r}_\perp)|^2 \tag{13}$$

resulting from (9) are together with (8) main predictions of this work.

The downstream variation of the above fluctuation spectra is governed by the filter function $\exp[2\kappa_{\rm r}(\omega) x]$ of the deterministic growth dynamics (3). It determines which modes are amplified out of the thermal fluctuation spectrum $D(\omega)$ at $x = 0$. Thus, very far downstream the spectrum of A is restricted to the frequency band $|\omega| \lesssim \omega_\pm$ and the spectrum of w contains practically only frequencies $|\omega - \omega_c| \lesssim \omega_\pm$. The amplification is largest in the band centre—the critical mode is amplified, *e.g.*, at $x = 60d$ by the factor $\exp[120\kappa_r(0)\,d] \simeq 10^{10}$ for the parameters of fig. 1. While the theoretical prediction for the band limits $\omega_\pm$ and the spatial variation of the spectrum, $C_{AA}(x;\omega)/C_{AA}(x';\omega) = \exp[2\kappa_r(\omega)(x - x')]$, can easily be checked experimentally, it only gives information of the deterministic growth dynamics (3). A more interesting test would be to divide the experimental amplitude spectrum by $\exp[2\kappa_r(\omega)\,x]$ to obtain the *experimental* noise spectrum $D_{\exp}(\omega)$. A comparison with the thermal spectrum $D(\omega)$ (cf. fig. 1) would then reveal whether the downstream velocity fluctuations are driven by molecular noise or other perturbations. A further test is the statistical dynamics of the phase fluctuations of the pattern. We find $\langle A_r\rangle = \langle A_i\rangle = 0$ and $\langle A_r(x,t)A_i(x,t)\rangle = 0$. Furthermore, the time-displaced correlation function $\langle A_r(x,t)A_i(x,t')\rangle = -(1/2)\,\mathrm{Im}\,C_{AA}(x;t-t')$ and its spectrum $(i/4)[C_{AA}(x;\omega) - C_{AA}(x;-\omega)]$ are very small since $\kappa_r(-\omega) \simeq \kappa_r(\omega)$, in particular for small throughflow, *i.e.* small c_n. For vortex patterns that are sustained in the convectively unstable range by perturbations other than molecular fluctuations we expect different correlation behaviour.

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