## **Convection at Finite Rayleigh Numbers in Large-Aspect-Ratio Containers**

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The phase diffusion and mean drift equations which describe the behavior of a convection pattern are derived, a step which is essential for obtaining quantitative comparisons between theory and experiment. The theory recovers the boundaries of the Busse balloon, agrees closely with the dominant wave numbers observed by Heutmaker and Gollub [Phys. Rev. A 35, 242 (1987)] and Steinberg, Ahlers, and Cannell [Phys. Scr. 32, 534 (1985)] in natural and target patterns, predicts a new instability which is important in facilitating wave-number adjustment in circular target patterns and in initiating time dependence, and predicts Rayleigh numbers at which loss of spatial correlation due to global defect nucleation will occur.

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Nonlinear systems, driven far from equilibrium by an external stress, can undergo a series of symmetrybreaking bifurcations leading to spatiotemporal patterns which generally become more complicated as the applied stress is increased. Such patterns are common in nature, and can be observed from weather maps to the surface of the saguaro cactus. In particular, Rayleigh-Bénard convection in large-aspect-ratio containers has long been the canonical paradigm for studying their behavior. In this Letter, we provide, for the first time in the literature, a self-consistent theory for a dynamical description of such convection patterns at finite amplitudes by deriving directly from the Navier-Stokes and heat equations the phase diffusion equation for

$$\mathbf{k} \left[ \mathbf{X}(X,Y) = \epsilon \frac{\bar{x}}{d}(x,y), T = \epsilon^2 \frac{\kappa t}{d^2} \right]$$

the pattern wave vector, and the mean drift equation for  $V(\mathbf{X},T)$  from which the mean drift horizontal velocity (which is a linear combination of V and slow gradients of  $\mathbf{k}$  with z-dependent coefficients) can be calculated. Here d denotes the depth of the container, L its horizontal size, and  $\kappa$  is the kinematic thermometric conductivity. The mean drift velocity field is driven by the pattern curvature and intensity gradients of the wave vector and in turn it advects and distorts the constant-phase contours. The small parameter in our theory is  $\epsilon = d/L$ , the inverse aspect ratio. It should be sufficiently small so that the band of stable wave numbers is densely populated. The derivation is valid in regions away from defects such as dislocations, disclinations, and foci where the macroscopic order parameters  $\mathbf{k} = \nabla \Theta$  and  $\mathbf{V} = \nabla \times \psi \hat{\mathbf{z}}$  are the gradient and curl of a single-valued phase and stream function, respectively. They vary by order 1 over distances of the container diameter L and over times of the order of the horizontal diffusion time  $L^2/\kappa$ .

The method by which the phase diffusion and mean drift equations are derived follows closely the ideas of Cross and Newell<sup>1</sup> who, in the early 1980s, derived the phase diffusion equation from a variety of model microscopic equations and, guided by the hand of experience and low-amplitude calculations, suggested the form of the mean drift equation. The idea is to look for slowly modulated finite-amplitude roll solutions to the governing equations (the Navier-Stokes and heat equations using the Oberbeck-Boussinesq approximation with rigidrigid boundary conditions), whose existence and linear stability properties have been found by Busse and colleagues.<sup>2</sup> The symmetry in the vertical direction about the midlayer means that rolls are the dominant planform, although the theory can equally well handle the slow modulation of hexagonal configurations (quasicrystals). Because the slowly varying roll is no longer an exact solution of the equations, corrections to the velocity (u,v,w), temperature  $(\phi)$ , and pressure (p) fields

$$\mathbf{v}(u,v,w,\phi,p) = \mathbf{f}(\theta = \epsilon^{-1}\Theta(X,Y,T), z, A(X,Y,T))$$
$$+ \epsilon \mathbf{v}_1 + \epsilon^2 \mathbf{v}_2 + \cdots,$$

where  $\mathbf{f}$  is  $2\pi$  periodic in  $\theta$  and  $\mathbf{k} = \nabla_{\mathbf{X}} \Theta$  (almost everywhere) must be sought. The algebraic equation for the amplitude A is determined by demanding that  $\mathbf{f}$  is  $2\pi$  periodic in  $\theta$ . The phase diffusion and mean drift equations for  $\mathbf{k} = \nabla \Theta$  and  $\mathbf{V} = \nabla \times \psi \hat{\mathbf{z}}$  (contained in  $\mathbf{v}_1$ ) arise as solvability conditions when one solves for  $\mathbf{v}_1$  and  $\mathbf{v}_2$ . These conditions are necessary because of the singular nature of the equations  $M\mathbf{v}_j = \mathbf{g}_j$ , j = 1, 2 where M is the operator obtained by linearizing the Navier-Stokes and heat equations about  $\mathbf{v} = \mathbf{f}$ , and result from the symmetries  $\partial \mathbf{f}/\partial \theta$  (translation of phase) and  $\partial \mathbf{f}/\partial p$  (one can add an arbitrary constant  $p_s$  to the pressure). The addition of the slowly varying pressure field  $p_s(\mathbf{X}, T)$  is necessary in order to ensure that the induced mean drift field satisfies mass conservation.

The key difficulty (and the novelty) in the derivation is that the phase diffusion equation arises as a solvability condition at order  $\epsilon$  and the mean drift equation at order  $\epsilon^2$ . Therefore one has to solve, after first removing the solvability condition, the singular equations for  $\mathbf{v}_1$  exactly retaining, in algebraic form, the dependence of  $\mathbf{v}_1$  on the wave vector  $\mathbf{k}$ . No approximation obtained by averaging the momentum equations over  $\theta$  and z will suffice because the vertical (z) structure of the induced mean drift fields is not trivial and, especially for low Prandtl numbers, is not well approximated by a Poiseuille-like profile. The key mathematical step in obtaining the generalized inverse of the singular equation for  $\mathbf{v}_1$  is the use of a singular-valued decomposition (SVD) of the matrix which represents M in an appropriate basis. SVD is ideally suited for our purposes because vectors are automatically decomposed into the range of the singular operator and the null space of its adjoint, and only poor conditioning of the nonsingular part requires further attention. The methods we use should have wide applicability.

The amplitude, phase diffusion, and mean drift equations are

$$\Omega(A,k,R) + O(\epsilon) = 0, \qquad (1)$$

$$\Theta_T + \rho(k) \mathbf{V} \cdot \mathbf{\nabla} \Theta + \frac{1}{\tau(k)} \mathbf{\nabla} \cdot \mathbf{k} B(k) + O(\epsilon) = 0, \qquad (2)$$

$$\hat{\mathbf{z}} \cdot \nabla \times \hat{\mathbf{k}} \, \alpha(k) (\hat{\mathbf{k}} \times \nabla \psi) \cdot \hat{\mathbf{z}} - \nabla \cdot \hat{\mathbf{k}} \, \beta(k) (\hat{\mathbf{k}} \cdot \nabla \psi) = \hat{\mathbf{z}} \cdot \nabla \times \left[ \frac{1}{P} \mathbf{k} \nabla \cdot \mathbf{k} \, A^2 - \frac{\hat{\mathbf{k}}}{\tau_a(k)} \nabla \cdot \mathbf{k} \, B_a(k) \right] - \nabla \cdot \hat{\mathbf{k}} [\nabla \times \mathbf{k} \, B_\beta(k)] \cdot \hat{\mathbf{z}} + O(\epsilon) \,, \quad (3)$$

where  $\mathbf{k} = \nabla \Theta$ ,  $\hat{\mathbf{k}} = \mathbf{k}/k$ ,  $\nabla = \nabla \times \psi \hat{\mathbf{z}}$ , and the quantities  $\rho(k), B(k), \tau(k), \alpha(k), \beta(k), A(k), B_{\alpha}(k), \tau_{\alpha}(k), \text{ and}$  $B_{\beta}(k)$  are all functions of k which are explicitly calculated and of which only two can be eliminated through combination. The function  $\Omega(A,k,R)$  is the algebraic relation through which the amplitude A is slaved to the wave number k. The  $O(\epsilon)$  correction term is equally important at singularities (dislocations, foci) at which points the amplitude A becomes an active order parameter. The mean drift is driven by the slow gradients (order  $L^{-1}$ ) of the Reynolds stresses of the short scale, locally periodic pattern which are nonzero when the pattern curvature is not constant everywhere. The fact that it cannot be written in terms of local phase gradients is a consequence of incompressibility. It plays a similar role to the long-wave ion acoustic field which is driven by the ponderomotive force generated by gradients in the intensity of short-scale Langmuir waves in plasmas<sup>3</sup> and to the large-scale pressure field which must be introduced for the description of two-dimensional gravity surface waves in a finite-depth inviscid fluid.<sup>4</sup>

The equations have the properties that they are translationally and rotationally invariant and also Galilean invariant even though the original rigid boundaryvalue problem is not. At infinite Prandtl numbers, no mean flow is induced [the forcing terms in (3) either vanish or cancel], and (2), in coordinates parallel (X)and perpendicular (Y) to **k**, is  $\Theta_T - D_{\parallel}(k)\Theta_{\chi\chi} - D_{\perp}(k)$  $\times \Theta_{YY} = 0$ , the Pomeau-Manneville<sup>5</sup> phase equation for which the parallel and perpendicular diffusion coefficients  $D_{\parallel} = -(1/\tau)(d/dk)kB$  and  $D_{\perp} = -(1/\tau)B$  are explicitly calculated. The loci  $D_{\parallel} = 0$  and  $D_{\perp} = 0$  are the Eckhaus and zigzag stability boundaries, respectively. Curved rolls patches select the wave number  $k_B(R,P)$ ,<sup>6</sup> the zero of B(k), which, in the infinite Prandtl number limit, is at the zigzag stability border where the rolls lose their resistance to lateral bending. As a consequence, an order  $d/\sqrt{\epsilon} = \sqrt{dL}$  length scale is introduced in this direction and higher-order correction terms proportional to  $\Theta_{YYYY}$  in (2) become equally important as  $\nabla \cdot \mathbf{k} B$ . The consequence is that at large P, the patterns take at least a time  $(L/d)L^2/\kappa$  to relax to equilibrium. As

 $R \rightarrow R_c$ , the critical Rayleigh number, the amplitude becomes small; the operator M has an additional null vector because one is effectively linearizing about the zero solution. The amplitude A becomes an active order parameter satisfying a partial differential equation rather than being passively slaved to k as in (1). When this equation is combined with the phase diffusion equation in the combination  $W = A \times \exp(i\Theta \epsilon^{-1})$ , one obtains the equation of Newell and Whitehead<sup>7</sup> and Segel<sup>7</sup> for lowamplitude convection.

At finite Prandtl numbers, the effect of mean drift is dramatic. It affects in a significant way the boundaries of instability (Busse balloon<sup>2</sup>) of the straight parallel roll solution  $\Theta = kX$ ,  $\psi = 0$  [see Figs. 1(a)-1(c)] by shifting the zigzag stability boundary to lower k and turning the one-dimensional Eckhaus instability into the two-dimensional skew varicose instability the finite-amplitude consequence of which is the generation of dislocation pairs. Our theory is in agreement with that of Busse<sup>2</sup> and has the advantage that we can follow the skew varicose instability into the finite-amplitude regime. The presence of mean drift can also balance wave-number diffusion  $\tau^{-1} \nabla \cdot \mathbf{k} B$  so that stationary patterns no longer have to relax to  $k_B$ . Nevertheless, because of the boundary constraints, natural convection patterns in cylindrical and rectangular geometries consist of almost circular patches whose center of curvature (called foci) are attracted to the sidewall. Our calculated  $k_B$  agrees with the wave number of maximum power at several Rayleigh numbers in the wave-number distributions found by Heutmaker and Gollub for natural convection in a cylindrical container of water with P = 2.5 [see Fig. 1(b)]. It also agrees with the results of Steinberg, Ahlers, and Cannell<sup>8</sup> for circular target patterns [see Fig. 1(a)] and with the theoretical calculations of Buell and Caton<sup>6</sup> made for exactly circular rolls.

Because almost circular patches are the dominant feature in natural convection, the stability of the circular roll patch  $\Theta = k_B r$ ,  $\psi = 0$  is relevant. We find a new instability which we call the focus instability. It breaks the axisymmetric symmetry of the circular roll pattern at a



FIG. 1. The long-wave borders of the Busse balloon marked E (Eckhaus), Z (zigzag), and SV (skew varicose), and the zeros  $k_B$  of B(k) as calculated from (2) and (3) for Prandtl numbers (a) 6.1, (b) 2.5, and (c) 0.71, respectively. The agreement with the calculations of Busse for the E, Z, and SV borders is so good that the two sets of curves superimpose exactly. (a) The wave numbers (as measured by  $2\pi$  where  $\lambda$  is the width of the second pair of rolls from the wall) of the  $3\frac{1}{2}$  (•) and 3 (•) roll equilibrium states as functions of Rayleigh number as the Rayleigh number is increased [taken from Steinberg, Ahlers, and Cannell (Ref. 8)]. (b) The maxima (×) and the support of the wave-number distribution are superimposed [taken from Heutmaker and Gollub (Ref. 9)].

value of the Rayleigh number when the mean flow  $\rho \mathbf{V} \cdot \mathbf{k}$ induced by an asymmetric deformation can overcome the stabilizing influence of parallel diffusion  $\tau^{-1} \mathbf{\nabla} \cdot \mathbf{k} B$ . For a circular target pattern as in Fig. 2(b), the deformation is  $\Theta = k_B [r + D(r)e^{\sigma t} \sin(m\theta)]$  and  $\psi = \phi(r)e^{\sigma t} \cos(m\theta)$ , with m = 1 and the mean flow has a dipole shape and compresses the rolls in the direction towards which the umbilicus has moved. The choice m = 2, relevant when the focus is attached to a sidewall, corresponds to a quadrupolelike mean flow in which the umbilicus does not move. The analysis is subtle and requires the introduction of the amplitude as an active order parameter near the focus (center) in order to ascertain the correct boundary conditions on the derivative of D(r) there. Details are discussed in Ref. 10.

The instability explains how circular target patterns adjust their pattern wave number and also may be of importance in understanding the onset of time dependence for natural convection patterns in which the texture is dominated by almost circular roll patches surrounding sidewall foci. The scenarios in each instance have the following common feature (e.g., see Refs. 9 and 11). In each case rolls are compressed to the point where the local wave number lies sufficiently outside the skew varicose, or for moderate to large Prandtl numbers, the Eckhaus stability boundary<sup>2</sup> for straight parallel rolls in an infinite horizontal geometry so that either a dislocation pair is nucleated or a roll directly disappears in the focus. In the first case and in a circular target pattern, the dislocations can glide to the focus thereby removing a roll pair. In natural convection patterns, the most compressed rolls are in the center of the container between two patches. In that case, the dislocations climb to the sidewall and vanish there or glide along and disappear in a focus. In the circular target patterns of Croquette, Le Gal, and Pocheau,<sup>11</sup> the relaxed pattern is again circular with wave number  $k < k_B$ . New rolls are nucleated at the focus [due to term 1 balancing term 3 in (2)], the pattern is returned to its former unstable state, and the cycle repeats. In the experiment of Steinberg, Ahlers, and Cannell,<sup>8</sup> the new circular  $2\frac{1}{2}$  roll-pair pattern in Fig. 2(b) is stable and the pattern remains in this



FIG. 2. Equilibrium patterns taken from Steinberg, Ahlers, and Cannel (Ref. 8) at P = 6.1,  $\Gamma = 6$  at two different Rayleigh numbers: (a) a stable three-roll state at  $R = 3R_c$  and (b) its distortion at  $R = 4R_c$ .

state until it reaches a Rayleigh number of another transition.

In natural patterns, there are several mechanisms through which roll compression sufficient to nucleate a dislocation pair occurs. At low Prandtl numbers, where the onset of time dependence occurs close to the onset of convection, boundary forcing, as described by Croquette, Le Gal, and Pocheau,<sup>11</sup> is important because a small change in Rayleigh number leads to a large change in roll curvature from nearly straight rolls which intersect the sidewall at an angle far from 90° to curved rolls whose axes are perpendicular to the boundary. This causes the rolls in the center of the container to be compressed. For low to moderate Prandtl numbers, on the other hand, the onset of time dependence occurs at Rayleigh numbers far from threshold at which values the boundary conditions force the pattern to consist of almost circular patches and two mechanisms for a roll compression sufficient to trigger the skew-varicose instability are important. First is the focus instability. The Rayleigh number must be sufficiently large so that it exceeds the critical value for the instability or else be close enough so that deformations from the circular state, which are forced on the pattern because  $k \neq k_B$ everywhere, and the corresponding mean flow are not severely inhibited. Second, the amplitude becomes an active order parameter at the focus and work on model equations reported in Ref. 10 shows that for moderate values of  $\epsilon$  (as is the case in these experiments), a significant part of the mean flow can be driven by amplitude gradients. For the range of Rayleigh numbers for which these scenarios are operative, the pattern remains spatially ordered and the dynamics low dimensional. For still larger Rayleigh numbers, the locus of the maximum  $k_B$  of the wave-number distribution will intersect the skew-varicose boundary (at  $7R_c$ ,  $2R_c$ , and  $\sim R_c$  for P = 2.5, 0.7, and 0.1, respectively) at which point one expects many defects to be nucleated. Spatial correlations will be lost and the spatial order will disappear.

A crucial ingredient for a complete macroscopic fieldparticle theory is the inclusion of a component which can handle the nucleation, annihilation, and motion of particlelike defect singularities. As a particular example, consider the dislocations which are nucleated as the result of a skew-varicose instability of straight parallel rolls. The induced mean flow acts to enhance the necking of the phase contours and locally the wave number k increases until it approaches the right border of the marginal stability boundary. At this point the amplitude becomes small and a weakly nonlinear version of (1)-(3), which preserves rotational invariance and includes the amplitude as an active order parameter satisfying a partial differential equation instead of (1), obtains. In contrast to the somewhat arbitrary introduction of an additional gauge field, <sup>12</sup> which has no physical origin in the hydrodynamic context and does not describe either the nucleation or annihilation of defects, the addition of the amplitude as an extra active order parameter near defects can be justified by rigorous asymptotics, has a concrete physical interpretation, and it can be shown that the polar combination of amplitude and phase satisfies an equation which has vortexlike defect solutions. A description of these new ideas and the matching between solutions in the outer region described by (1)-(3) and in the defect core will be given elsewhere.

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