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The state-space structure around spiral-defect chaos in Rayleigh–Bénard convection

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The co-existence of ideal straight rolls (ISRs) and spiral-defect chaos (SDC) as bistable states in Rayleigh–Bénard convection (RBC) above the onset of the linear instability is well established in extended spatial domains ($\Gamma \geq 80$, where Γ is the aspect ratio of the domain). However, multiple stable states have also been found independently, raising questions about the precise understanding of this observed bistability in extended domains. In this study, we isolate the localized structures of SDC by gradually reducing the spatial domain. By minimizing the domain systematically to $\Gamma = 4\pi$, SDC appears transiently and eventually stabilizes into new stable states referred to as elementary states. These elementary states are visibly and statistically similar to the spatially local patterns of SDC, indicative of invariant solutions underpinning the pattern formation in SDC. To understand the state-space structure further, we have examined the edge between ISRs and the elementary states, revealing multiple edge states, and conducted a series of numerical simulations along the unstable manifolds of unstable ISRs. The unstable ISRs near the Busse balloon are connected to stable ISRs and the base state through networks of heteroclinic orbits, forming a basin of attraction for each stable ISR. In contrast, the unstable ISRs farther from the Busse balloon contain some unstable manifolds, along which

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the solution trajectory leads to SDC, suggesting that these unstable ISRs sit on the boundary between stable ISRs and SDC. Finally, we propose a state-space structure around the basic heat conduction state, stable/unstable ISRs, elementary states and transient SDC.

1. Introduction

Rayleigh–Bénard convection (RBC) concerns the fluid motion confined between two parallel horizontal, good conducting walls, separated by a distance d , heated from below. The motion of the fluid is effectively driven by unstable stratification due to temperature gradients ($\Delta T/d$) across the walls. Given a large enough temperature gradient, a non-trivial fluid motion occurs, often developing into a spatially varying structure known as a convection pattern. This motion is described in terms of the Rayleigh number $Ra = \alpha g d^3 \Delta T / \nu \kappa$, Prandtl number $Pr = \nu / \kappa$ and aspect ratio of the experimental/computational domain $\Gamma = L/d$, where $\alpha, g, \Delta T, \nu, \kappa, L$ refer to the thermal expansion coefficient, acceleration due to gravity, temperature difference between the bottom and top wall, kinematic viscosity, thermal diffusivity, domain length and span, respectively. An important question that underpins RBC is often as follows: Given the Rayleigh number (Ra), Prandtl number (Pr) and aspect ratio (Γ) of a fluid system, what convection pattern arises and what is its associated heat flux?

(a) Multiple convection states

The Busse balloon describes the secondary neutral stability curves of ideal straight rolls (ISRs) of RBC over a continuum of wavenumbers, delineating regions in wavenumber space into stable and unstable ISRs at a given Ra and Pr . While the Busse balloon is well established, predicting the wavenumber of an ISR state remains an ongoing challenge [1]. Experimental investigations of RBC in moderate domains ($\Gamma \geq 14$) showed that ISRs in rectangular (straight rolls) and cylindrical (concentric rolls) domains are stable. Consider $\varepsilon (\varepsilon \equiv (Ra - Ra_c)/Ra_c)$, where Ra_c is the critical Ra for the onset of linear instability for ISRs) as a control parameter referred to as the reduced Rayleigh number. As ε is increased continuously from below the onset, the initial ISRs become unstable and transform into another set of ISRs with a different wavelength. With the marginal increase of ε , this process is repeated and the ISRs undergo hysteretic transverse wavelength adjustments, adhering to the stability boundaries of the Busse balloon [2,3]. When ISRs become unstable, roll dislocations and defects can be nucleated near the boundary or bulk, modifying the effective roll wavenumber as they travel through the domain [3]. This observation implies that the wavenumber of an ISR state depends on the state's history or the system's initial condition [1].

Note that the solutions in the form of ISRs appear to be an exception rather than the rule [4]. The coexistence of multiple 'non-ISR' states, in the form of squares, travelling/stationary targets, giant rotating spirals and oscillatory convection patterns have been found over several years [3,5–9]. Investigation of cylindrical RBC with small aspect ratio ($\Gamma = 2$) revealed eight stationary states (at the same $Ra = 142\,000$) and two oscillatory states ($Ra > 14\,200$) [7]. These findings were later supported by numerical experiments and bifurcation analyses [9–11]. In particular, bifurcation analyses performed by [10] revealed 12 stable branches in the form of symmetric and asymmetric convection rolls near the onset ($Ra \leq 2500$), with the potential emergence of hundreds of branches at higher Rayleigh numbers, $Ra \leq 30\,000$ [11]. In larger domains ($\Gamma \geq 28$), giant rotating spirals were identified and thoroughly investigated [6,12]. Experimental and numerical studies of RBC with varying sidewall boundary conditions (i.e. thermally insulating, conducting and no-slip) [13–16], non-Boussinesq convection [17,18] and rotational effects [19] were investigated, where multiple states were also reported. More recently, [20,21] computed up to 16 stable and unstable invariant states and identified heteroclinic orbits between the multiple states in an inclined RBC.

(b) Spiral-defect chaos

Convection rolls exhibiting spatio-temporal chaotic behaviour known as spiral-defect chaos (SDC) are found in the same parameter space of ε , where ISRs were expected [22–32]. It is well established that SDC exists as an intrinsic state of RBC, independent of sidewall conditions [27]. SDC has also been found in numerical simulations of the two-dimensional Swift–Hohenberg equations [33–37]. Some investigations into quantifying the onset of SDC in terms of Rayleigh number remain inconclusive. The critical reduced Rayleigh number for the onset of SDC, ε_s , has been observed to decrease with increasing Γ and increase with increasing Pr [1,25,26,28,38]. Note that SDC has been reported in larger domains ($\Gamma \geq 40$) only, implying that there exists a minimal Γ for SDC to occur [1], further supporting the dependence of ε_s on Γ mentioned above. This is also consistent with the leading Lyapunov exponents, which become smaller with decreasing aspect ratios, Γ , albeit at larger $\varepsilon = 2.5$ [39,40]. Investigations into the spatial-temporal characteristics of SDC, such as the quantification of the averaged roll-curvature [25,26], probability of spirals [41,42] and correlation length and time scales [22,27,28] have been performed. Specifically, the correlation length scales [22,27,28] of SDC appear to scale exponentially as ε is increased. Furthermore, spatio-temporal chaotic behaviour reminiscent to SDC has been found in other pattern-formation systems such as rotating RBC [19], dielectric barrier discharge [43] and chemical systems [44].

Given the co-existence of ISRs and SDC in the parameter space of ε , it is known that they form bistability at $Pr \approx 1$ in a spatially extended domain, supported by experiments over a range of $\varepsilon (> 0)$ [28]. Only carefully prepared experiment set-ups led to ISRs while most initial conditions yield SDC. In other words, the asymptotic state of RBC depends on its initial conditions, reminiscent of the hysteretic behaviour of RBC discussed in §1a. The chaotic state of SDC is unstable at $Pr = 4$, where multiple spiral patterns coarsen into a single spiral, before evolving into straight-curved rolls over a long period [38]. This implies that the behaviour of SDC depends on Pr .

(c) Scope of this study

The bistability between SDC and ISR is well established, but this also opens a question of how it is connected with the previous findings of multiple stable states. Note that a possible parameter in exploring this connection appears to be the domain size. Bistability has been reported in domains much larger ($\Gamma = 100$) than the multiple states found in small-to-moderate domains ($\Gamma \leq 20$) [28]. Furthermore, giant rotating spirals have been found in domains comparable to the horizontal length scale of SDC [6,12]. We consider a nonlinear dynamical systems approach in this study, well adopted in the study of transitional wall-bounded shear flows. In the context of wall-bounded shear flows, turbulence occurs subcritically, organized as chaotic trajectories evolving around the unstable manifolds of invariant solutions. These invariant solutions and their unstable manifolds offer a building-block description of turbulence, providing insights into the dynamical process of turbulence [45–51]. The scope of this study is to explore how SDC, ISRs and multiple states are linked within the state space, where stable/unstable equilibria and their manifolds (or linear stability) could provide useful physical insights into the state transition dynamics.

Motivated by the observation that SDC consists of several localized structures that resemble multiple states (i.e. travelling waves, spirals, asymmetric states), we first seek to isolate these states by minimizing the domain systematically. Confined within the minimal domain, SDC is found to appear only transiently and does not sustain for a long time. The transient SDC state eventually stabilizes into a large number of stable multiple states, which we refer to as the ‘elementary’ states of SDC, and they are subsequently found within the minimal domain. As we shall see later, these elementary states remarkably resemble local structures of SDC observed in wide computational domains, indicating that they possibly underpin the formation of SDC. Next, the state-space boundaries between SDC and ISRs are explored by employing the edge-tracking technique [52,53], unveiling the existence of multiple edge states sitting on the boundaries. Finally,

to understand the role of the unstable ISRs outside the Busse balloon, we perform a series of numerical experiments, in which a small perturbation is added along the unstable manifolds of several (unstable) ISRs outside of the Busse balloon. We shall see that some of their unstable manifolds are connected to stable ISRs within the Busse balloon, while the others are linked to transient SDC, which is subsequently stabilized into an elementary state. This suggests that some of the unstable ISRs act as signposts for the state-space boundary between stable ISRs and SDC (and/or elementary states).

The main contributions of the present study can be briefly summarized as follows:

- (i) discovery of a number of stable invariant solutions which underpin the localized structures of SDC by minimizing the computational domain for SDC (§3);
- (ii) computation of some of multiple ‘edge states’ sitting on the separatrix between SDC and ISRs (§4);
- (iii) several heteroclinic orbits connecting unstable ISRs and stable ISRs near the boundaries of the Busse balloon (§5a); and
- (iv) the role of unstable ISRs far from the Busse balloon acting as a signpost between ISRs and SDC (§5b).

2. Problem formulation

(a) Rayleigh–Benard convection (RBC)

We consider a buoyancy-driven flow of an incompressible fluid separated by a vertical height of d , confined between an upper wall of uniform temperature T_U and a lower wall of uniform temperature T_L . The temperature of the lower wall is higher than the temperature of the upper wall ($\Delta T = T_L - T_U > 0$) such that the fluid is unstably stratified. The fluid has a density of ρ , a thermal diffusivity of κ and a kinematic viscosity of ν . The non-dimensionalized governing equations with the Boussinesq approximation for buoyancy-driven flows are given by

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + Pr \nabla^2 \mathbf{u} + Ra Pr \theta \mathbf{j}, \quad (2.1a)$$

$$\frac{\partial \theta}{\partial t} + (\mathbf{u} \cdot \nabla) \theta = \nabla^2 \theta \quad (2.1b)$$

$$\text{and} \quad \nabla \cdot \mathbf{u} = 0, \quad (2.1c)$$

with the following boundary conditions at the wall:

$$\mathbf{u}|_{y=0,1} = 0, \quad \theta|_{y=0} = 1 \quad \text{and} \quad \theta|_{y=1} = 0, \quad (2.2a)$$

and the periodic boundary condition in the horizontal direction. Here, t denotes the time scaled by the vertical thermal diffusion time, d^2/κ , and $\mathbf{x} = (x, y, z)$ is the spatial coordinates non-dimensionalized by d , where x and z are two orthogonal horizontal directions and y is the vertical direction. $\mathbf{u} = (u, v, w)$ is the velocity vector scaled with κ/d , p the pressure scaled with $\rho \kappa^2/d^2$, $\theta \equiv (T - T_U)/\Delta T$ the non-dimensional temperature with T being the absolute temperature, and $\mathbf{j}$ denotes the unit vector in y -direction. The Rayleigh number and the Prandtl numbers are defined as in §1: $Ra = \alpha g d^3 \Delta T / \nu \kappa$, Prandtl number $Pr = \nu / \kappa$. Throughout this study, $Pr = 1$ is set, and the reduced Rayleigh number $\varepsilon = 0.7$ is considered.

(b) Numerical method

The governing equations are solved numerically using Nektar++, an open-source spectral/hp-element method framework [54]. An initial computational mesh, composed of quadrilateral elements, in the x – y plane is generated using Gmsh [55] and then refined by Nekmesh, the mesh generator available in Nektar++. Several periodic computational domains of different sizes are prepared: $(L_x, L_y, L_z) = (16\pi, 1, 16\pi), (8\pi, 1, 8\pi), (4\pi, 1, 4\pi)$. The spatial domain is discretized using

a quasi-three-dimensional (3D) approach with spectral/ hp elements in x - y domain and Fourier expansions in the z -direction. The discretized equations are subsequently solved using a velocity-correction method based on a second-order implicit–explicit temporal scheme [56–58]. Since different computational domain sizes were considered, the spatial distribution of spectral/ hp elements in the x - y plane and Fourier expansions along z was kept constant. A spatial resolution of $(\Delta x, \Delta y|_{y=0,d}, \Delta y|_{y=d/2}, \Delta z) = (0.1\pi, 0.0549, 0.367, 0.25\pi)$ with polynomial order $P=4$, and temporal resolution of $\Delta t=0.0125$ was sufficient to establish numerical independence—for example, the Nusselt number, $Nu(= -\int_{x,z} \partial\theta/\partial y|_{y=0} dx dz)$, varies less than 10^{-5} when P was increased to $P=5$.

(c) Linear stability analysis of ISRs

As discussed in §1c, we perform a set of numerical experiments, in which a small perturbation about several unstable ISRs is added along their unstable manifolds. To obtain the direction of the unstable manifolds (i.e. linear instability eigenfunctions), we consider a small perturbation about the ISR (base) state:

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{u}_{\text{ISR},q}(\mathbf{x}) + \mathbf{u}'(\mathbf{x}, t), \quad (2.3a)$$

$$\theta(\mathbf{x}, t) = \theta_{\text{ISR},q}(\mathbf{x}) + \theta'(\mathbf{x}, t) \quad (2.3b)$$

$$\text{and} \quad p(\mathbf{x}, t) = p_{\text{ISR},q}(\mathbf{x}) + p'(\mathbf{x}, t), \quad (2.3c)$$

where $\mathbf{s} = [\mathbf{u}, \theta, p]^T$, $\mathbf{s}_{\text{ISR},q} = [\mathbf{u}_{\text{ISR},q}, \theta_{\text{ISR},q}, p_{\text{ISR},q}]^T$ and $\mathbf{s}' = [\mathbf{u}', \theta', p']^T$ refer to the solution vector, the ISR (base) state of a given wavenumber, q and the perturbation, respectively. Substitution of equation (2.3) into equation (2.1) leads to the following linearized equations:

$$\frac{\partial \mathbf{s}'}{\partial t} = \mathcal{A}(\mathbf{s}_{\text{ISR},q}; Ra, Pr) \mathbf{s}', \quad (2.4a)$$

where

$$\mathcal{A}(\mathbf{s}_{\text{ISR},q}; Ra, Pr) = \begin{pmatrix} -(\mathbf{U} \cdot \nabla) - (\nabla \mathbf{U} \cdot) + Pr \nabla^2 & Ra Pr \hat{\mathbf{j}} & -\nabla \\ -(\nabla \Theta \cdot) & -(\mathbf{U} \cdot \nabla) + \nabla^2 & 0 \\ \nabla \cdot & 0 & 0 \end{pmatrix}. \quad (2.4b)$$

For the sake of simplicity here, we only consider the ISRs invariant along the z -direction. Since the ISRs are also assumed periodic in the x -direction, the following form of normal-mode solution can be considered:

$$\mathbf{s}'(\mathbf{x}, t) = \check{\mathbf{s}}(x, y) e^{i(\alpha x + \beta z) + \lambda t} + \text{c.c.}, \quad (2.5)$$

where λ, α and β are the complex frequency, the streamwise wavenumber (or the Floquet exponent) and the spanwise wavenumber, respectively (c.c. stands for complex conjugate). Using the periodic nature of $\check{\mathbf{s}}(x, y)$ in the x -direction, equation (2.5) can also be written as

$$\mathbf{s}'(\mathbf{x}, t) = \left[\sum_{n=-\infty}^{\infty} \check{\mathbf{s}}_n(y) e^{i \frac{2\pi}{L_x} (n+\sigma)x} \right] e^{i\beta z + \lambda t} + \text{c.c.}, \quad (2.6)$$

where $\sigma(=\alpha L_x/(2\pi))$ is the Floquet detuning parameter with $0 \leq \sigma \leq 1/2$. Since the stability analysis here is limited to the identification of unstable manifolds of ISRs in a fixed computational domain, $\sigma=0$ (fundamental mode) is considered only—note that the modes associated with $\sigma \neq 0$ are only observed in the x domains greater than L_x .

Substituting equation (2.6) into equation (2.4) leads to a discretized eigenvalue problem in terms of the eigenvalue λ , where the wavenumber in the z -direction must be restricted to be $\beta = 2\pi m/L_z$, and m is a positive integer, for the given computational domain. The resulting eigenvalue problems are solved using a time-stepper-based iterative Arnoldi algorithm [59], implemented in Nektar++, which has been verified in various applications [54]. The eigenvalues of primary instabilities of RBC computed in Nektar++ are also verified against those obtained with a Chebyshev-collocation method shown in appendix A.

3. Transient SDC and elementary states in minimal domain

In this section, we seek to capture localized structures of SDC using a minimal domain by systematically reducing the domain by half in the homogeneous (x - z) directions. A random noise, characterized by Gaussian white noise (0 mean and 1 variance), generated with a total energy of

$$\delta = \frac{1}{V} \int_{\Omega} \tilde{\mathbf{u}}(\mathbf{x})^T \tilde{\mathbf{u}}(\mathbf{x}) + RaPr\tilde{\theta}(\mathbf{x})^2 d\Omega \approx O(10^{-3}), \quad (3.1)$$

where $\tilde{\mathbf{u}}(\mathbf{x})$ and $\tilde{\theta}(\mathbf{x})$ refer, respectively, to the perturbation velocity and temperature about the base state $\mathbf{U}(\mathbf{x}) = \mathbf{0}$ and $\Theta(y) = 1 - y$, is introduced as an initial condition to the system. Here, we note that the first term of the integrand in equation (3.1) is the kinetic energy of the perturbation velocity and the second one measures the potential energy from the perturbation temperature.

The system is time integrated for 300 units of vertical thermal diffusion time t ($=d^2/\kappa$). The resulting mid-plane temperature snapshots $\theta(x, z)|_{y=d/2}$ at $t = 300$ exhibit features of spiral defect chaos, as shown in figure 1. When the domain size is large, for instance, $\Gamma = 16\pi$ shown in figure 1a, features of SDC consist of many repeating localized spirals, defects and dislocations. Reducing the domain in half to $\Gamma = 8\pi$, shown in figure 1b, led to a spatially less-extensive chaotic state, revealing a single spiral, with some defects and dislocations. Surprisingly, a further reduction of the domain in half, $\Gamma = 4\pi$, does not lead to sustained SDC, but rather, a transient SDC state before settling into stable ‘elementary’ states. These elementary states are identified as *pacman* (PM), *spiral-defect* (SD), *hooked* (HK) and *peanut* (PN) states in figure 1c–f, which resemble the localized features of SDC (see the coloured bounding boxes in figure 1a,b). We note that these illustrative names (see appendix C for a summary of acronyms) are intended to serve as a visual guide rather than referring to established terminology in the literature. These states represent stable invariant solutions of equation (2.1). Specifically, the PM state represents a steady equilibrium, the SD and HK states are characterized by relative periodic orbits,¹ and the PN state is a periodic orbit [60].

An example of a transient SDC state is shown in figure 2a, where spirals, a typical feature of SDC [22], form spontaneously with a chaotic transient (figure 2c–e), before stabilizing into an SD state with a period of $T \approx 75$ (figure 2f,g). In addition to the elementary states presented in figure 1c–f, we have identified 10 additional elementary states, each independently preceded by a transient SDC state, and 14 stable ISRs of varying wavenumbers (see appendix B). We intentionally restrict the spatial domain to identify non-trivial invariant solutions apart from ISRs. This method follows the well-established approach of the minimal flow unit of plane Couette flow [61], where non-trivial solutions within small domains exhibit coherent ‘streak-roll’ structures that reproduce the statistics of turbulent [48]. In total, we have identified 28 states with $\Gamma = 4\pi$. Minimizing the domain further to $\Gamma = 2\pi$ only led to stable ISRs at least for the random initial conditions we have examined in this study. We, therefore, consider $\Gamma = 4\pi$ as the minimal domain, in which both transient SDC and elementary states exist. Note that solutions to multiple states were obtained in smaller domains with $\Gamma = 4$, but in a cylindrical domain [10,11].

To show whether SDC and elementary states are related, we compare their state-space trajectories and the averaged wall-normal temperature profiles. Since the full state space is very high-dimensional, with its dimensionality determined by the number of degrees of freedom dictated by the spatial discretization scheme, it is, therefore, very challenging, if not impossible, to visualize the full state space in its entirety. Here, we choose the volume ($\bar{V} = L_x L_z L_y$) normalized L2-norms of velocity ($\|(1/\bar{V})\tilde{\mathbf{u}}\|_2$) and temperature ($\|(1/\bar{V})RaPr\tilde{\theta}\|_2$) perturbations as state-space observables, describing the deviation from the conduction state and providing a consistent depiction across different domain sizes, as we shall see later. Note, too, that the perturbation kinetic/thermal energies are integral quantities and, therefore, may not distinguish between states that are spatially symmetric or are translations of one another (i.e. ISRs of the same wavenumber that differ in phase). Other integral quantities, such as the Nusselt number, do not

¹Relative periodic orbit is a type of periodic orbit whereby the solution trajectory after a period T returns to its initial state that is continuously translated in the horizontal directions.

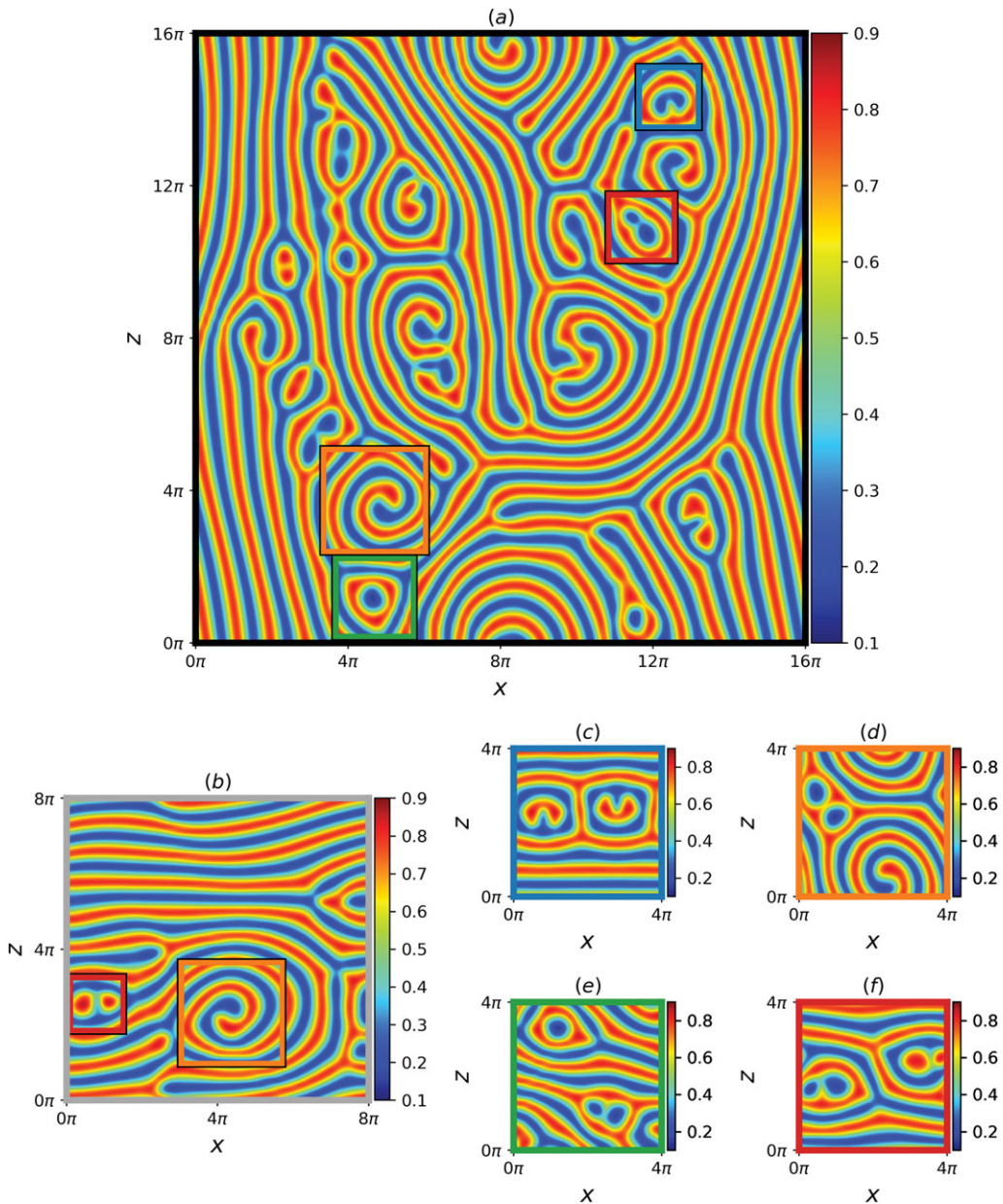


Figure 1. Mid-plane temperature snapshots, $\theta(x, z)|_{y=d/2}$, of SDC for a domain aspect ratio of (a) $\Gamma = 16\pi$ and (b) 8π . Elementary states of SDC captured when $\Gamma = 4\pi$: (c) steady *pacman* (PM), (d) relative periodic orbit *spiral-defect* (SD), (e) relative periodic orbit *hooked* (HK) and (f) periodic *peanut* (PN) elementary state. Note that the localized structures indicated by bounding boxes in (a) and (b) resemble structures in (c–f). Snapshots are captured at 300 diffusive time units, t .

provide a clear separation between SDC and ISR. We emphasize that our choice of projection does not capture the full dimensionality of the system, and our intent in using this projection is to provide a qualitative ‘slice’ of its high-dimensional dynamics. As in other studies of turbulent shear flow [48,51], low-dimensional projections are commonly used to visualize an otherwise high-dimensional state space. We also note that different choices of projection will naturally change the figures.

Figure 3 presents the two chaotic trajectories of SDC from $\Gamma = 16\pi, 8\pi, 4$ of 14 transient SDC trajectories obtained and 14 stable fixed points of ISRs from $\Gamma = 4\pi$ on a two-dimensional state

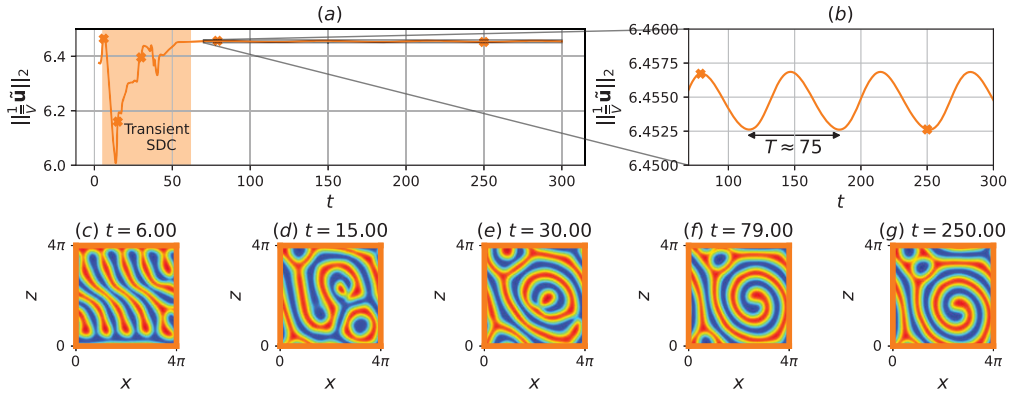


Figure 2. (a,b) Time history of the volume ($\bar{V} = L_x L_y L_z$) normalized L2-norm of velocity perturbations from a random initial condition with $\delta = 0.001$ and (c–g) mid-plane temperature snapshots at $t = 6, 15, 30, 79, 250$. Here, transient chaotic SDC lasts up to $t \approx 70$, before stabilizing into an SD state, emerging as a relative periodic orbit with the time period $T \approx 75$ propagating diagonally in the negative x - and z -directions.

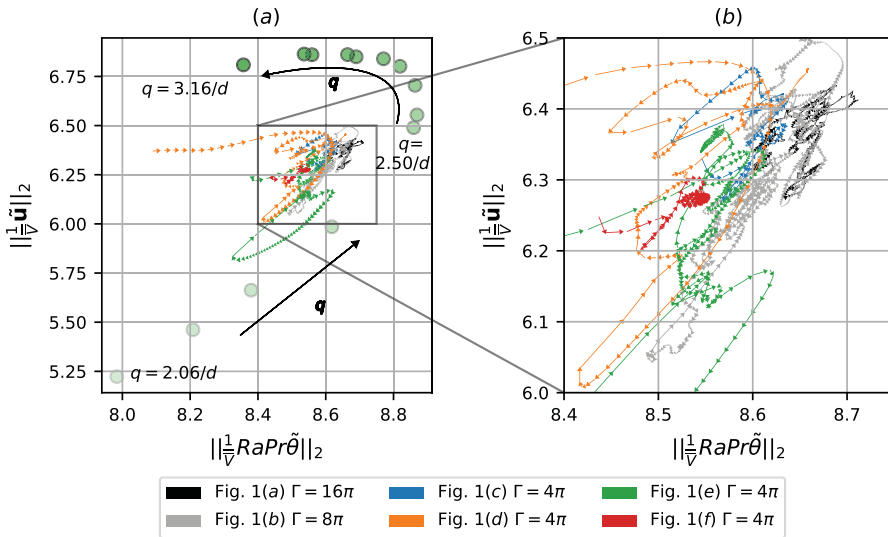


Figure 3. (a) State-space portrait in the plane of $\|(1/\bar{V})\tilde{\mathbf{u}}\|_2$ and $\|(1/\bar{V})RaPr\tilde{\theta}\|_2$ for SDC from $\Gamma = 16\pi, 8\pi$ (figure 1a,b), four transient SDC state proceeding to stable elementary states (figure 1c–f and 20), and 14 stable stationary ISRs of wavenumbers $2.0 \leq qd \leq 3.35$. Here, the magnitude of q is denoted by the opacity of the filled symbol ($\bullet$), increasing from the bottom left and turning towards the top left shown as arrows; (b) zoomed-in view of (a). The legend refers to the figures for respective trajectories preceding snapshots in figure 1.

portrait based on the volume normalized L2-norms of velocity and temperature perturbations. The trajectories begin from $t = 3$, as those for $t < 3$ contain artificial transients and are omitted for clarity. The state-space trajectories of SDC ($\Gamma = 16\pi, 8\pi$) and the transient SDC states for $\Gamma = 4\pi$ appear approximately between $(8.4, 6) \lesssim (\|(1/\bar{V})\tilde{\mathbf{u}}\|_2, \|(1/\bar{V})RaPr\tilde{\theta}\|_2) \lesssim (8.7, 6.5)$ shown in figure 3b. This suggests that they are presumably the same type of SDC emerging in different domains. The closely packed chaotic trajectories are in contrast to the ISRs populating sparsely.

The transient SDC trajectories eventually stabilize into 14 elementary states in figure 4, where the transient SDC trajectories from figure 3 are now omitted. Obscured by the transient SDC trajectories initially, the elementary states in figure 4 emerge as seven steady states ($\blacksquare$), two

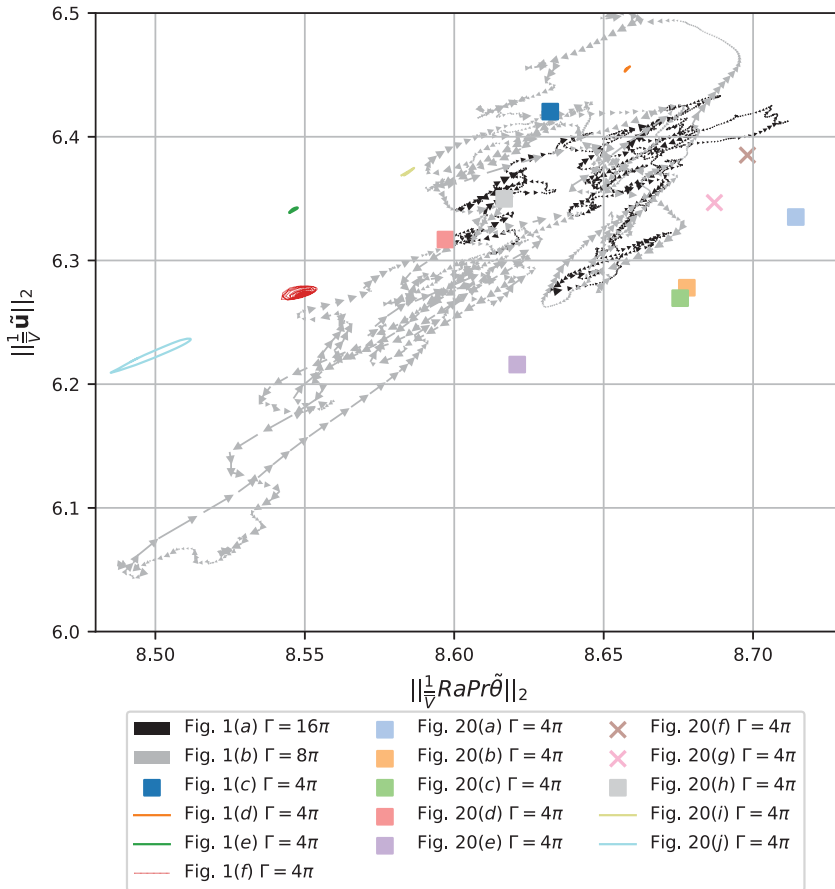


Figure 4. State-space portrait (from figure 3) highlighting the transient SDC states for $\Gamma = 4\pi$ proceeding towards stable elementary states (see figures 1c–f and 20): steady states (■), travelling waves (×), periodic orbit (dashed–dotted line) and relative periodic orbits (solid lines).

travelling waves (×), one periodic orbit (dashed–dotted line) and four relative periodic orbits (solid line). The SDC trajectories for $\Gamma = 16\pi, 8\pi, 4\pi$ appear near the 14 elementary states, approximately bounded between $(8.5, 6) \lesssim (||1/\sqrt{V}\tilde{\mathbf{u}}||_2, ||1/\sqrt{V}RaPr\tilde{\theta}||_2) \lesssim (8.7, 6.5)$ (figure 4), in contrast to the larger region occupied by ISRs between $(8, 5.25) \lesssim (||1/\sqrt{V}\tilde{\mathbf{u}}||_2, ||1/\sqrt{V}RaPr\tilde{\theta}||_2) \lesssim (8.8, 7)$ (figure 3a). Notably, the state-space trajectories of SDC and the elementary states are in close vicinity to the ISR of wavenumbers $q = 2.5/d$ (see figure 3), which corroborates the averaged wavenumber of SDC, $q_{\text{avg}} \approx 2.5/d$ [22,24].

The comparison between the time-averaged mean temperature profile, mean-squared temperature fluctuations and mean-squared velocity fluctuations of SDC (figure 1a,b) and elementary states (figures 1c–f and 20) are presented in figure 5. In figure 5c, we present the sum of mean-squared x - and z -velocity fluctuations due to horizontal isotropy. The mean temperature profiles of the elementary states closely match those of SDC (figure 5a). Notably, the mean-squared temperature and velocity fluctuations between SDC states (grey and black dashed curves) of figure 5b–d are similar. The mean-squared temperature and velocity fluctuations profiles of elementary states are comparable to those of SDC but are, in general, slightly larger in magnitude.

The spatial–temporal complexity of SDC reduces when the domain size is reduced from $\Gamma = 16\pi$ to $\Gamma = 8\pi$, i.e. less disordered spatial features. Reducing the domain from $\Gamma = 8\pi$ to $\Gamma = 4\pi$ led to transient SDC before stabilizing into many elementary states. From the conventional view, especially made in the context of shear flow turbulence, this is unexpected as the chaotic

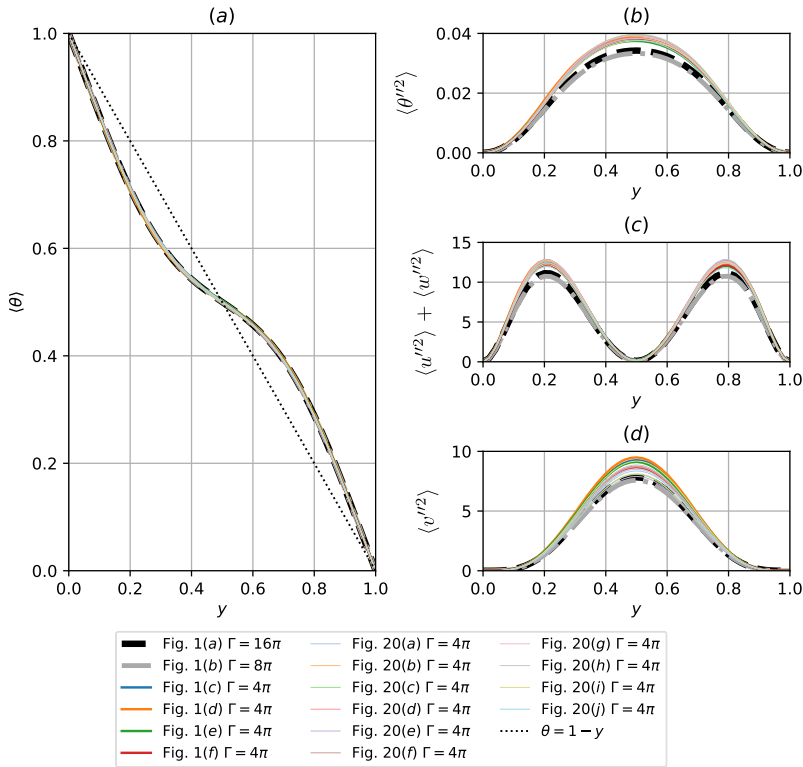


Figure 5. Profiles of (a) averaged temperature, (b) root-mean-squared temperature fluctuation, (c) sum of root-mean-squared x - z velocity fluctuations and (d) root-mean-squared wall-normal velocity fluctuations for the SDC and elementary states shown in figure 1*a–f* and in appendix B. Note that $\langle \cdot \rangle = 1/TL_xL_z \int_{t,x,z} \times dt dx dz$ refers to the time- and plane-averaged operator, where T was chosen to be sufficiently long to ensure temporal convergence. The double-primed variable indicates the deviation from its time and plane averaged, i.e. $\theta'' = \theta - \langle \theta \rangle$.

state (i.e. turbulence) is commonly described as solution trajectories wandering around unstable invariant solutions [62–65]. However, in this particular case observed in RBC, the chaotic state (i.e. SDC) stabilized into stable invariant solutions (elementary states) instead, in contrast to shear flow turbulence where invariant solutions are expected to be unstable. Despite this distinguished feature of the state space, each of the elementary states is still seen to emerge in a spatially localized manner of SDC in an extended domain (figure 1), and their spatially averaged statistics are remarkably similar to those of SDC in extended domains (figure 5). Therefore, we consider the elementary states in the minimal domain to be the ‘building block’ structure of SDC.

4. Multiplicity of edge states

The stable nature of many ISRs and elementary states underpinning SDC implies the existence of state-space boundaries between them (i.e. edge). In this section, we perform the edge tracking between the stable manifolds of ISRs and elementary states to compute the attractors on the edge. These attractors that sit along the edge are referred to as the edge states. For the edge tracking, we use the bisection method [52,53,66], with an initial condition given by

$$\mathbf{s}_0(\mathbf{x}, t = 0) = \chi \mathbf{s}_{\text{ISR},q} + (1 - \chi) \mathbf{s}_{\text{elementary}}, \quad (4.1)$$

where $\mathbf{s}_0 = [\mathbf{u}_0, \theta_0, p_0]^T$ refers to an initial condition consisting of a weighted sum, $\chi \in [0, 1]$, between a stable ISR state, $\mathbf{s}_{\text{ISR},q}$ of a wavenumber q , and an elementary state, $\mathbf{s}_{\text{elementary}}$ where the subscript refers to its names in figure 1*c–f*.

Table 1. A summary of the edge states computed. The first two columns denote the pair of initial conditions considered for edge tracking in equation (4.1). The names and classification of the edge states are described in the third column. The last column describes the state transitioned from $s_{\text{ISR},q}$ for sufficiently large χ in equation (4.1).

$s_{\text{ISR},q}$	$s_{\text{elementary}}$	edge state	state transitioned
$s_{\text{ISR},q=2.06/d}$	$s_{\text{spiral-defect}}$	<i>jagged</i> (stationary)	transient chaos
$s_{\text{ISR},q=2.06/d}$	s_{pacman}	<i>jagged</i> (stationary)	transient chaos
$s_{\text{ISR},q=2.24/d}$	$s_{\text{spiral-defect}}$	<i>point-defect</i> (travelling wave)	$s_{\text{bubble-defect}}$
$s_{\text{ISR},q=2.24/d}$	s_{pacman}	<i>forked</i> (relative periodic orbit)	transient chaos
$s_{\text{ISR},q=3.16/d}$	$s_{\text{spiral-defect}}$	<i>skewed-varicose</i> (stationary)	transient chaos
$s_{\text{ISR},q=3.16/d}$	s_{pacman}	<i>skewed-varicose</i> (stationary)	transient chaos

Given the large number of stable ISRs and elementary states, we shall focus on the computation of the edge states considering three of the stable ISRs and two of the elementary states. However, in principle, the edge tracking is technically possible with other stable ISRs and elementary states. As such, in general, multiple edge states are expected. The three ISRs are related to three different wavenumbers, denoted by $s_{\text{ISR},q=2.06/d}$, $s_{\text{ISR},q=2.24/d}$, $s_{\text{ISR},q=3.16/d}$ (figure 21*b,d,j*), respectively, and the two elementary states are SD state, $s_{\text{spiral-defect}}$ (figure 1*c*), and PM state, s_{pacman} (figure 1*d*). Using this set of stable ISRs and elementary states, we aim to track the edge near $s_{\text{ISR},q}$ in the direction of $s_{\text{elementary}}$ by bisecting the initial condition with χ in equation (4.1), whereby one of the two trajectories across the edge decays towards $s_{\text{ISR},q}$ and the other is attracted towards the transient chaotic state (i.e. SDC), referred to as the ‘lower’ and ‘upper’ trajectories, respectively. The bisection of the initial condition is carried out by monitoring the difference in two trajectories with Nu (i.e. ΔNu). When the two trajectories reach a certain time at which $\Delta Nu > 0.0007$, the bisection of the initial condition is repeated using the flow fields from the two different trajectories by replacing $s_{\text{ISR},q}$ and $s_{\text{elementary}}$ in equation (4.1) with them. This process is repeated until the edge trajectory reaches an attractor (i.e. an edge state).

Table 1 lists a summary of the edge states and their dynamical properties computed from six combinations of $s_{\text{ISR},q}$ and $s_{\text{elementary}}$ states, and they are visualized with the mid-plane temperature field in figure 6. The convection patterns of edge states are often featured with mild spatial complexity compared to SDC and the elementary states. In particular, their patterns contain the underlying convection pattern of $s_{\text{ISR},q}$ with spatially localized defects. We obtained four edge states: specifically, the *jagged* and *skewed-varicose* edge states are stationary, and the *point-defect* and *forked* edge states are travelling wave and a relative periodic orbit, respectively. The *jagged*, *skewed-varicose* and *forked* edge states lie on the boundary, separating the basins of attraction of stable $s_{\text{ISR},q}$ from transient SDC. In the case of the *point-defect* edge state, the solution trajectory is found to bypass the transient SDC state, directly settling into a stable elementary state characterized by bubble-like convection roll defects, $s_{\text{bubble-defect}}$. Since the *jagged*, *skewed-varicose*, *forked* edge states are similar, acting as separatrices between $s_{\text{ISR},q}$ states and transient SDC, we focus our analysis on the *jagged* edge state only, alongside the *point-defect* edge state.

Using Nu as an observable, successive bisections between $s_{\text{ISR},q=2.06/d}$ and $s_{\text{spiral-defect}}$ reveal the trajectory along the edge, as illustrated in figure 7. The trajectory along the edge spans from $t \approx 0$ –15 and is initially characterized by a ‘speckled’ defect (figure 7*b*). The speckled defect grows into a spatially localized jagged-like defect as the trajectory is attracted to the *jagged* stationary edge state from $t \approx 6.5$ onwards (figure 7*c–e*). We further examine the two trajectories in the opposite directions along the unstable manifold of the *jagged* edge state in figure 8, where the upper trajectory evolves into a transient SDC and the lower trajectory decays into the original stable $s_{\text{ISR},q=2.06/d}$ state. Starting from the upper trajectory (figure 8*a*), the spatially localized jagged defect grew in the direction normal to the roll orientation at $t = 80.5$ (figure 8*b*), contaminating the adjacent roll structure and propagating through the domain where

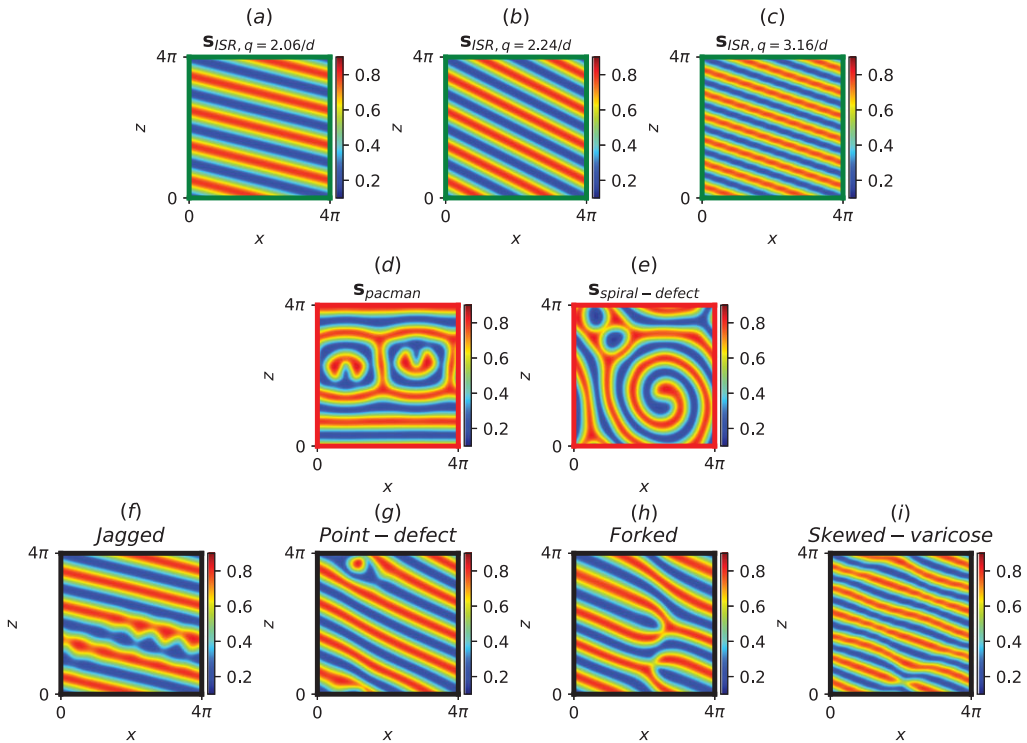


Figure 6. Mid-plane temperature fields of ISRs and elementary states used in equation (4.1), and the resulting edge states. Here, ISRs (green borders): (a) $s_{\text{ISR}, q=2.06/d}$, (b) $s_{\text{ISR}, q=2.24/d}$, (c) $s_{\text{ISR}, q=3.16/d}$; elementary states: (d) s_{pacman} , (e) $s_{\text{spiral-defect}}$; edge states (black borders): (f) *jagged*, (g) *point-defect*, (h) *forked* and (i) *skewed-varicose* edge state.

transient SDC emerges from $t > 80.5$, lasting up to $t \approx 120$ (a snapshot of transient chaotic SDC regime at $t = 90.5$ is shown in figure 8c). The trajectory subsequently stabilizes into a travelling-wave PM elementary state described by ‘pacman’ like patterns, propagating along the $-x$ direction from $t = 125.5$ to $t = 170.5$ (figure 8d,e). This is reminiscent of a secondary cross-roll instabilities experienced by low-wavenumber ISRs (such as $s_{\text{ISR}, q=2.06/d}$ considered here), where a defect propagates in the direction perpendicular to the rolls [1]. Along the lower trajectory (figure 8f), the jagged defects diffuses from $t = 70.5$ to $t = 75.5$, decaying into the stable $s_{\text{ISR}, q=2.06/d}$ state at $t = 80.5$ (figure 8g–j).

Next, we analyse the edge trajectory obtained bisecting between $s_{\text{spiral-defect}}$ and $s_{\text{ISR}, q=2.24}$ in figure 9. The trajectory along the edge from $t = 4$ (figure 9b) is described by time-dependent convection structures. The edge trajectory began to be stabilized into the *point-defect* edge state from $t = 13$ onwards (figure 9c), propagating along the x direction from $t = 22.5$ (figure 9d,e). It is characterized by the convection structure of the $s_{\text{ISR}, q=2.24}$ state with a pointed defect structure, hence referred to as the *point-defect* edge state. The upper and lower trajectories through two opposite directions of the unstable manifold of the travelling wave *point-defect* edge state are subsequently examined in figure 10. Integrating along the upper trajectory (figure 10a), the spatially localized point-defect structure grew from $t = 43$ to $t = 83$ (figure 10b–d), saturating into a stationary elementary state at $t = 163$ (figure 10e) characterized by $s_{\text{ISR}, q=2.24}$ with a large bubble defect. Along the lower trajectory (figure 10f), the spatially localized point defect merged onto the adjacent convection roll from $t = 38$ to $t = 44.5$ (figure 10g–i), stabilizing into the $s_{\text{ISR}, q=2.24/d}$ state at $t = 53$ (figure 10j). Note that, in this particular case, no chaotic transient in the form of SDC has been observed.

Finally, figure 11 depicts a state-space portrait of stable ISRs, SDC and the edge/elementary states found here. As seen previously, SDC and elementary states appear between $(8.5, 6.1) \lesssim$

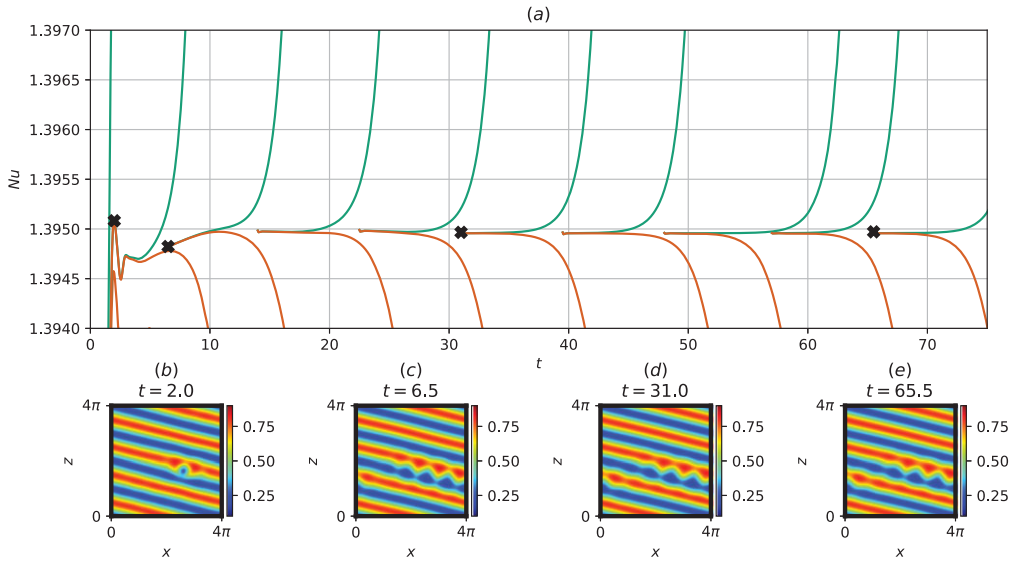


Figure 7. (a) Time history of Nu and (b–e) the corresponding mid-plane temperature field snapshots at $t = 2.0, 6.5, 31.0, 65.5$ along the edge trajectory obtained by bisecting $s_{\text{ISR},q}=2.06/d$ and $s_{\text{spiral-defect}}$.

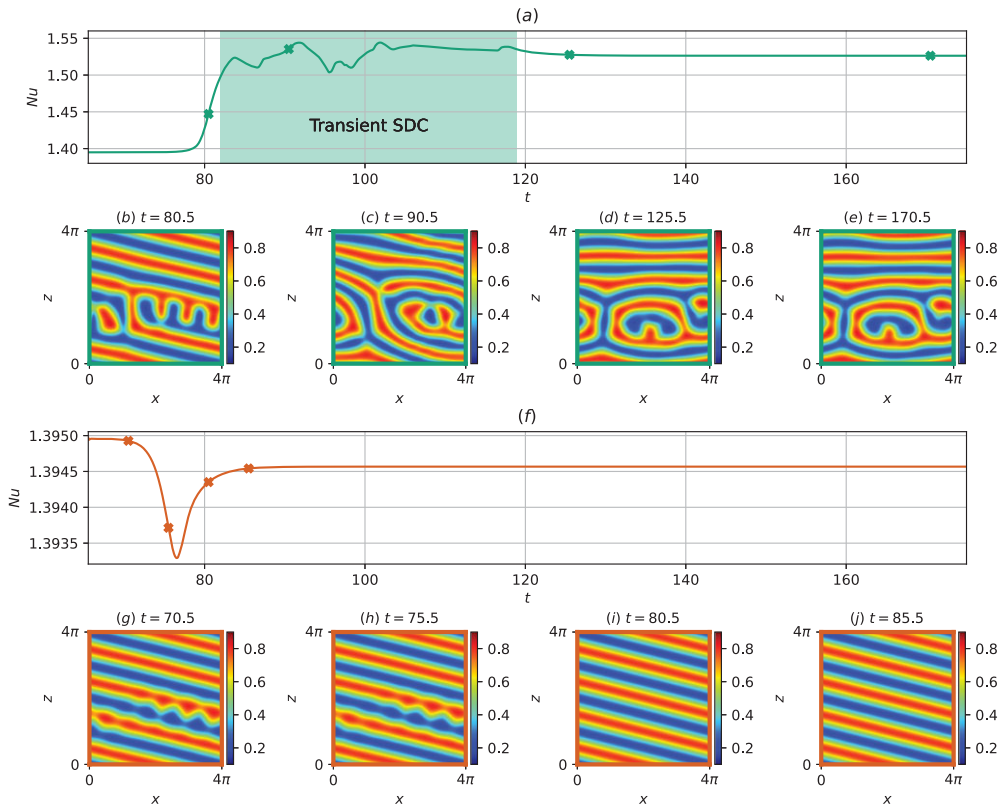


Figure 8. Time history of Nu along two opposite directions along the unstable manifold of the *jagged* edge state: (a) upper trajectory leading to a transient SDC for $t \approx 85 - 120$ and subsequently to PM state for $t > 120$ and (f) lower trajectory stabilizing into $s_{\text{ISR},q}=2.06/d$. Mid-plane temperature fields are visualized in (b–e) along the upper trajectory at $t = 80.5, 90.5, 125.5, 170.5$, and in (g–j) along the lower trajectory at $t = 70.5, 75.5, 80.5, 85.5$.

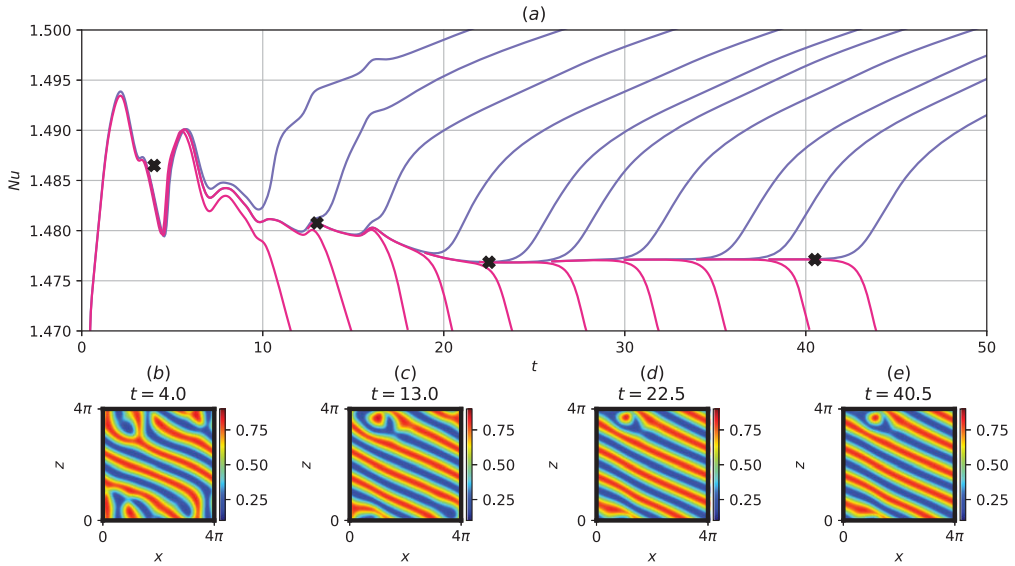


Figure 9. (a) Time history of Nu and (b–e) the corresponding mid-plane temperature field snapshots at $t = 4, 13, 22.5, 40.5$ along the edge trajectory obtained by bisecting $s_{\text{SR},q=2.24}$ and $s_{\text{spiral-defect}}$.

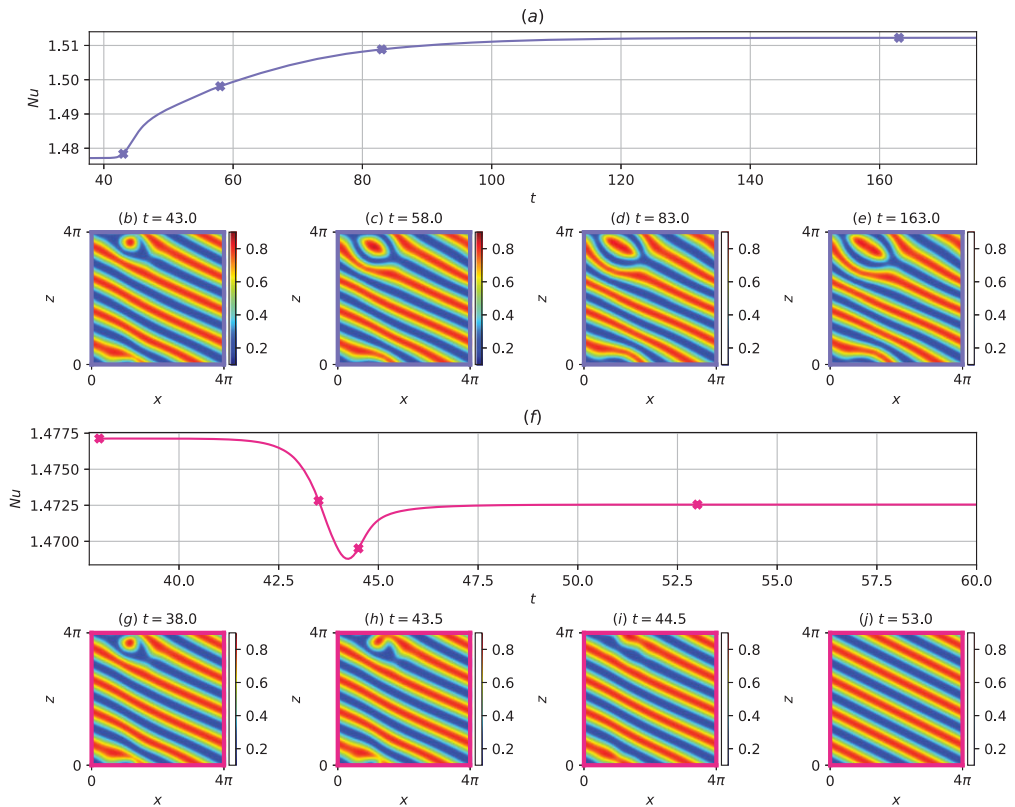


Figure 10. Time history of Nu along two opposite directions of the unstable manifold of the *point-defect* edge state: (a) upper trajectory leading a stationary elementary state with bubble defect from $t \approx 43 - 163$ and (f) lower trajectory decaying to the stable $s_{\text{SR},q=2.24}$ state. Mid-plane temperature fields are visualized in (b–e) along the upper trajectory at $t = 43.0, 58.0, 83.0, 163.0$, and in (g–j) along the lower trajectory at $t = 38.0, 43.5, 44.5, 53.0$.

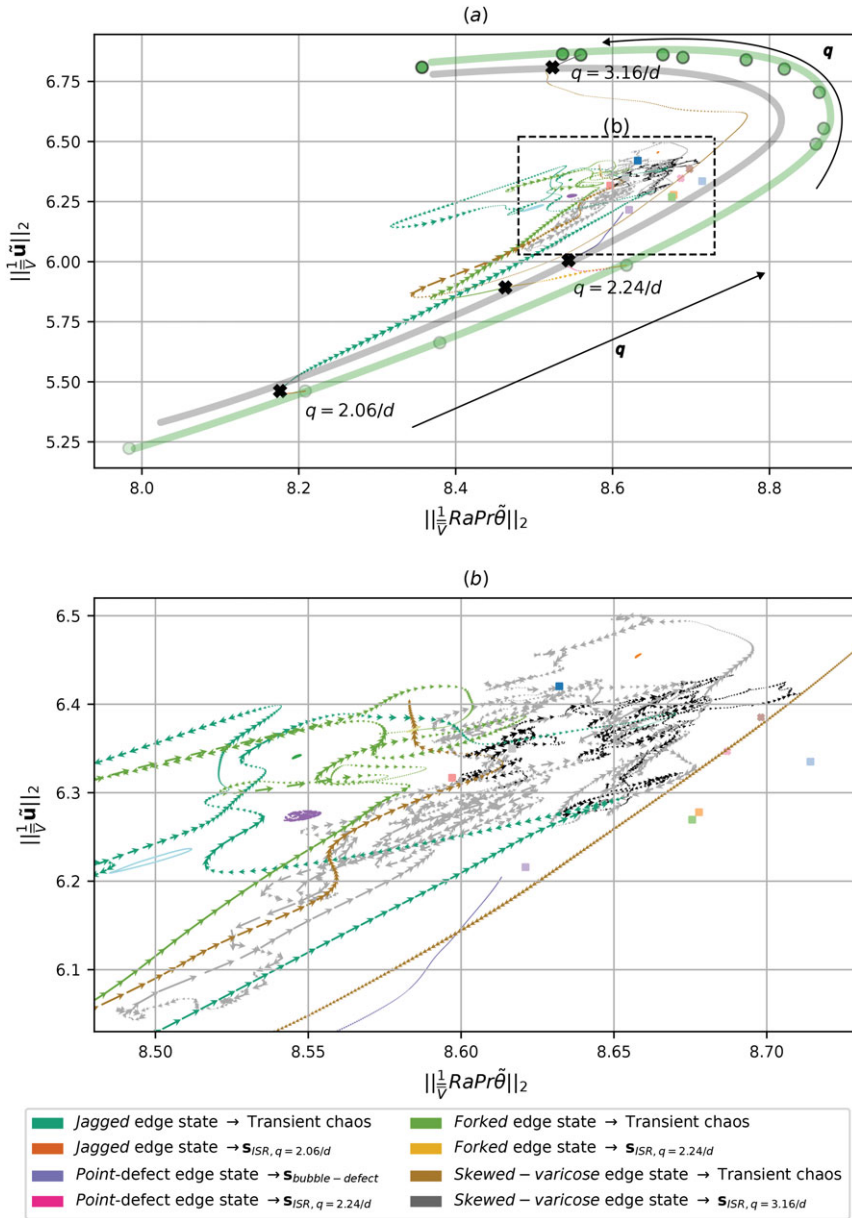


Figure 11. Phase portrait of the *jagged*, *point-defect*, *defect* and *skewed-varicose* edge states, along with stable ISRs, elementary states and transient SDC (based on the colour scheme from figure 4). Green and grey horseshoe lines are the regions, where stable ISRs and edge attractors are expected to be distributed when different sizes of the computational domain are considered. Panel (b) is a zoomed-in plot of panel (a). The arrows are plotted at every $t = 1$ interval with sizes that provide a qualitative representation for the rate of change of trajectories.

$(\| (1/\bar{V})\tilde{u} \|_2, \| (1/\bar{V})RaPr\tilde{\theta} \|_2) \lesssim (8.7, 6.5)$, whereas stable ISRs are distributed along a horseshoe-shaped band (green line), occupying a larger region $(8.8, 6.75) \lesssim (\| (1/\bar{V})\tilde{u} \|_2, \| (1/\bar{V})RaPr\tilde{\theta} \|_2) \lesssim (8.8, 6.75)$, consistent with figure 3. Note that the edge states we found here contain the underlying ISR structure ($\mathbf{s}_{q=2.06/d, 2.24/d, 3.16/d}$) modified by spatially localized defects and ‘pinches’ between rolls, supporting its proximity with ISRs in the state space. This feature is also reminiscent of spatially localized edge states identified in boundary-layer flows [66]. Finally, we would like to emphasize that we have only considered initial conditions from the states between $\mathbf{s}_{ISR, q}$ and

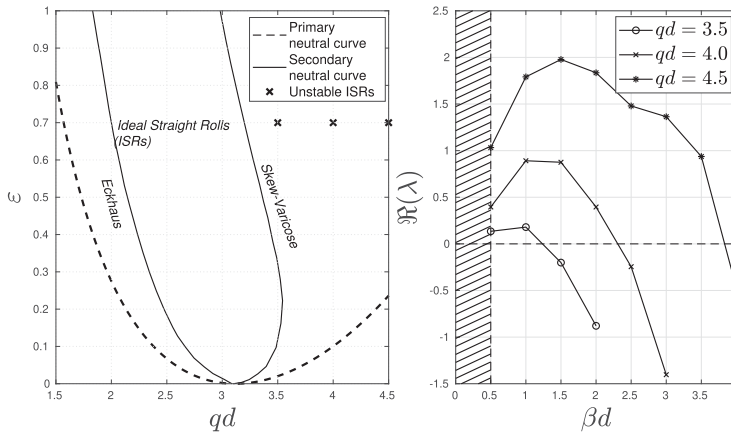


Figure 12. (a) Primary and secondary (Busse balloon from figure 1 [24]) stability curves and unstable ISRs with $q = 3.5/d, 4.0/d, 4.5/d$ and (b) variation of the growth rate of instabilities of unstable ISRs as a function of spanwise wavenumber β . (Note that there are a total 13 unstable eigenmodes. Linear stability analysis has been omitted in the shaded region for wavenumbers smaller than the fundamental wavenumber ($\beta d = 0.5$) of the minimal domain ($\Gamma = 4\pi$).

elementary and not strictly between $\mathbf{s}_{\text{ISR},q}$ and a transient SDC state. Nevertheless, three of the edge states are found to lie on the boundary separating the stable ISRs from transient SDC, supporting previous findings that the transient chaotic SDC are related to elementary states.

5. Unstable ideal straight rolls

Thus far, we have studied the edge and the edge states between some of the stable ISRs and elementary states. The dynamics associated with the unstable ISRs outside of the Busse balloon, however, remain unclear [67]. Given that the stable ISRs and SDC form a bistable system, it is expected that some of the unstable ISRs near the Busse balloon would asymptotically reach one of the stable ISRs as the difference between the stable and unstable ISRs would be sufficiently small [2,3]. On the other hand, the unstable ISRs, which exist far from the boundary of the Busse balloon, may well have a sufficiently large deviation from the stable ISRs, implying that they are possibly associated with a state-space route to the SDC. The purpose of this section is to test this hypothesis by examining the long-term behaviour of the linear instabilities of the unstable ISRs.

We consider the linear instabilities of three unstable ISRs on the right-hand side of the Busse balloon, with increasing wavenumber of $q = 3.5/d, 4.0/d, 4.5/d$, as shown in figure 12a. The identification of the linear instability mode (or unstable manifold) with the different spanwise wavenumbers β is considered (see equation (2.6)). Figure 12b presents the unstable eigenvalues as a function of β . There are two, four and seven unstable eigenmodes ($\Re(\lambda) > 0$) for unstable ISRs of $q = 3.5/d, 4.0/d, 4.5/d$, respectively, forming total 13 unstable eigenmodes. In general, the growth rate and the number of linear instability modes (i.e. the repelling strength and the number of unstable manifolds) increase as q increases. Note that the solutions of unstable ISRs of $\mathbf{s}_{\text{ISR},q}(x, y)$ (required for linear stability analysis) are obtained by restricting the computational domain to the two-dimensional x - y plane which artificially suppresses 3D linear instabilities. We also note that the stability analysis of the unstable ISR, $q = 5.0/d$ was not considered as it quickly evolved into an unstable ISR of $q = 3.5/d$, which is discussed in section §5a.

To consider the long-term behaviour in the direction of the unstable manifolds, an initial condition,

$$\mathbf{s}_0(\mathbf{x}, t = 0) = \mathbf{s}_{\text{ISR},q}(\mathbf{x}) + \hat{\mathbf{s}}_\beta(x, y) e^{i\beta z}, \quad (5.1)$$

is prescribed to equation (2.1). Here, $\hat{\mathbf{s}}_\beta e^{i\beta z}$ is the unstable eigenmode, the amplitude of which was scaled such that its total energies (defined in equation (2.6)) of $\delta = 10^{-5}, 10^{-4}, 10^{-3}$ were

Table 2. Asymptotic state of secondary linear instabilities of $q = 3.5/d, 4.0/d, 4.5/d$. Subscripts in ISR refer to asymptotic wavenumber q , e.g. $\text{ISR}_{2.5}$ refers to ISRs with wavenumber of $q = 2.5/d$. The asymptotic behaviours of (a–c) and (d), (e) are discussed further in §5a,b, respectively.

cases	$\beta = 0.25$	$\beta = 0.50$	$\beta = 0.75$	$\beta = 1.00$	$\beta = 1.25$	$\beta = 1.50$	$\beta = 1.75$
$q = 3.5/d$	$\text{ISR}_{3.04}$	(a) $\text{ISR}_{2.50}$	stable	stable	stable	stable	stable
$q = 4.0/d$	$\text{ISR}_{2.50}$	(b) $\text{ISR}_{3.16}$	$\text{ISR}_{3.00}$	$\text{ISR}_{2.83}$	stable	stable	stable
$q = 4.5/d$	$\text{ISR}_{2.50}$	$\text{ISR}_{2.50}$	(c) $\text{ISR}_{3.00}$	$\text{ISR}_{3.20}$	(d) elementary	$\text{ISR}_{2.50}$	(e) elementary

considered. The total energy of the eigenmode, $\delta = 10^{-4}$ was found to be sufficiently small enough to ensure linear growth, while large enough to prevent other eigenmodes from being excited. Next, the initial condition is time integrated over an extended period until an asymptotic state is reached. Table 2 lists the asymptotic states of 13 linear instabilities, depicted in figure 12b, of which 11 linear instabilities led to ISRs states, forming a network of heteroclinic orbits which are discussed in §5a. Only the remaining two instabilities led to a transient SDC state before settling into an elementary state discussed further in §5b.

(a) Pathways leading to ISRs—heteroclinic orbits

In this section, the asymptotic behaviour of the most unstable linear modes of ISRs (table 2a–c) are discussed. Solution trajectories that connect two invariant states referred to as heteroclinic orbits, are shown in figure 13 which depicts the state-space plot of volume normalized L2-norms of velocity and temperature. It reveals a number of heteroclinic orbits, connecting the base state (•), stable (•) and unstable (•) ISRs. Figure 13a exhibits several solution trajectories linking the base state, stable and unstable ISRs: three orbits connecting the base state to all the stable and unstable ISRs shown, one from the ISR of $q = 3.5/d$ to that of $q = 2.5/d$, and one from the ISR of $q = 5.0/d$ to that of $q = 3.5/d$. Here, caution will need to be taken in interpreting each of the connections as a heteroclinic orbit, because there appears to be an invariant state at which the speed of the solution trajectory nearly vanishes (a sign of the existence of unstable invariant states or ghost states [68]): for example, see the solution trajectory between the ISR of $q = 3.5/d$ to that of $q = 2.5/d$ (in the inset of figure 13a), which is discussed below with figure 14. Starting from the primary base state, the system saturates into an ISR of wavenumber $q = 5.0/d$. Since this ISR is linearly unstable, it evolves into another unstable ISR of $q = 3.5/d$, before ultimately stabilizing into an ISR of $q = 2.5/d$. Next, figure 13b shows three solution trajectories connecting the base state, an unstable and stable ISR. Starting from the base state, the system transitions into an unstable ISR of $q = 4/d$ before stabilizing into an ISR of $q = 3.16/d$. Finally, figure 13c presents three solution trajectories connecting the base state, a stable and unstable ISR. Starting from the base state, it can evolve to an unstable ISR of $q = 4.5/d$ before settling into a stable ISR of $q = 3.0/d$. Figure 13 suggests that each of the stable ISRs within the Busse balloon has the basin of attraction, characterized by a web of heteroclinic orbits connecting some of the unstable ISRs outside of the Busse balloon. Note that the connections between the solutions presented here were obtained by time integrating the dominant unstable manifolds of ISRs. In practice, there are many more unstable manifolds (see table 2) which have not been presented, potentially leading to more complex networks of heteroclinic orbits that form the basin of attraction for each stable ISR.

Figure 14 describes the asymptotic behaviour with the most unstable eigenmode for $q = 3.5/d$ (table 2a) in detail, corresponding to the connection between the unstable ISR of $q = 3.5/d$ and the stable ISR of $q = 2.5/d$ in figure 13a. To observe the linear instability defined in equation (5.1), we report contribution of modal energy (figure 14a) as

$$E_k(t) = \frac{1}{2} \int_{\Omega} |\hat{\mathbf{u}}_k(t)|^2 d\Omega, \quad (5.2)$$

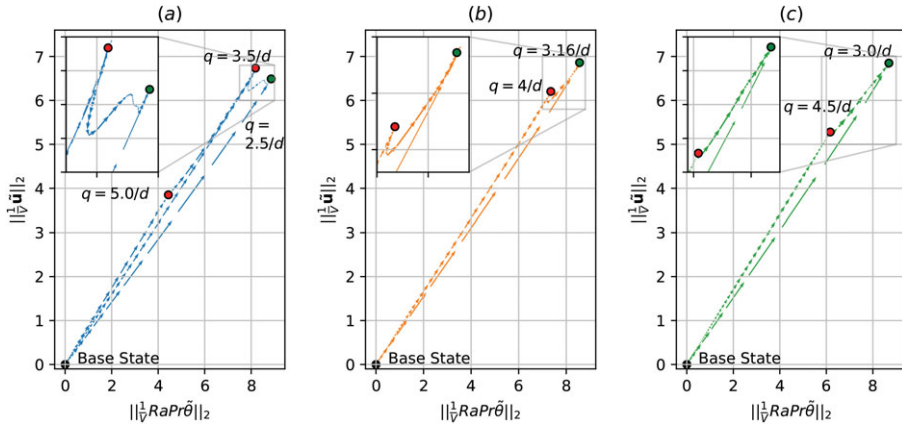


Figure 13. The phase-space solution trajectories connecting: (a) unstable base (conductive) state between 10 unstable rolls ($q = 5/d$), 7 unstable rolls ($q = 3.5/d$) and 5 stable rolls ($q = 2.5/d$) and (b) unstable base (conductive) state between eight unstable rolls ($q = 5/d$) and six stable rolls ($q = 3.16/d$); (c) unstable base (conductive) state between nine unstable rolls ($q = 4.5/d$) and six stable rolls ($q = 3/d$). Here, the size of the arrows indicates the speed of the solution trajectory (or flow).

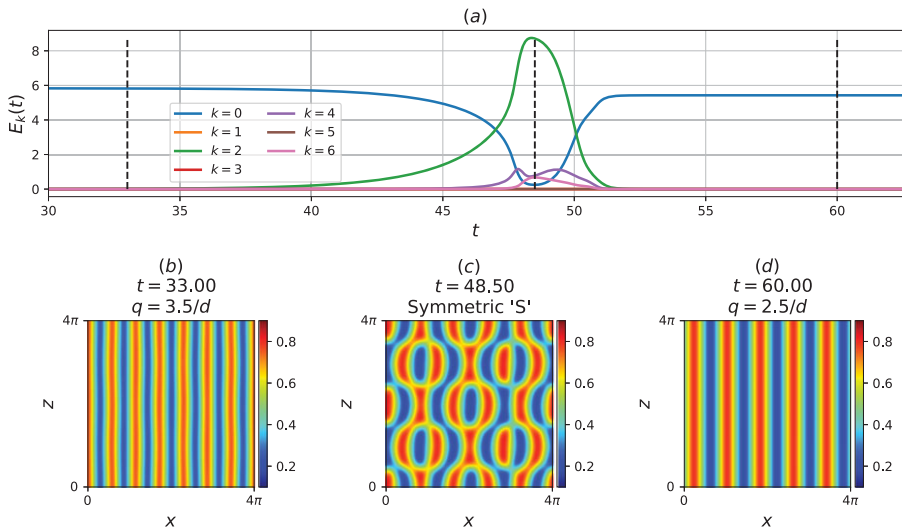


Figure 14. Asymptotic behaviour of the linear instability ($\hat{q}_{\beta=0.50}$) about unstable ISR $q = 3.5/d$. (a) Modal energy $E_k(t)$, and temperature snapshots, $\theta(x, z)|_{y=d/2}$ at (b) $t = 33$, (c) $t = 48.5$ and (d) $t = 60$.

where $\hat{u}_k$ refers to the k th Fourier coefficient in the z -direction. Initially, the simulation starts from the ISR state of seven rolls ($t = 33$), corresponding to a roll-wavenumber of $q = 3.5/d$. The unstable eigenmode $\hat{s}_{\beta=0.50}$ grows exponentially before peaking at $t = 48.50$, forming an ‘S’-like symmetric state (figure 14c). Note that, at this point, the time derivative of $E_k(t)$ nearly vanishes, indicating that the snapshot taken at $t = 48.50$ is potentially close to an unstable invariant state. Finally, the modal energy of $N_z = 2$ decays and the system settles into an ISR state of $q = 2.5/d$ (five rolls aligned in the x -direction), which is within the Busse balloon. The asymptotic behaviour along the dominant unstable eigenmode for $q = 4.0/d$ and $q = 4.5/d$ is qualitatively similar to figure 14, where an unstable ISR stabilizes into a stable ISR.

All three cases examined here show that the transition from an unstable ISR to a stable ISR involves an intermediate state, at which $dE_k(t)/dt$ is seen to be relatively small. In the transition

pathway from the unstable to stable ISR, it is presumable that there exists an unstable equilibrium (i.e. fixed point/travelling waves etc.) in the form of the original unstable ISR with its nonlinearly saturated instability, or ghost states [68]. The existence of such a stationary solution can probably be computed with a typical Newton iteration or variational methods [69,70], but this is beyond the scope of the present study. In any case, the numerical experiments here suggest that each of the stable ISR has a basin of attraction composed of a network of heteroclinic orbits involving connections between the base state and unstable ISRs.

(b) Pathways leading to elementary states

Now, we discuss the asymptotic behaviour with linear instabilities of $\hat{s}_{\beta=1.75}$ about the unstable ISR of $q = 4.5/d$ (table 2e). Contrary to the transitions presented in the previous section, the asymptotic states did not result in ISRs, but transient SDC before settling into an elementary state for case (e) (table 2e).

The asymptotic behaviour with $\hat{s}_{\beta=1.75}$ of unstable ISR $q = 4.5/d$ (table 2(e)) is presented in figure 15. Starting from $t = 1.25$, the unstable ISR state is characterized by nine convection rolls aligned along the x -axis. The state experiences the linear instability imposed from $t = 1.25$ to $t = 7$, corresponding to an exponential growth in the grey curve ($E_7(t)$ in figure 15a), marked by cross-convection rolls in figure 15c. Subsequently, the state exhibits a transient SDC behaviour from $t \approx 7$ to $t \approx 80$, characterized by an ‘O’-ring and pacman liked convection pattern illustrated in figure 15d. Following this, the system stabilizes into a short-period ($T \approx 1.8$) oscillatory behaviour between $t = 90$ and $t = 110$ (figure 15e), before transitioning into a long-period time-periodic state from $t = 110$ to $t = 201.75$ (figure 15a cont.), with a period of $T = 51.75$. The convection pattern appears to be travelling diagonally in the negative x - z directions (compare figure 15f,g), indicating that this state is a relative periodic orbit. Interestingly, the asymptotic behaviour of $\hat{s}_{\beta=1.25}$ about the unstable ISR of $q = 4.5/d$ (table 2d) also led to an elementary state.

Figure 16 presents the state-space trajectories of two pathways discussed above, represented by the volume-normalized L2-norms of velocity perturbations, temperature perturbations and Nusselt number. These trajectories are superimposed upon the state-space trajectories of SDC and 14 elementary states (figure 4). The purple trajectory represents the one along the linear instability direction (i.e. the unstable manifold) of $q = 4.5/d$ with $\beta = 1.25$. Originating from the unstable ISR ($q = 4.5/d$), briefly saturates at $\|(1/\bar{V})\tilde{u}\| \approx 6.25$ and $\|(1/\bar{V})RaPr\tilde{\theta}\|_2 \approx 8$, before stabilizing into a periodic orbit near the *spiral-defect* elementary state (see figure 1, represented by the orange trajectory in figure 4). The case of $q = 4.5/d$ along the linear instability direction for $\beta = 1.75$ is represented by the brown trajectory. Emanating from the unstable ISR ($q = 4.5/d$), the trajectory experiences a period of transient SDC behaviour in the vicinity of elementary states before converging onto a relative periodic orbit, as expected from figure 15. It is evident that the two trajectories arising from linear instabilities about the unstable ISR ($q = 4.5/d$) lie within the vicinity of SDC.

(c) A pathway to SDC in an extended domain $\Gamma = 8\pi$

In §5b, we have identified two distinct pathways to elementary states along some unstable manifolds from an unstable ISR. In particular, one of the trajectories evolved into transient SDC before stabilizing into an elementary state. This is reminiscent of a chaotic saddle, but with a considerably shorter lifetime. The transient SDC behaviour observed within the minimal domain implies that if the same initial condition is added in an extended computational domain, it would trigger a chaotic state at least with a longer lifetime. This chaotic state is expected to be SDC in an extended domain, given the analysis in §5b. To examine this hypothesis, we conduct a numerical simulation with an initial condition from the case of table 2e (i.e. the unstable ISR $q = 4.5/d$ with the instability mode of $\hat{s}_{\beta=1.75}$) in a domain twice larger than each horizontal direction ($\Gamma = 8\pi$).

The solution trajectory along the unstable manifold, $\mathbf{s}_{\beta=1.75}$, of ISR $q = 4.5/d$ in an extended domain ($\Gamma = 8\pi$) is presented in figure 17. The state, characterized by 18 convection rolls

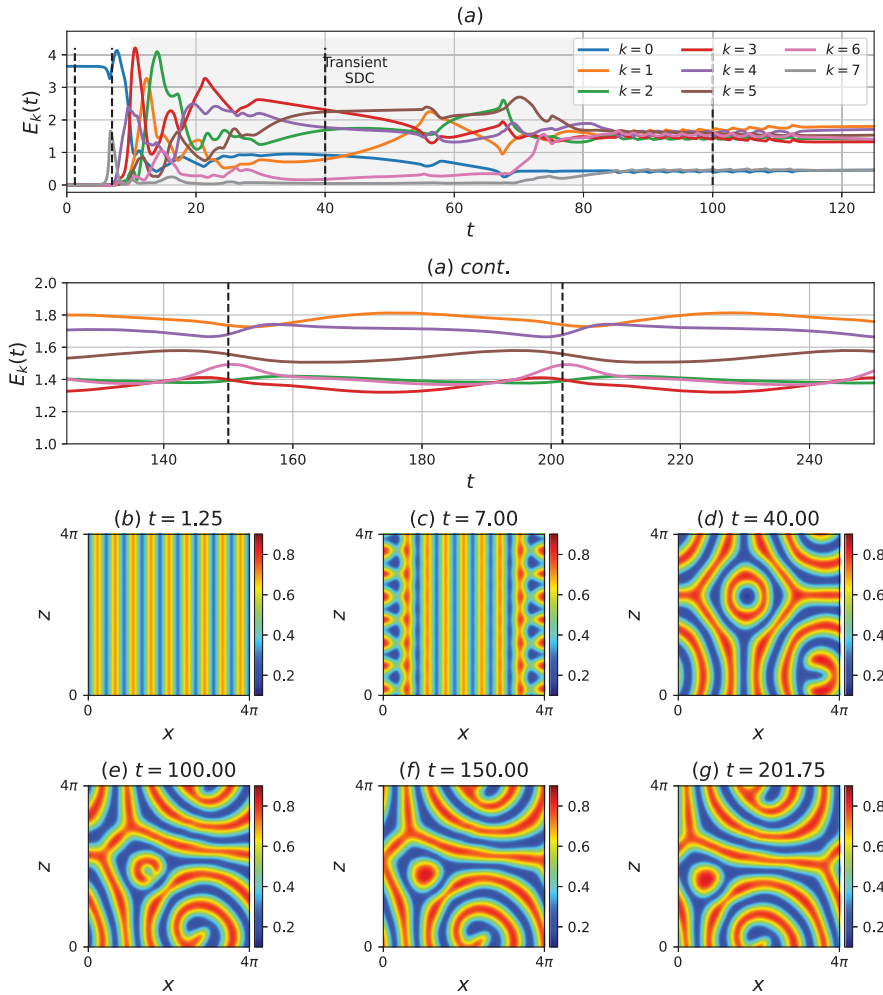


Figure 15. Asymptotic behaviour along the linear instability of $\hat{s}_{\beta=1.75}$ about unstable ISR $q = 4.5/d$. (a) Modal energy $E_k(t)$, and temperature snapshots $\theta(x, z)|_{y=d/2}$ at the onset of secondary instability at (b) $t = 1.25$, (c) $t = 7$, following a transient SDC behaviour at (d) $t = 40$, and settling into a elementary state at (e) $t = 100$, (f) $t = 150$ and (g) $t = 201.75$.

(figure 17b), experiences the linear instability from $t = 1.25$ to $t = 7$, marked by cross-convective rolls shown in figure 17c. Subsequently, the state exhibits a prolonged period of chaotic behaviour, starting from $t = 7$ and lasting beyond $t = 200$. This is in stark contrast to the transient SDC behaviour observed in the minimal domain (figure 15), confirming the hypothesis above. Finally, we note that the convection patterns of figure 17f,g contain localized structures that bear resemblance with the stationary *pacman* (figure 1c) and oscillatory *peanut* (figure 1f) elementary states.

6. Concluding remarks

SDC has been considered one of the bistable states within a large spatial domain in RBC. However, existing studies have also shown the presence of multiple stable states in small and large domains, puzzling one's understanding of the bistable system in an extended spatial domain. Starting with numerical simulation in an extended domain ($\Gamma = 16\pi$), we have systematically reduced the computational domain, such that the fundamental patterns of SDC can be isolated.

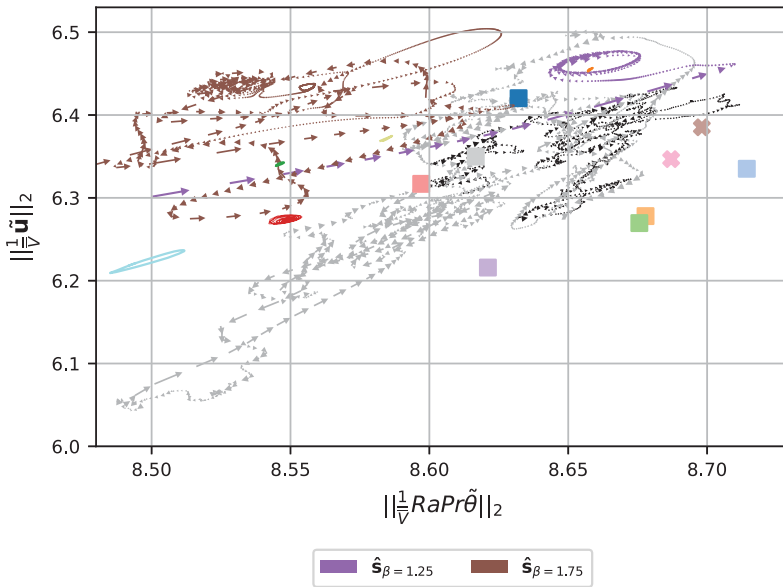


Figure 16. State-space visualizations using $\|(1/\bar{V})\tilde{u}\|_2$ and $\|(1/\bar{V})RaPr\tilde{\theta}\|_2$, of SDC, and 14 elementary states with colour schemes based upon figure 4. The trajectories of two linear instabilities (purple) $\hat{s}_{\beta=1.25}$, (brown) $\hat{s}_{\beta=1.75}$ about an unstable ISR $q = 4.5/d$ leading to elementary states (see figure 15) are shown.

Through numerical experiments confined within a minimal domain of $\Gamma = 4\pi$, we have identified transient SDC before stabilizing in/to stable elementary states of SDC, and 14 different elementary states have been found in this way. From a dynamical system perspective of turbulence in shear flow, chaotic trajectories (representing turbulence) are typically envisioned to wander among a set of unstable invariant solutions [48,50,51,69], and in some cases, may decay towards the base (laminar) state [71–73]. Our results for the chaotic trajectories of SDC in a confined spatial domain reveal a distinct scenario, where chaotic trajectories, once tangled into SDC, stabilize into a non-trivial elementary state instead of returning to the base (ISR) state. This finding is new and challenges the understanding of the transition between the conduction state and SDC from a dynamical system viewpoint. Despite this, the elementary states are still situated around the chaotic trajectories of SDC in the state space (figure 4), and their statistical properties (figure 5) and localized spatial structures (figure 1) are similar to those of SDC. This suggests that the computed elementary states may serve as spatially local building block structures of SDC that interact with each other to form SDC in an extended domain. Within the minimal domain $\Gamma = 4\pi$, we have identified 14 stable elementary states, with a possibility of additional states yet to be found. Notably, the large number of invariant states seem to be characteristic feature of Rayleigh–Bénard fluid systems such as cylindrical RBC [9,11] and inclined RBC [74,75].

To further understand the state-space structure of SDC, ISRs and possible gateways towards SDC, we furnish a state-space sketch of the solution trajectories connecting the base, stable and unstable ISRs, edge, elementary states and SDC, shown in figure 18. Starting from the base state, time integrating along the unstable manifold guided by primary instabilities leads to either stable or unstable ISRs, denoted by solid trajectories. Notably, the most unstable primary instability leads to a seven-roll ISR ($q = 3.5/d$), before saturating into a stable five-roll ISR ($q = 2.5/d$), following the most unstable secondary instability, depicted by dashed trajectories. These solution trajectories form a network of heteroclinic orbits, connecting the base state with stable ($q = 2.5/d$) and unstable ($q = 3.5/d, 5/d$) ISRs, represented in blue. Farther from the boundaries of the Busse balloon, we have identified two more heteroclinic orbits that form a basin of attraction between the base state, and stable, unstable ISRs, labelled as a group of orange and green trajectories. These

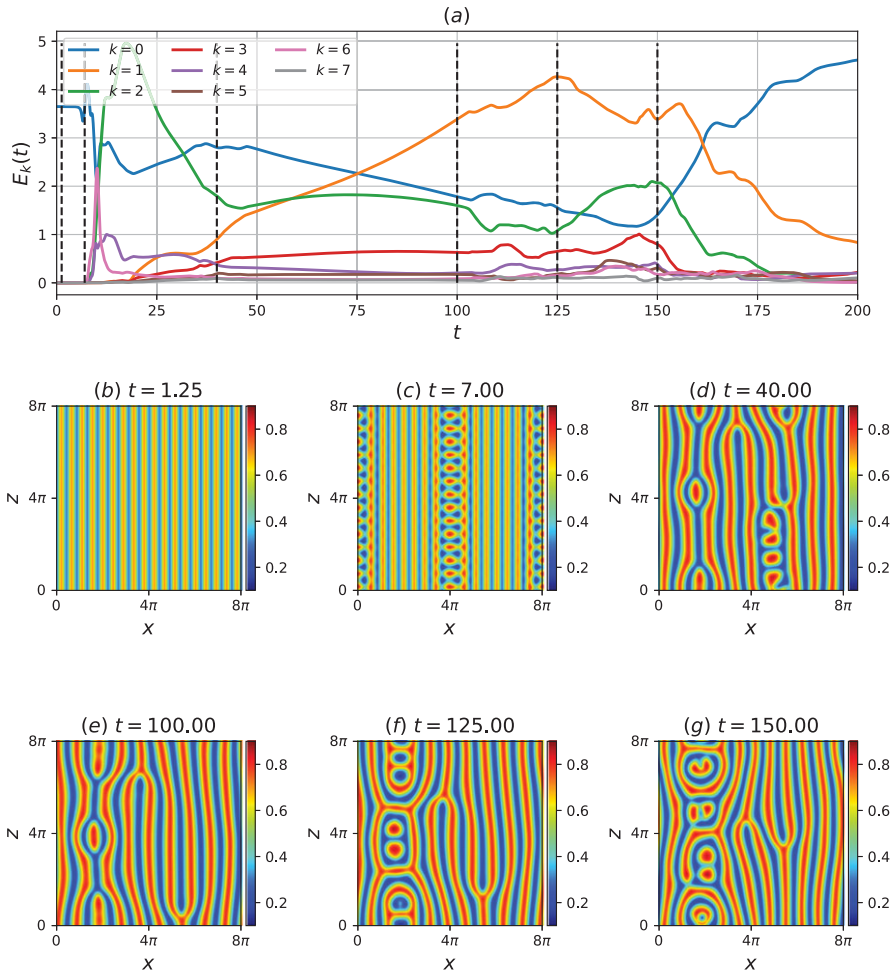


Figure 17. Asymptotic behaviour along the linear instability $\hat{s}_{\beta=1.75}$ about unstable ISR $q = 4.50/d$, in an extended domain $\Gamma = 8\pi$. (a) Modal energy $E_k(t)$, and temperature snapshots $\theta(x, z)|_{y=d/2}$, at (b) $t = 1.25$, (c) $t = 7$, (d) $t = 40$, (e) $t = 100$, (f) $t = 125$, (g) $t = 150$.

heteroclinic orbits are expected in experimental settings where initial conditions and background noise can be controlled precisely. In practice, where precise controls are inaccessible, it is more likely to observe SDC ($\Gamma = 8\pi, 16\pi$) or stable elementary states ($\Gamma = 4\pi$), which are embedded in the chaotic trajectories of SDC (see coloured squares), supporting the notion that SDC is underpinned by elementary states presumably interacting with each other.

We have identified four edge states that lie on the boundary between stable ISRs and transient SDC, where the upper and lower trajectories emerging from their unstable manifold are represented by dashed–dotted trajectories. Farther from the Busse balloon, we have identified an unstable manifold of a nine-roll ($q = 4.5/d$) ISR, leading to the onset of SDC. Consequently, the unstable base state is also expected to lie on the boundary, as a controlled initial condition could guide the system towards the unstable nine-roll ISR, and subsequently the onset of SDC. Finally, the dotted line represents the boundary between ISRs and SDC, consisting of the base state, edge states and unstable nine-roll ISR ($q = 4.5/d$), illustrating four possible routes towards SDC. Although we have considered the unstable manifolds of ISRs for $\Gamma = 4\pi$, we acknowledge that the dimension of such manifolds depends on the domain size and that the spatially subharmonic instabilities may arise as the domain size increases. In addition, there may well be other unstable

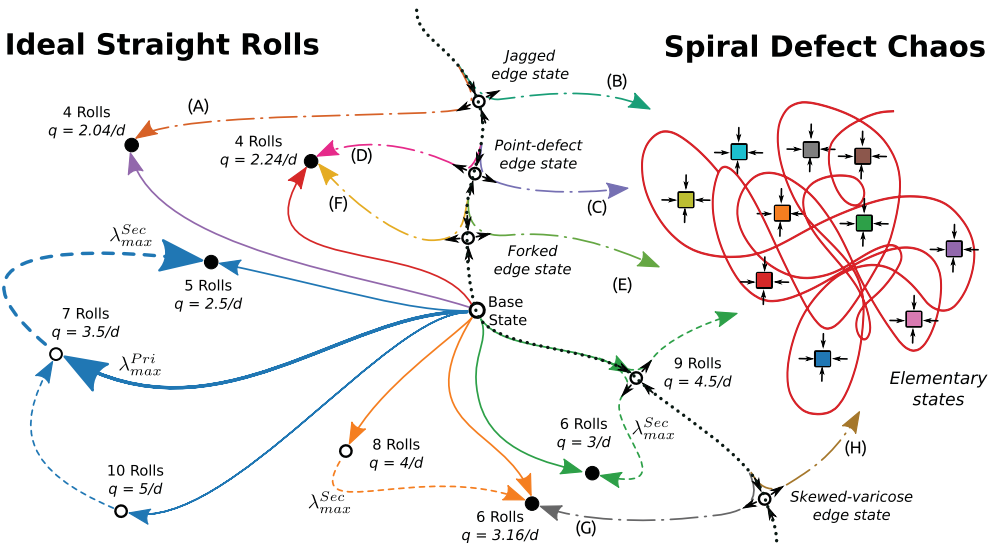


Figure 18. State-space sketch containing the base, stable and unstable ISRs, edge, elementary states and SDC in a confined domain. Open circles ($\circ$) and filled circles/squares ($\bullet$, $\blacksquare$) refer to unstable and stable states. Solid (—) and dashed lines (---) are the solution trajectories along the primary and secondary instabilities, respectively, $\lambda_{\text{Pri}}^{\text{max}}$ refers to the most unstable primary and secondary linear instability manifolds. Blue, orange and Green trajectories denote heteroclinic connections leading towards stable ISRs (trajectories labelled (A–G) and colours adapted from figure 13). Dashed–dotted trajectories (— · —) refer to solution trajectories emerging from the edge states (colour-coded from figure 11). The dotted line ($\cdots$) represents the boundary between ISRs and SDC, consisting of many stable elementary states.

ISRs and edge states along the boundary. However, the investigation into the existence of such states is challenging owing to the daunting computational efforts required. Recent advances, such as the framework proposed in [76], may help to accelerate linear stability analysis and facilitate further investigations.

Data accessibility. This article has no additional data.

Declaration of AI use. We have not used AI-assisted technologies in creating this article.

Authors' contributions. CH.C.: conceptualization, data curation, formal analysis, funding acquisition, investigation, methodology, project administration, resources, software, validation, visualization, writing—original draft; M.H.: conceptualization, project administration, resources, software, supervision, validation, writing—review and editing; S.S.: conceptualization, funding acquisition, project administration, resources, software, supervision, writing—review and editing; Y.H.: conceptualization, funding acquisition, project administration, resources, software, supervision, writing—review and editing.

All authors gave final approval for publication and agreed to be held accountable for the work performed therein.

Conflict of interest declaration. We declare we have no competing interests.

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Appendix A. Verification of linear stability analysis

Figure 19 shows the eigenvalues as a function of spanwise wavenumber β of RBC at $\varepsilon = 0.7$. The results are obtained using Nektar++ and compared against a Chebyshev-collocation method discretized by 101 Chebyshev polynomials [77].

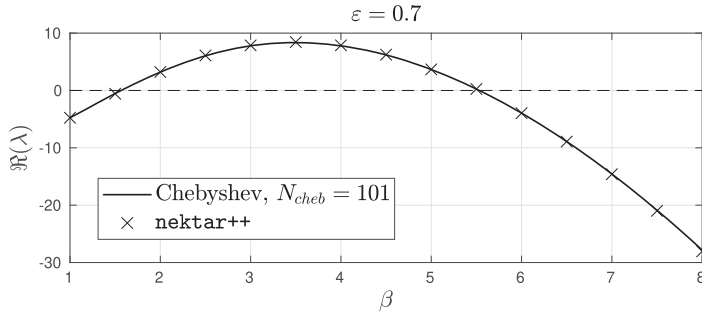


Figure 19. Eigenvalues of primary instabilities of RBC at $\varepsilon = 0.7$ computed in Nektar++ compared against a Chebyshev-collocation method with 101 Chebyshev expansions.

Appendix B. Other elementary states and ISRS

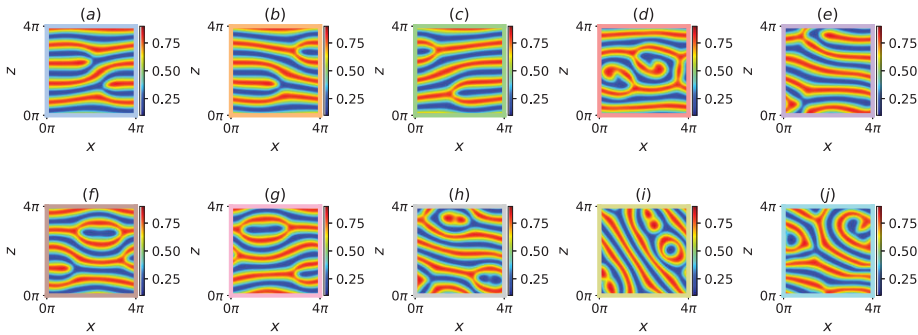


Figure 20. Temperature snapshots, $\theta(x, z)|_{y=d/2}$, of 10 elementary states confined within a minimal domain $\Gamma = 4\pi$: (a) steady ‘forked-A’ state, (b) steady ‘forked-B’ state, (c) steady ‘forked-C’ state, (d) steady ‘twin-armed’ state, (e) steady ‘tri-rolls’ state, (f) travelling-wave ‘O-a’ state, (g) travelling-wave ‘O-b’ state, (h) steady ‘keyhole’ state, (i) relative periodic orbit ‘eye’ state, (j) relative periodic orbit ‘S’ state

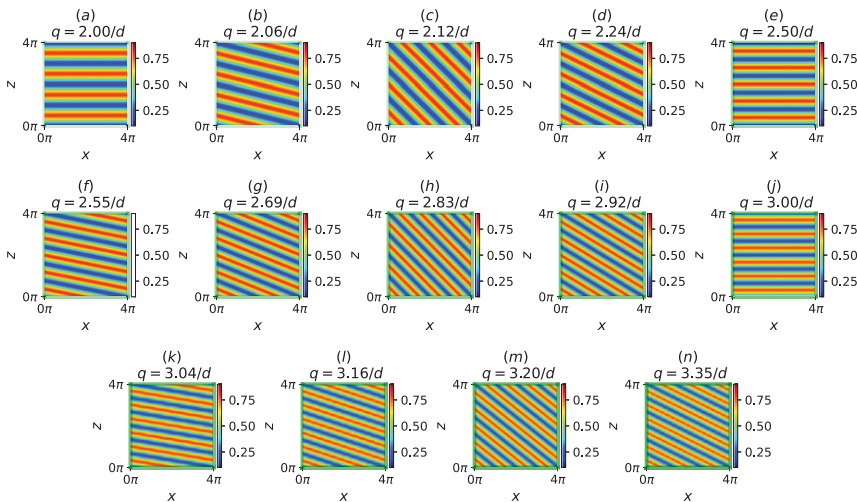


Figure 21. Temperature snapshots, $\theta(x, z)|_{y=d/2}$, of 14 stable ISRs confined within a minimal domain, $\Gamma = 4\pi$. Plots (a–n) are ordered in increasing wavenumbers, $q \in (2/d, 3.35/d)$.

Table 3. Table of acronyms.

acronyms	description
ISRs	ideal straight rolls
RBC	Rayleigh–Bénard convection
SDC	spiral-defect chaos
PM	pacman
SD	spiral defect
HK	hooked
PN	peanut

Figure 20 presents snapshots of temperature slices ($\theta(x, z)|_{d/2}$), depicting 10 distinct elementary states. These states are obtained within a minimal domain $\Gamma = 4\pi$, consisting of eight stationary states (figure 20*a–h*) and two travelling-wave states (figure 20*i* and *j*). Figure 21 features a snapshot of 14 ISRs, and they satisfy rotational symmetry about the y -axis and mirror symmetries about the x - and z -axes owing to the horizontal isotropy of the present system. These ISRs represent stable fixed points in the state space of figures 3, 4, 11 and 16.

Appendix C. Acronyms

Table 3 shows describes the acronyms used in this work.

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