


Bifurcation analysis of two-dimensional Rayleigh-Bénard convection using deflationN. Boullé^{✉,*}, V. Dallas^{✉,†} and P. E. Farrell^{✉,‡}*Mathematical Institute, University of Oxford, Woodstock Road, Oxford OX2 6GG, United Kingdom* (Received 21 February 2021; revised 17 April 2022; accepted 22 April 2022; published 18 May 2022)

We perform a bifurcation analysis of the steady states of Rayleigh-Bénard convection with no-slip boundary conditions in two dimensions using a numerical method called deflated continuation. By combining this method with an initialization strategy based on the eigenmodes of the conducting state, we are able to discover multiple solutions to this nonlinear problem, including disconnected branches of the bifurcation diagram, without the need for any prior knowledge of the solutions. One of the disconnected branches we find contains an S-shaped curve with hysteresis, which is the origin of a flow pattern that may be related to the dynamics of flow reversals in the turbulent regime. Linear stability analysis is also performed to analyze the steady and unsteady regimes of the solutions in the parameter space and to characterise the type of instabilities.

DOI: [10.1103/PhysRevE.105.055106](https://doi.org/10.1103/PhysRevE.105.055106)**I. INTRODUCTION**

This paper considers the bifurcations of the two-dimensional Rayleigh-Bénard convection, which supports a profusion of states. There have been numerous investigations trying to visualize solutions and characterize the steady states of Rayleigh-Bénard convection, as well as computing its bifurcation diagrams with respect to Ra , the Rayleigh number, in various settings and for different geometries [1,2]. Ouertatani *et al.* [3] performed numerical simulations of Rayleigh-Bénard convection in a square cavity using the finite volume method and computed fluid flow profiles and temperature patterns at $Ra = 10^4, 10^5, 10^6$. Numerical studies have been conducted to understand the existence of bifurcating solutions to this problem in a two-dimensional domain with periodic boundary conditions in the horizontal direction [4,5]. Mishra *et al.* [6] analyzed the effect of low Prandtl number on the bifurcation structures, while Peterson [7] used arclength continuation [8] to study the evolution of cell solutions with respect to the aspect ratio of the domain. Bifurcation structures of Rayleigh-Bénard convection have been extensively studied in cylindrical geometry by Ma *et al.* [9] as well as by Borońska and Tuckerman [10,11]. In particular, Refs. [10,11] adapted a time-dependent code to perform branch continuation and then analyzed the linear stability of the computed solutions using Arnoldi iterations [12]. Finally, Puigjaner *et al.* [13,14] computed bifurcation diagrams for Rayleigh-Bénard convection in a cubical cavity over different intervals of $Ra < 1.5 \times 10^5$.

A common way to reconstruct bifurcation diagrams is to use arclength continuation and branch switching techniques [8,15,16] to continue known solutions in a given parameter. These solutions can be computed by applying Newton's

method to suitably chosen initial guesses or by using time-evolution algorithms. A standard numerical technique in fluid dynamics for finding initial states for the continuation algorithm is to perform time-dependent simulation of initial solutions until a steady state is reached [17–19]. These numerical techniques have been widely used and are extremely successful at computing bifurcation diagrams of nonlinear partial differential equations (PDEs).

In this paper we employ a recently developed algorithm called deflation for computing multiple solutions to nonlinear PDEs [20,21]. This method has been successfully applied to compute bifurcations to a wide range of physical problems such as the deformation of a hyperelastic beam [21], Carrier's problem [22], cholesteric liquid crystals [23], and the nonlinear Schrödinger equation in two and three dimensions [24–26]. We emphasize that deflation offers some advantages that could be combined with the standard bifurcation analysis tools. The main strength of deflation is that it detects disconnected branches, in addition to those connected to known branches. An additional advantage is that it does not require the solution of augmented problems to find new solutions. Using perturbed solutions to the linearized equations as initial conditions, we are able to discover numerous steady states of Rayleigh-Bénard convection. These solutions can be obtained without prior knowledge and regardless of the stability of the solutions.

While much progress in fluid dynamics has been made on the study of hydrodynamic instabilities, instabilities that occur when a control parameter is varied within the turbulent regime remain poorly understood [27]. The difficulty in studying such transitions arises from the underlying turbulent fluctuations which make analytical approaches cumbersome. These types of transitions resemble more closely phase transitions in statistical mechanics because the instability occurs on a fluctuating background [28]. In Rayleigh-Bénard convection, such transitions have been observed in the form of reversals of the large-scale circulation in an enclosed rectangular geometry, in both experiments and numerical simulations [29–31].

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Although we do not study the turbulent case, we investigate the bifurcations of Rayleigh-Bénard convection in an enclosed rectangular geometry to attempt to understand the genesis of the flow patterns that play the central role in flow reversals in the turbulent regime.

The paper is organized as follows. We first discuss the problem setup and the choice of parameters in Sec. II. Then, in Sec. III, we briefly review deflation and present the methods used to improve its initialization procedure and compute the linear stability of the solutions. Next we analyze the different branches discovered by deflation and their stability in Sec. IV. Finally, in Sec. V, we recapitulate the main conclusions of this study and propose potential extensions for future work.

II. PROBLEM SETUP

We consider Rayleigh-Bénard convection [32–34] in a confined fluid heated from below and maintained at a constant temperature difference $\Delta T = T - T_0$ across a two-dimensional square cell of height d . For simplicity, we employ the Oberbeck-Boussinesq approximation [35–37], in which the kinematic viscosity ν and the thermal diffusivity κ do not depend on temperature while the fluid density ρ is assumed to be constant except in the buoyancy term of the momentum equation. In this case, we assume the density to depend linearly on the temperature $\rho(T) \simeq \rho(T_0)[1 - \alpha \Delta T]$, where α is the thermal expansion coefficient. Then the governing equations of the problem are

$$\nabla \cdot \mathbf{u} = 0, \tag{1a}$$

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \text{Pr} \nabla^2 \mathbf{u} + \text{Pr} \text{Ra} T \hat{\mathbf{z}}, \tag{1b}$$

$$\partial_t T + \mathbf{u} \cdot \nabla T = \nabla^2 T, \tag{1c}$$

where $\mathbf{u} = (u, w)$ is the velocity field, T is the temperature field, p is the pressure, and $\hat{\mathbf{z}}$ is the buoyancy direction. The above equations have been nondimensionalized using $d, d^2/\kappa$, and ΔT as the relevant scales for length, time, and temperature, respectively. The two dimensionless parameters of the problem are the Rayleigh and Prandtl numbers

$$\text{Ra} = g\alpha \Delta T d^3 / \nu \kappa, \quad \text{Pr} = \nu / \kappa, \tag{2}$$

where g is the gravitational acceleration. The Rayleigh number represents the ratio of the acceleration $g\alpha \Delta T$ related to buoyancy to the stabilizing effects of ν and κ . The bifurcation parameter in the problem we study is Ra by setting $\text{Pr} = 1$. The cell is assumed to have rigid walls, with thermally conducting horizontal walls and thermally insulating sidewalls, i.e.,

$$u = w = 0, \quad x = 0, 1 \text{ or } z = 0, 1, \tag{3a}$$

$$T = 1, \quad z = 0, \tag{3b}$$

$$T = 0, \quad z = 1, \tag{3c}$$

$$\partial_x T = 0, \quad x = 0, 1. \tag{3d}$$

The trivial steady state is motionless with a negative thermal gradient through the layer,

$$\mathbf{u} = 0, \quad T = 1 - z, \tag{4}$$

and is called the conducting state. This is because the fluid acts as a conducting material. The cooler fluid near the top of

the layer is denser than the warmer fluid underneath it. The symmetries of the problem are (a) the mirror symmetry with respect to the axis $x = 1/2$,

$$[u, w, T](x, z) \rightarrow [-u, w, T](1 - x, z), \tag{5}$$

which leaves the velocity and temperature field invariant, and (b) the Boussinesq symmetry

$$[u, w, T](x, z) \rightarrow [u, -w, 1 - T](x, 1 - z), \tag{6}$$

which leaves the velocity field invariant but transforms the temperature field into its opposite. These symmetries (and the combination of both) dictate the bifurcations that the system can undergo.

III. NUMERICAL METHODS

A. Computation of multiple solutions with deflation

Steady states of Rayleigh-Bénard convection are computed using a recent numerical technique called deflation [20]. This algorithm is based on Newton’s method and can compute multiple solutions to a nonlinear system of equations $F(\phi, \lambda) = 0$, where ϕ is the solution and $\lambda \in \mathbb{R}$ is a bifurcation parameter. First, fix $\lambda \in \mathbb{R}$ and assume a solution ϕ_1 to $F(\cdot, \lambda)$ has been previously discovered by Newton’s method. One can then construct a deflated problem

$$G(\phi, \lambda) := \left(\frac{1}{\|\phi - \phi_1\|^2} + 1 \right) F(\phi, \lambda) \tag{7}$$

such that $G(\phi, \lambda)$ does not converge to zero as $\phi \rightarrow \phi_1$. The term $\mathcal{M}(\phi, \phi_1) := \|\phi - \phi_1\|^{-2} + 1$ is called a deflation operator and ensures that Newton’s method applied again to G will not converge to a previously computed solution. By adding one to the expression of the deflation operator, we impose that the new problem G behaves similarly to F away from the root ϕ_1 . This process can be repeated to obtain a set of solutions $S(\lambda)$ to a nonlinear problem $F(\phi, \lambda) = 0$ at the bifurcation parameter λ . Deflated continuation is the combination of this idea with continuation. The previously discovered solutions are continued to a new bifurcation parameter $\lambda - \Delta\lambda$: Each $\phi \in S(\lambda)$ is used as an initial guess for the deflation procedure in order to construct a new set of solutions $S(\lambda - \Delta\lambda)$ at $\lambda - \Delta\lambda$.

We apply this algorithm repeatedly to discover multiple solutions to the steady-state Rayleigh-Bénard problem

$$\begin{aligned} F(\phi, \text{Ra}) &:= -\mathbf{u} \cdot \nabla \mathbf{u} - \nabla p + \text{Pr} \nabla^2 \mathbf{u} + \text{Pr} \text{Ra} T \hat{\mathbf{z}} = 0 \\ &:= \nabla \cdot \mathbf{u} = 0 \\ &:= -\mathbf{u} \cdot \nabla T + \nabla^2 T = 0, \end{aligned} \tag{8}$$

where $\phi = (\mathbf{u}, p, T)$ and Ra is the bifurcation parameter. This equation is discretized with Taylor-Hood finite elements for the velocity and pressure (piecewise biquadratic and piecewise bilinear, respectively), together with piecewise bilinear polynomials for the temperature, using the FIREDRAKE finite element library [38]. The unit square domain is represented by a mesh with 50×50 square cells to preserve the symmetries of the problem and avoid spurious symmetry-breaking solutions. A coarse discretization is needed due to the complexity of the problem and number of distinct solutions discovered. However, we did not observe significant differences in selected experiments where we refined the mesh.

Deflated continuation requires two different computational tasks. The first is the continuation of a previously discovered branch by the continuation step, which usually results in the convergence of the Newton solver in an average of three iterations. The convergence criterion is defined to be when the Euclidean l^2 -norm of the discretized PDE residual is below 10^{-8} . The second task is the deflation step to discover new branches. Most of the time, the solver does not converge, which means that it does not discover any new branch within the maximum number of Newton iterations allowed, which is set to 100. Typically, when the deflation step is successful, it requires around 80 iterations to find a new solution. Since the deflation step is employed for each of the steady states in the different branches, this yields at least hundreds of thousands of Newton iterations in total and a few weeks of calculation on a desktop with 32 cores. The linear systems resulting from Newton's method are solved using the sparse direct solver MUMPS [39].

A crucial question in the deflation technique is the choice of the deflation operator \mathcal{M} because it can affect the convergence of Newton's method. We use the operator

$$\begin{aligned} \mathcal{M}((\mathbf{u}, p, T), (\mathbf{u}_1, p_1, T_1)) \\ = \left(\frac{1}{\|\mathbf{u} - \mathbf{u}_1\|_2^2 + \|\nabla(\mathbf{u} - \mathbf{u}_1)\|_2^2 + \|T - T_1\|_2^2} + 1 \right), \end{aligned} \quad (9)$$

where $\|\cdot\|_2$ denotes the L^2 -norm. Note that the deflation operator \mathcal{M} does not depend on the pressure p because we wish to deflate all the solutions of the form $(u_1, p_1 + c, T_1)$, where $c \in \mathbb{R}$, to avoid discovering solutions trivially related to known ones.

We perform bifurcation analysis of Rayleigh-Bénard convection and compute solutions to the nonlinear system of Eq. (8) for $0 \leq \text{Ra} \leq 10^5$ using deflated continuation for $\text{Ra} = 10^5, 10^5 - \Delta \text{Ra}, \dots, 0$. Here ΔRa denotes the continuation step size in the bifurcation parameter, which is chosen as $\Delta \text{Ra} = 100$. In a previous work on the computation of solutions to the three-dimensional nonlinear Schrödinger equation [26], we found that having good initial guesses (e.g., solutions of the linearized problem) for the initial deflation steps facilitates the convergence of Newton's method and leads to more complex and interesting states. However, contrary to [26], we do not have the analytic expressions of the linear solutions to the Rayleigh-Bénard convection due to the no-slip boundary conditions. Therefore, we numerically solve an eigenvalue problem (see Sec. III B) to obtain the first ten unstable eigenmodes $(\mathbf{u}_1, T_1), \dots, (\mathbf{u}_{10}, T_{10})$ linearized around the conducting steady state (4) (see Fig. 2). Then the sums of the conducting state with the respective normalized perturbations $(\mathbf{u}_1, 1 - z + T_1), \dots, (\mathbf{u}_{10}, 1 - z + T_{10})$ are used as initial guesses for deflated continuation.

B. Linear stability analysis

The stability analysis of a given steady state (\mathbf{u}_0, T_0) is performed by considering the perturbation ansatz

$$\mathbf{u}(x, z, t) = \mathbf{u}_0 + \mathbf{v}e^{\lambda t}, \quad (10a)$$

$$T(x, z, t) = T_0 + \theta e^{\lambda t}, \quad (10b)$$

where the velocity perturbation $\mathbf{v} \ll 1$ and the temperature perturbation $\theta \ll 1$ have an eigenvalue λ , whose real part is the growth rate and imaginary part is the frequency of the corresponding eigenvector. When at least one of the eigenvalues has a positive real part $\mathcal{R}(\lambda) > 0$, we can have two types of instabilities: to a real eigenmode, occurring when the imaginary part of the eigenvalue $\mathcal{I}(\lambda) = 0$, and to a complex eigenmode, occurring when $\mathcal{I}(\lambda) \neq 0$. If all the eigenvalues have negative real parts, then the steady state is stable. Inserting Eq. (10) into Eq. (1) and considering the linearized system of equations, we obtain the generalized eigenvalue problem at leading order

$$\begin{pmatrix} A & -\nabla & \text{Ra Pr} \hat{\mathbf{z}} \\ \nabla \cdot & 0 & 0 \\ -\nabla T_0 \cdot & 0 & \nabla^2 - \mathbf{u}_0 \cdot \nabla \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ p \\ \theta \end{pmatrix} = \lambda \begin{pmatrix} I & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & I \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ p \\ \theta \end{pmatrix}, \quad (11)$$

where I is the relevant identity operator and A is the linear operator defined by

$$A\mathbf{v} = \nabla^2 \mathbf{v} - \mathbf{u}_0 \cdot \nabla \mathbf{v} - \mathbf{v} \cdot \nabla \mathbf{u}_0.$$

The eigenvalue problem described in Eq. (11) is solved with a Krylov-Schur method [40] using the SLEPC library [41].

To obtain the critical value of the Rayleigh number Ra_c at which the conducting state (4) becomes unstable, we modify the eigenvalue problem in Eq. (11). Inserting Eq. (4) into Eq. (11), we obtain the generalized eigenvalue problem

$$\begin{pmatrix} \nabla^2 & -\nabla & \text{Ra Pr} \hat{\mathbf{z}} \\ \nabla \cdot & 0 & 0 \\ \hat{\mathbf{z}} \cdot & 0 & \nabla^2 \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ p \\ \theta \end{pmatrix} = \lambda \begin{pmatrix} I & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & I \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ p \\ \theta \end{pmatrix}. \quad (12)$$

A steady state becomes unstable when $\lambda = 0$ and this corresponds to the critical Rayleigh number Ra_c , which is the smallest Ra satisfying Eq. (12) for $\lambda = 0$. So, to obtain the critical value of the Rayleigh number for different base states we have reformulated the problem to a generalized eigenvalue problem for Ra_c as

$$\begin{pmatrix} \nabla^2 & -\nabla & 0 \\ \nabla \cdot & 0 & 0 \\ \hat{\mathbf{z}} \cdot & 0 & \nabla^2 \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ p \\ \theta \end{pmatrix} = \text{Ra}_c \begin{pmatrix} 0 & 0 & -\text{Pr} \hat{\mathbf{z}} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ p \\ \theta \end{pmatrix}. \quad (13)$$

In the following sections this linear analysis will be used to study the stability of the conducting state (4) and of the nonlinear steady states that we obtain from deflated continuation.

IV. RESULTS

A. Primary instabilities

In this section we analyze the stability of the conducting steady state defined by Eq. (4). We find that the first instability of this state arises at $\text{Ra}_c^{(1)} := \text{Ra}_c \approx 2586$. It is well known [42] that the critical Rayleigh number is approximately equal to $\text{Ra}_c^* \approx 1707.762$ for a domain with periodic side boundaries and no-slip top and bottom boundaries. This difference in the value of Ra_c is due to the effect of the sidewalls on the instability. This effect should decrease when the length of the domain, L , becomes large such that the behavior predicted for

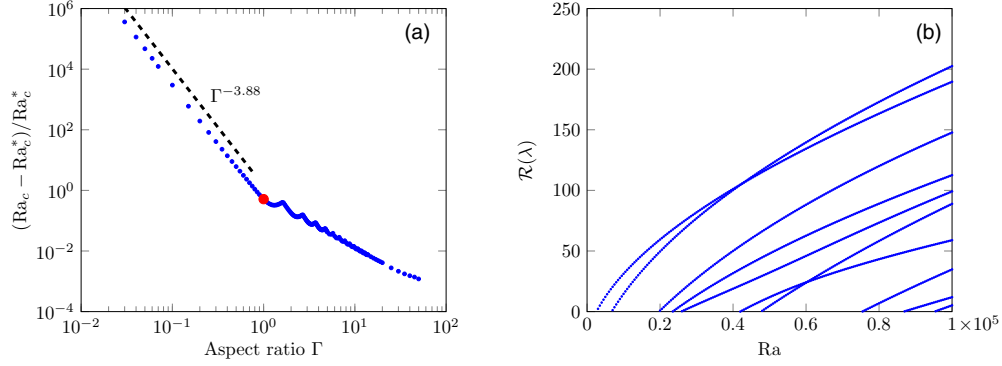


FIG. 1. (a) Critical Rayleigh number with respect to the aspect ratio Γ (blue dots). The red dot indicates the aspect ratio $\Gamma = 1$, which is the focus of our study. (b) Growth rates of the eigenmodes that emanate from the conducting steady state.

an unbounded domain is recovered. To demonstrate this, we systematically increase the aspect ratio

$$\Gamma = \frac{L}{d}. \quad (14)$$

Figure 1(a) clearly shows that for $\Gamma \gg 1$ the $Ra_c^{(1)}$ converges to Ra_c^* . In addition, for aspect ratios $\Gamma < 1$ we observe $Ra_c \propto \Gamma^{-3.88}$. The critical Rayleigh number for Rayleigh-Bénard convection with stress-free boundary conditions is $Ra_c^*(k) = (\pi^2 + k^2)^3/k^2$ [43], where k is the horizontal wave number. For $k \gg 1$ the critical Rayleigh number scales like $Ra_c^*(k) \propto k^4 \propto \Gamma^{-4}$ using Eq. (14). This scaling relation is very close to the observed one, which implies that the exponent is not affected much by the no-slip boundary conditions. The exponent we find is in agreement with [44].

The case on which we focus for the rest of the paper is the square cell ($\Gamma = 1$), which is denoted by a red dot in Fig. 1(a). We first study the linear stability of the conducting state (4). In the range $0 \leq Ra \leq 10^5$ we observe ten supercritical stationary bifurcations that arise from the conducting state. Figure 1(b) shows the growth rates of the unstable eigenmodes as a function of Ra . These bifurcations occur when $\mathcal{R}(\lambda) = 0$. The critical values of the Rayleigh number at the onsets are listed in Table I. Figure 1(b) demonstrates that the growth rates of the eigenmodes vary with Rayleigh number such that the curves can cross. The eigenmode which bifurcated from the

conducting state at $Ra_c^{(2)} = 6746$ ends up being the most unstable as $Ra \rightarrow 10^5$. The velocity magnitude and temperature fields of the eigenmodes from these primary bifurcations of the flow are shown in Fig. 2 with the corresponding critical Rayleigh numbers indicated on the top of each flow pattern. In Table I we characterize the flow patterns by the number of rolls (m_x, m_z) , where m_x and m_z are the number of rolls in the temperature field in the horizontal and vertical directions, respectively. Note that, due to the aspect ratio $\Gamma = 1$ of the domain, the flow pattern of the first bifurcation at $Ra_c^{(1)} = 2586$ is just a single convection roll (see Fig. 2) according to the classical result [33]. In the following sections we first analyze the branches of solutions that are created from some of these primary bifurcations before moving to disconnected branches.

B. Bifurcation diagrams

The combination of deflation and the initialization strategy presented in Sec. III A identified 43 branches for the two-dimensional steady-state Rayleigh-Bénard convection at $Ra = 10^5$, leading to 129 branches when reflections are included. Here we analyze the evolution and the linear stability of some of the branches arising from the first four excited states (see Fig. 2) as well as two disconnected branches. Moreover, we discard the mirror symmetric solutions with respect to the $x = 1/2$ and $z = 1/2$ axes (see symmetries in Sec. II). Our diagnostics for the bifurcation diagrams, representing the evolution of the steady states as a function of Ra , are the kinetic energy $\|\mathbf{u}\|_2^2$, the potential energy $\|T\|_2^2$, and the Nusselt number Nu , which are defined as

$$\begin{aligned} \|\mathbf{u}\|_2^2 &= \int \mathbf{u}^2 d^2x, & \|T\|_2^2 &= \int T^2 d^2x, \\ Nu &= \int |\nabla T|^2 d^2x. \end{aligned} \quad (15)$$

The Nusselt number characterizes the efficiency of convective heat transfer and is given by the ratio of the total heat transfer (i.e., both advective and diffusive) to the conductive heat transfer $Nu \equiv HL/\kappa d = \langle wT \rangle - \kappa \partial_z \langle T \rangle = \langle (\nabla T)^2 \rangle$, where H is the heat flux and $\langle \cdot \rangle$ stands for the area average. A Nusselt number of one represents heat transfer by pure conduction. Here the Nusselt number is essentially defined as the dissipation rate of the temperature variance (see the second

TABLE I. The ten primary bifurcations from the conductive state within the range $0 \leq Ra \leq 10^5$. Here n enumerates the eigenmodes by order of appearance as Ra increases. Here (m_x, m_z) are the number of rolls in the horizontal and vertical directions.

| n | $Ra_c^{(n)}$ | (m_x, m_z) |
|-----|--------------|--------------|
| 1 | 2586 | (1,1) |
| 2 | 6746 | (2,1) |
| 3 | 19655 | (3,1) |
| 4 | 23346 | (2,2) |
| 5 | 25780 | (1,2) |
| 6 | 41772 | (3,2) |
| 7 | 47431 | (4,1) |
| 8 | 74878 | (4,2) |
| 9 | 86313 | (2,3) |
| 10 | 94543 | (3,3) |

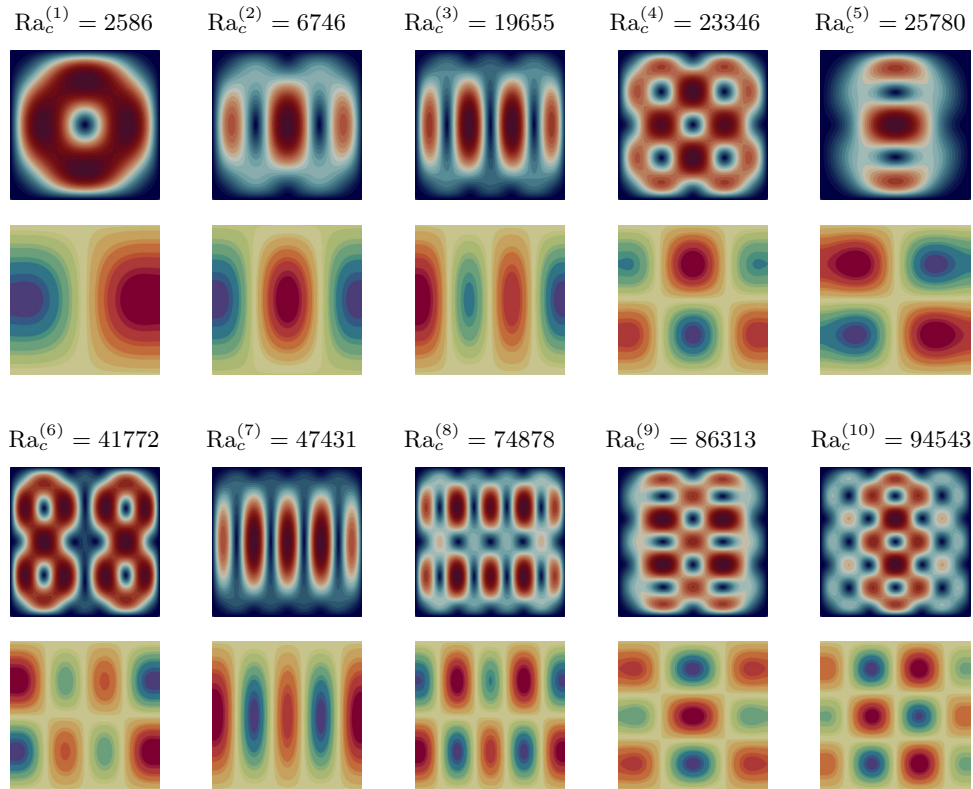


FIG. 2. Eigenmodes of the primary bifurcations emanating from the conducting steady state (4) in the Rayleigh number range $0 \leq Ra \leq 10^5$. The top rows show the magnitude of the velocity \mathbf{v} (red color indicates a high magnitude and blue a zero-velocity magnitude), while the bottom rows show the temperature θ (red and blue display positive and negative temperature values, respectively).

equality). This is obtained by integrating the equation for potential energy over the entire area [45].

The bifurcation diagrams are presented in Fig. 3, where the numbers denote the different branches of steady solutions, indicating the values of kinetic energy, potential energy, and Nusselt number that correspond to each branch on each diagram. The first steady solutions that we obtain from deflated continuation as Ra is varied are four branches that arise from the first four bifurcations of the conducting steady state: branch (1) at $Ra_c^{(1)} = 2586$, branch (2) at $Ra_c^{(2)} = 6746$, branch (3) at $Ra_c^{(3)} = 19655$, and branch (4) at $Ra_c^{(4)} = 23346$. Moreover, a secondary branch (10) bifurcates at $Ra \approx 13550$ from branch (2), which originates from the second instability of the conducting state. A similar behavior is observed for the fourth instability, where branch (6) bifurcates at $Ra \approx 27300$ from branch (4). We also focus on two disconnected branches (11) and (8) obtained directly by deflated continuation. In Fig. 3(a), branch (11) is close to branch (12). However, note that the bifurcation diagram using the potential energy [see Fig. 3(b)] shows that branch (11) does not bifurcate from branch (12). On the other hand, branch (8) bifurcates from branch (11) at $Ra \approx 37000$ (see Fig. 3). It is interesting to point out that in the range $0 \leq Ra \leq 10^5$ branch (1) has the highest kinetic energy while branch (6) has the highest potential energy [see Figs. 3(a) and 3(b)]. The steady states that are most effective in convecting heat transfer for $0 \leq Ra \lesssim 3 \times 10^4$ are in branch (1) from the first instability of the conducting state while for $3 \times 10^4 \lesssim Ra \leq 9.5 \times 10^4$ they

are in branch (2) and for $Ra \gtrsim 9.5 \times 10^4$ they are in branch (11) [see Fig. 3(c)].

C. Bifurcations from the conducting steady state

In this section we analyze the states that emanate from the conducting steady state and their evolution as a function of the bifurcation parameter Ra . Our analysis involves the detailed evolution of the velocity magnitude and the temperature on the branches of the bifurcation diagrams using the kinetic and potential energies, respectively. In addition, we present the largest growth rates and corresponding frequencies from the linear stability analysis we have performed on the steady states.

Figure 4 shows results of the aforementioned analysis for branch (1), which arises at $Ra_c^{(1)} = 2586$ from the first eigenmode (see Fig. 2). This bifurcation breaks the x -reflection symmetry but the branch has the Boussinesq symmetry. As Ra increases, the magnitude of the velocity field evolves from a circular to a bent convection roll at $Ra \approx 4 \times 10^4$ [see Fig. 4(a)]. On the other hand, the Z-shaped interface of the temperature field is sheared [see Fig. 4(b)], enhancing the heat transfer in the convection cell [see also branch (1) in Fig. 3(c)]. Figure 4(c) demonstrates that the solutions on this branch remain stable [$\mathcal{R}(\lambda) < 0$] with an almost constant growth rate over the whole range of Rayleigh numbers we consider. The frequency corresponding to the largest growth rate is zero from the stationary bifurcation at $Ra_c^{(1)} = 2586$ to $Ra = 10^5$

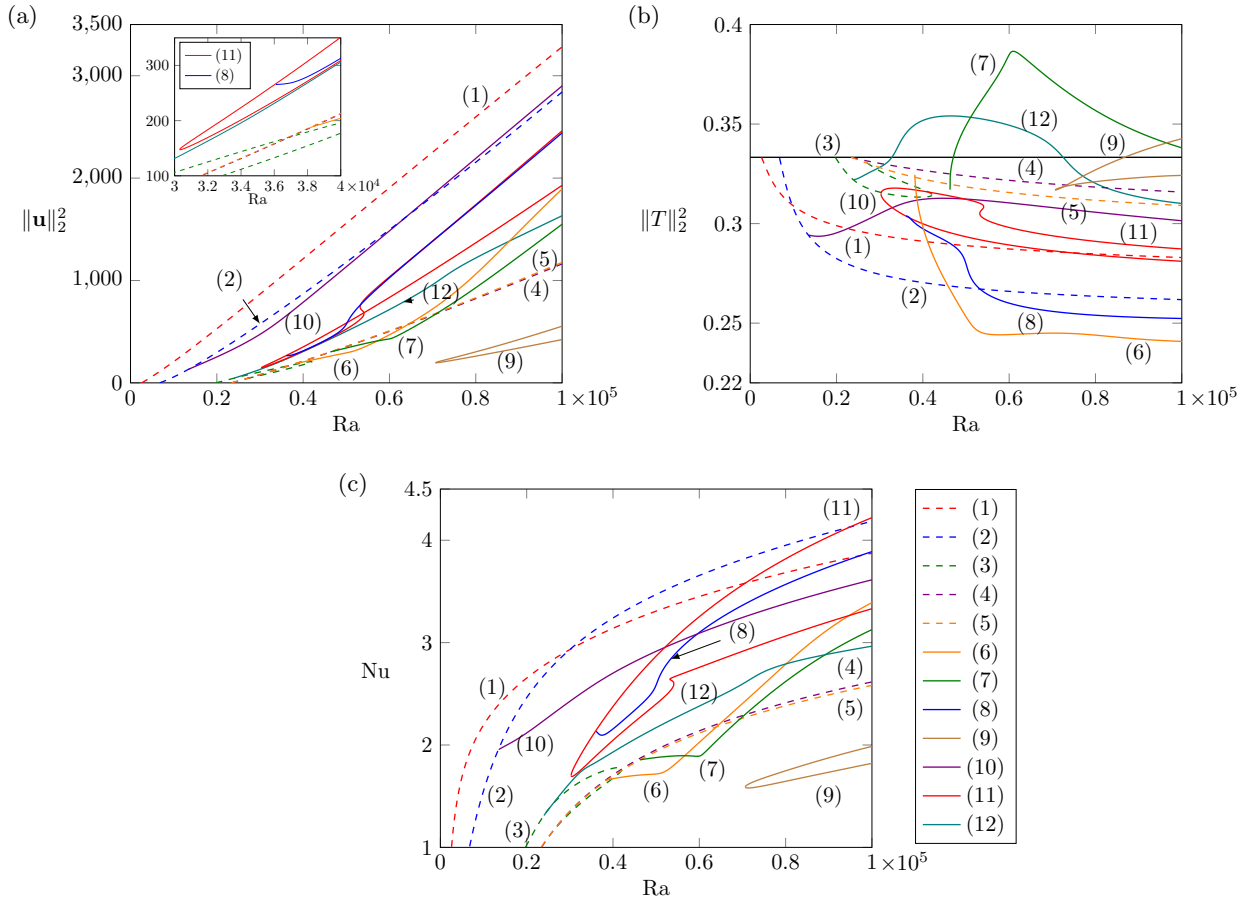


FIG. 3. (a) Bifurcation diagram using the kinetic energy $\|\mathbf{u}\|_2^2$ of the branches studied in the paper. Also represented are (b) the potential energy $\|T\|_2^2$ and (c) the Nusselt number Nu of the branches as a function of Ra . The branches that originate from the linear conducting state are plotted with dashed lines, while branches emanating from secondary instabilities and disconnected branches are depicted with solid lines. The horizontal black line in (b) indicates the potential energy of the conducting steady state.

[see Fig. 4(d)], while the next eigenvalue has a negative real part and a large imaginary part.

The second eigenmode introduced in Fig. 2 gives birth to branch (2) at $Ra_c^{(2)} = 6746$, which is depicted in Figs. 5(a) and 5(b). The bifurcation is transcritical and preserves the symmetries of the eigenmode in the velocity and temperature profiles. Then the largest growth rate in Fig. 5(c) indicates that the solutions on this branch are stable over the interval $Ra \in [13\,500, 85\,500]$ and unstable outside. A bifurcation occurs at $Ra \approx 13\,500$ when $\mathcal{R}(\lambda) = \mathcal{I}(\lambda) = 0$, which is analyzed later and illustrated in Fig. 6. The bifurcation from branch (2) to branch (10) is accompanied by a loss of Boussinesq symmetry. Another bifurcation is observed at $Ra \approx 85\,500$ and has been obtained by deflated continuation. Figure 6(a) demonstrates that the two symmetries of the second eigenmode (see Sec. II) are rapidly broken as Ra increases after the bifurcation from branch (2) to the secondary branch (10). This symmetry breaking leads to a primary large-scale circulation spanning the domain and a secondary vortex with smaller amplitude in one of the corners depending on which symmetric solution one is referring to. As $Ra \rightarrow 10^5$, the difference in the flow pattern of the velocity magnitude between branches (1) and (10) is the secondary vortex in the corner of the convection cell. The symmetry breaking is also obvious in the

temperature field [see Fig. 6(b)] with the potential energy of the flow increasing and then decreasing slightly in contrast to the increase of the kinetic energy and the convective heat transfer [see also Fig. 3(c)]. The largest growth rate shows that the states are unstable to a real eigenmode [see Fig. 6(d)]. The subsequent growth rates shown in Fig. 6(c) are negative and almost constant in this range of Rayleigh numbers.

Branch (3) originates from the eigenmode of the conducting state at $Ra_c^{(3)} = 19\,655$, which is depicted in Fig. 7. This branch preserves the centrosymmetry of the third eigenmode and has a turning point located at $Ra \approx 42\,130$. Interestingly, the lower part of the branch, colored in red in Figs. 7(a) and 7(b), bifurcates from branch (5) around $Ra \approx 27\,000$. The latter branch emanates from the fourth eigenmode and is illustrated later in Fig. 10. The largest growth rates of the upper and lower parts of branch (3) are displayed in Figs. 7(c) and 7(e), together with their associated frequencies in Figs. 7(d) and 7(f). We find that the steady states in the branch are unstable with a zero frequency throughout the range of Rayleigh numbers for which the branch exists. Moreover, we observe that the eigenmode colored in purple in Fig. 7(c) traverses zero at $Ra \approx 23\,800$, indicating the presence of a secondary bifurcation, which we will analyze in the following paragraph. We point out that this branch was not originally discovered by

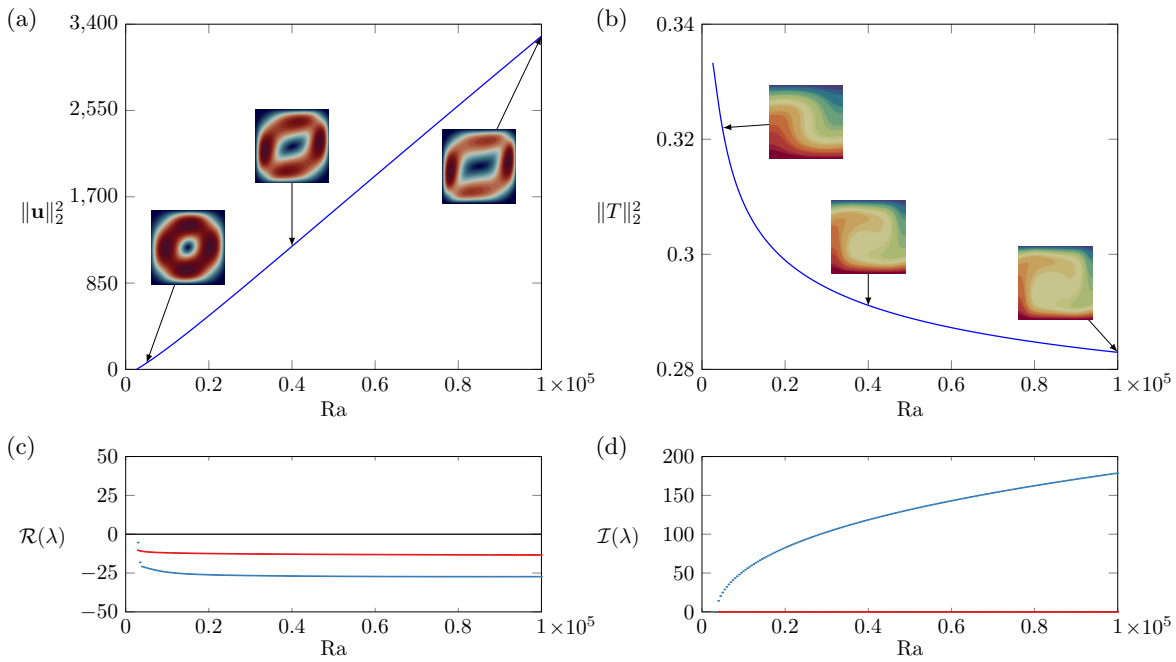


FIG. 4. Evolution of the steady states in branch (1) arising from the first eigenmode, illustrated via (a) the kinetic energy and (b) the potential energy. The color scheme for the temperature ranges from 0 (blue) to 1 (red). Also shown are (c) the largest growth rates and (d) the corresponding frequencies.

deflated continuation (our method does not guarantee finding all the steady states of a problem) but obtained by continuing the third linear state with finer steps in the Rayleigh number. This illustrates that deflated continuation may be complemented by standard bifurcation analysis techniques,

such as arclength continuation and branch-switching algorithms. We now focus on branch (12), which bifurcates from branch (3) at $Ra \approx 23\,800$, and display the evolution of the steady states in the branch in Fig. 8 along with its stability analysis. This branch breaks the centrosymmetry of branch

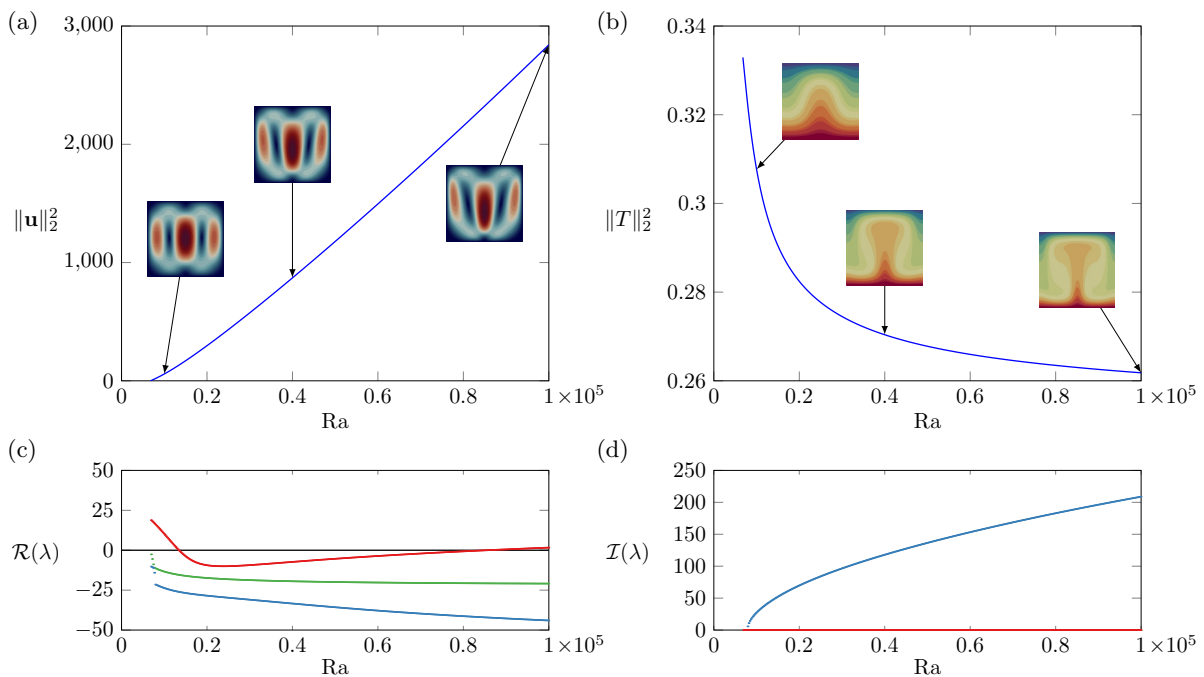


FIG. 5. Evolution of the steady states in branch (2) arising from the second eigenmode, illustrated via (a) the kinetic energy and (b) the potential energy. Also shown are (c) the largest growth rates and (d) the corresponding frequencies. The two largest growth rates are shown in red and green, while the subsequent ones are depicted in blue.

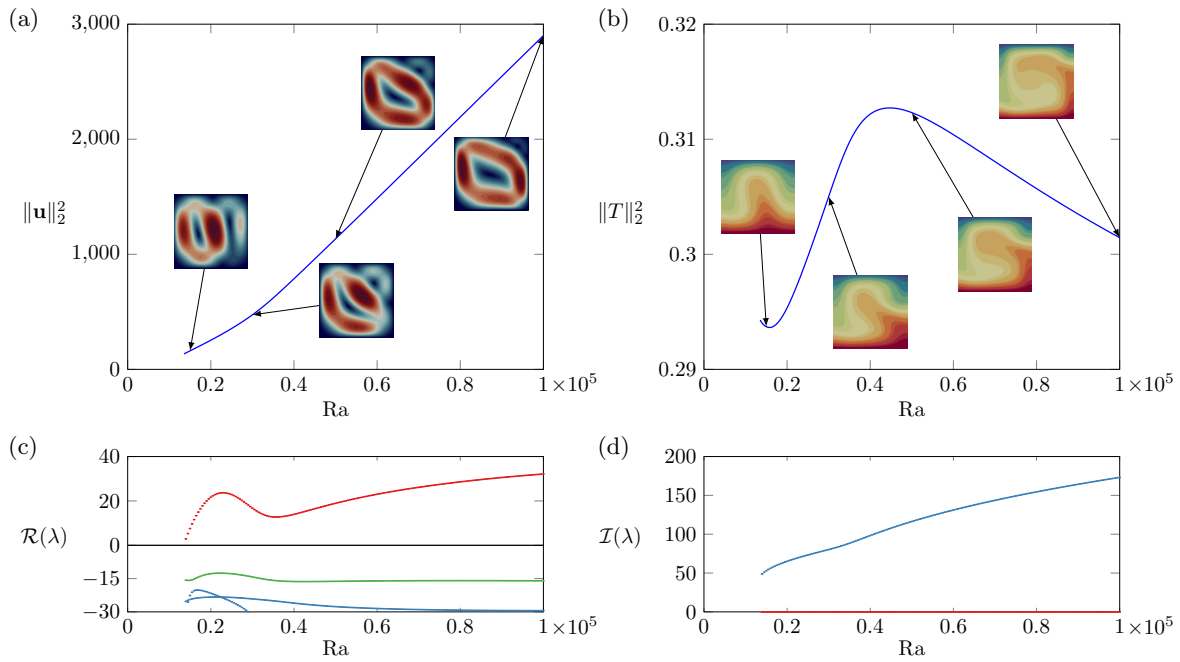


FIG. 6. Evolution of the steady states in branch (10), bifurcating from branch (2) at $Ra \approx 13\,550$, illustrated via (a) the kinetic energy and (b) the potential energy of branch (10). Also shown are (c) the largest growth rates and (d) the corresponding frequencies.

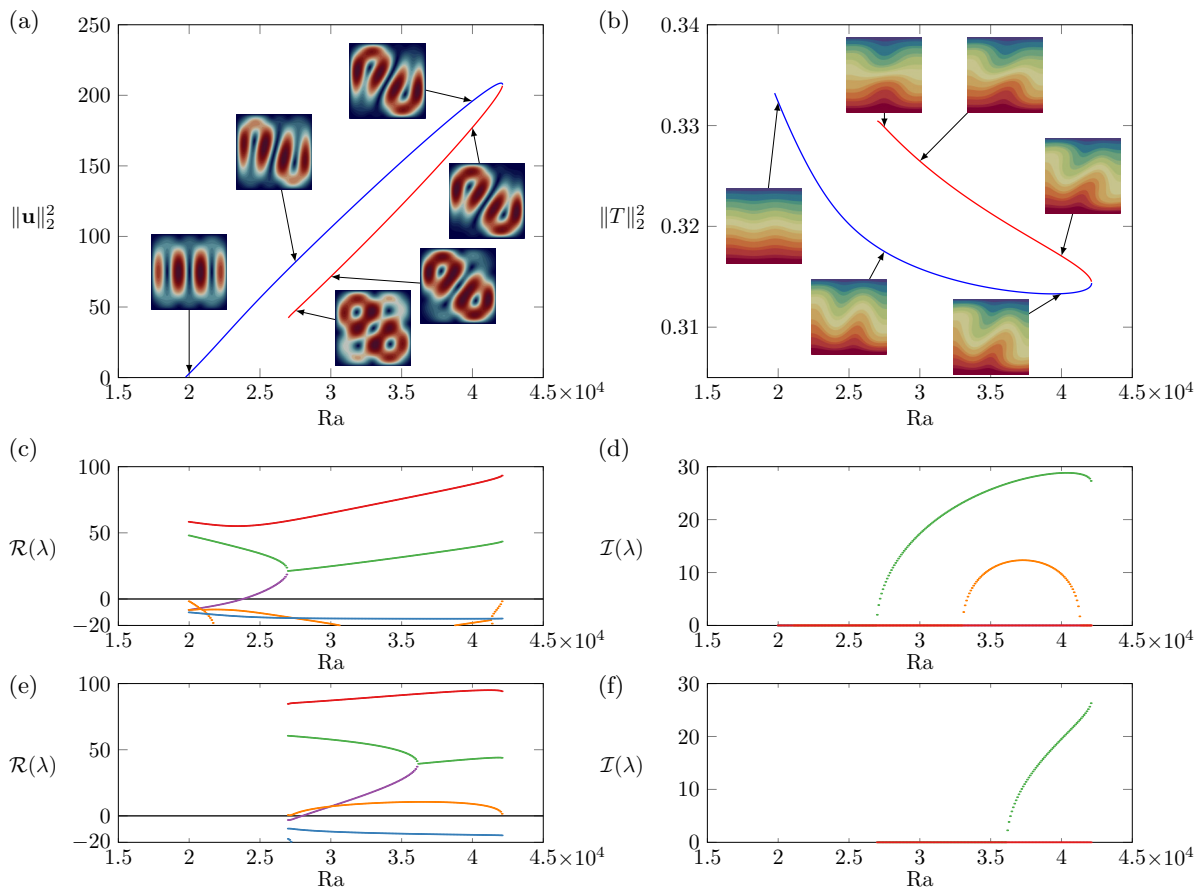


FIG. 7. Evolution of the steady states in branch (3) arising from the third eigenmode, illustrated via (a) the kinetic energy and (b) the potential energy. The upper and lower parts of the branch are colored in blue and red, respectively. Also shown are (c) the largest growth rates and (d) the corresponding frequencies of the upper part of the branch. (e) and (f) Same as (c) and (d) but for the lower part of the branch.

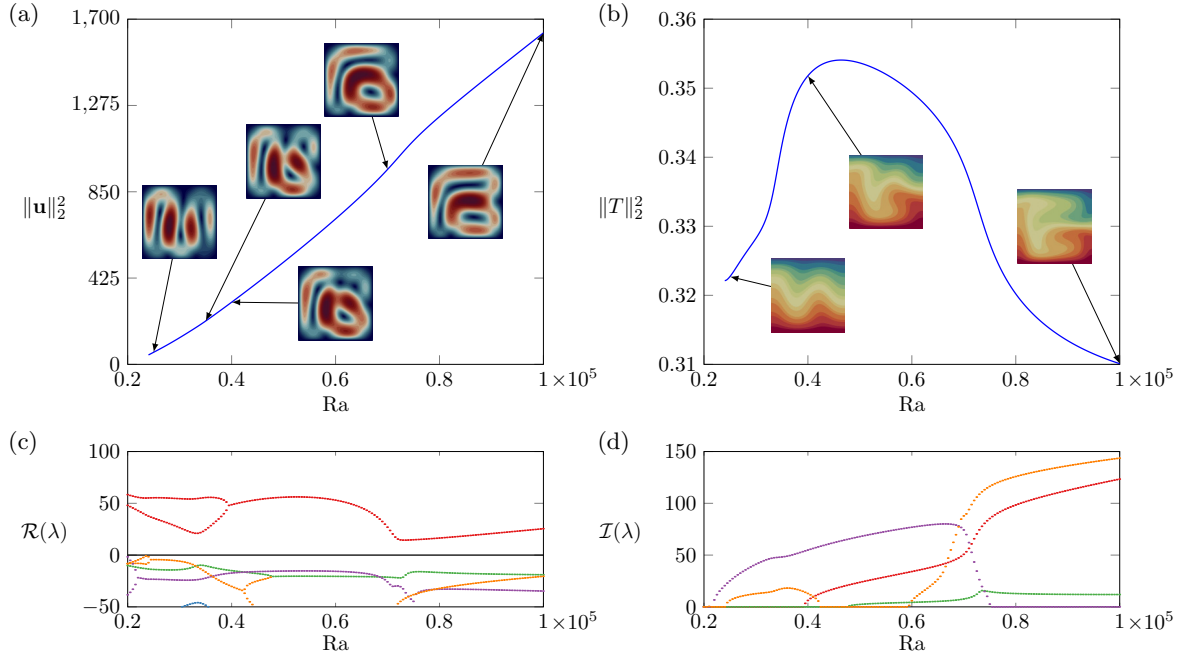


FIG. 8. Evolution of the steady states in branch (12), bifurcating from branch (3) around $Ra \approx 23\,800$ and illustrated via (a) the kinetic energy and (b) the potential energy. Also shown are (c) the largest growth rates and (d) the corresponding frequencies.

(3) and the pattern of the velocity magnitude becomes more complex as Ra increases. This complex pattern is one reason for the meandering of the potential energy in this range of Rayleigh numbers and enhances the convective heat transfer [see Fig. 3(c)] by mixing the temperature field. Figure 8(c) shows that the steady states of branch (12) are unstable to two eigenmodes until $Ra \approx 39\,500$, where they coalesce. At this Rayleigh number, we see that the two most unstable eigenmodes coalesce into an unstable complex conjugate pair of eigenvalues [see Fig. 8(d)]. All the subsequent eigenmodes are found to be stable with either $\mathcal{I}(\lambda) = 0$ or $\mathcal{I}(\lambda) \neq 0$.

Figure 9 shows bifurcation diagrams and the linear stability results of branch (4), which originates from the fourth eigenmode at $Ra_c^{(4)} = 23\,346$ through a transcritical bifurcation. The flow pattern of the velocity magnitude has a symmetric form of an array of four vortices, which is conserved over the whole range of Rayleigh numbers we consider, as Fig. 9(a) suggests. Similarly, the symmetric pattern of the temperature field remains unaffected in the regime $23\,346 \leq Ra \leq 10^5$ [see Fig. 9(b)]. We have verified numerically that the symmetries are conserved within this range of Ra . Figure 9(c) shows the four largest growth rates as a function of Ra . At Rayleigh numbers close to $Ra_c^{(4)} = 23\,346$ we see that three of the eigenmodes are real and unstable, while the fourth one is real and stable. As Ra increases, the two most unstable eigenmodes [colored in red and green, respectively, in Fig. 9(c)] coalesce at $Ra \approx 56\,000$ into a complex unstable eigenmode whose growth rate and oscillation frequency increases as $Ra \rightarrow 10^5$. Similarly, the other two real unstable modes coalesce at $Ra \approx 40\,000$ into a complex conjugate pair of eigenmodes which are unstable for $40\,000 < Ra \leq 10^5$. At $Ra \approx 52\,000$ and $Ra \approx 73\,500$, we observe in Fig. 9(c) that the growth rate colored in blue vanishes with a nonzero

frequency, leading to Hopf bifurcations where periodic solutions to the time-dependent problem (1) arise.

We close our discussion on the branches arising from the conducting steady state with branch (5), presented in Fig. 10. This branch originates from the fourth eigenmode of the conducting state at $Ra \approx 23\,346$ through the same transcritical bifurcation as branch (4). The steady states in branch (5) conserve the Boussinesq and x symmetries, with a velocity field consisting of four vortices, located symmetrically at each corner of the domain. The velocity fields of branches (4) and (5), illustrated in Fig. 11, are different, indicating that branch (5) is not a symmetric version of branch (4). The stability analysis reveals that the steady states in this branch are very sensitive to perturbations and unstable to a real eigenmode throughout the range of Ra considered in this study. Moreover, the largest growth rate at $Ra = 10^5$ is equal to $\mathcal{R}(\lambda) \approx 188$, which is approximately three times larger than the largest growth rate of the steady state in branch (4) at the same Rayleigh number [see Figs. 9(c) and 10(c)]. One of the eigenmodes vanishes at $Ra \approx 27\,000$, giving rise to branch (3), depicted in Fig. 7. Finally, the real part of the eigenvalue depicted in blue in Figs. 10(c) and 10(d) crosses zero at $Ra \approx 57\,500$, which shows the existence of a Hopf bifurcation.

We now analyze the branches bifurcating from branches (4) and (5). The fourth largest growth rate of branch (4), colored in blue in Fig. 9(c), crosses zero at $Ra \approx 38\,150$, leading to the bifurcating branch (6) depicted in Fig. 12. We observe that the Boussinesq symmetry of branch (4) is broken by the bifurcation, while the symmetry with respect to the x axis is preserved. Additionally, the linear stability analysis indicates that this branch is unstable with a zero frequency except in the interval $Ra \in [72\,500, 93\,000]$, where the largest growth rate is associated with a positive frequency, as shown

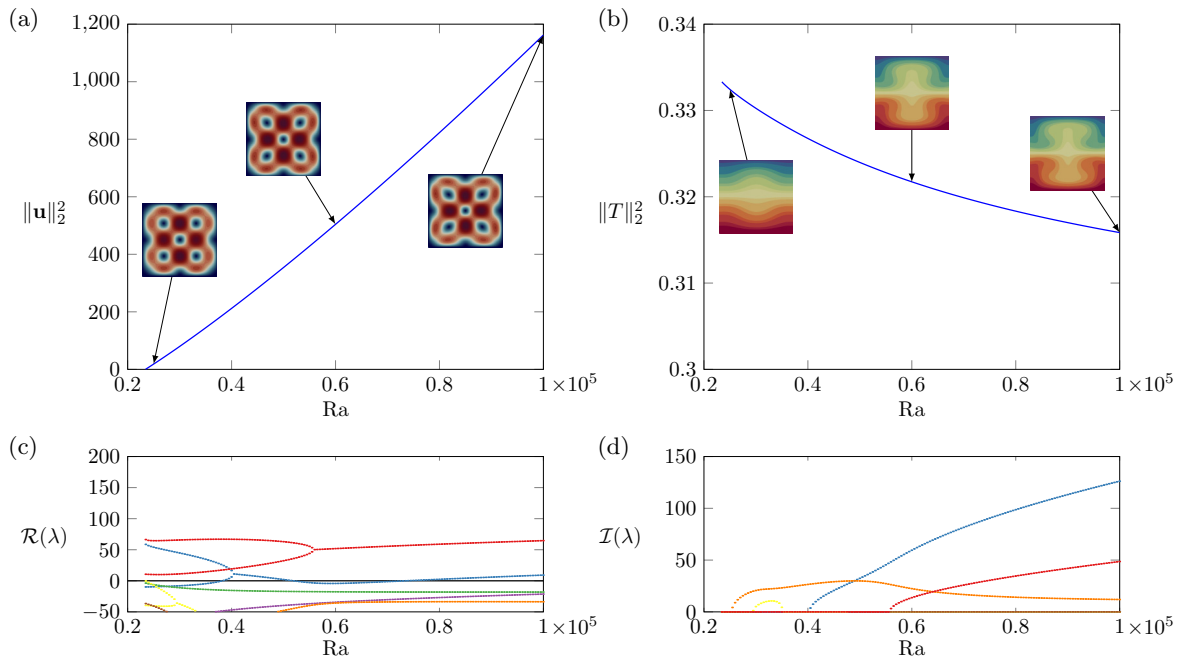


FIG. 9. Evolution of the steady states in branch (4) arising from the fourth eigenmode, illustrated via (a) the kinetic energy and (b) the potential energy. Also shown are (c) the largest growth rates and (d) the corresponding frequencies.

by the eigenvalues colored in blue in Figs. 12(a) and 12(c). Moreover, the third largest growth rate (colored in orange) crosses zero around $Ra \approx 63\,500$, indicating the presence of a bifurcation which has not been discovered by deflation. Finally, a branch, denoted by (7), bifurcates from branch (5) at $Ra \approx 46\,300$. The steady states in this branch are illustrated in Fig. 13. We observe on the velocity magnitude and

temperature field that the symmetry of branch (5) with respect to the x axis is maintained while the Boussinesq symmetry is broken. Branches (6) and (7) might seem nearly symmetric but they arise at different Rayleigh numbers and have different eigenvalues. The linear stability analysis of branch (7) shows that the steady states are unstable to a real eigenmode, with a largest growth rate around $\mathcal{R}(\lambda) \approx 150$ throughout

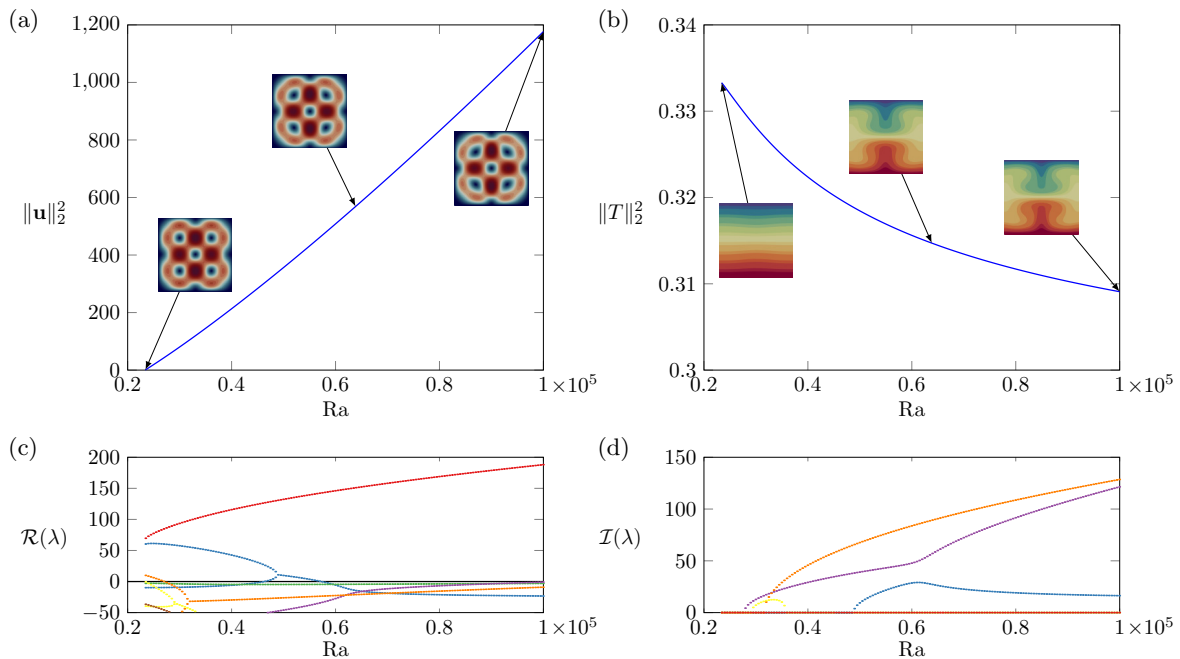


FIG. 10. Evolution of the steady states in branch (5) illustrated via (a) the kinetic energy and (b) the potential energy. Similarly to branch (4), this branch bifurcates from the fourth eigenmode. Also shown are (c) the largest growth rates and (d) the corresponding frequencies.

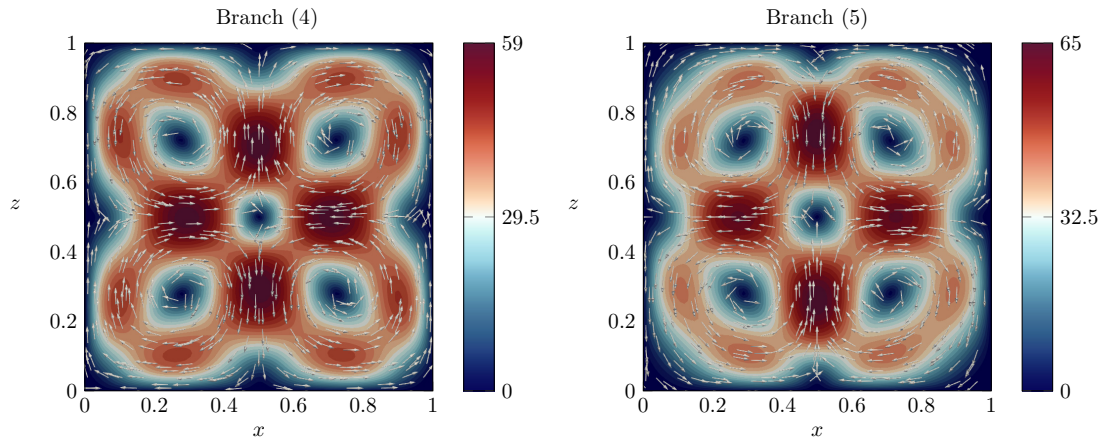


FIG. 11. Velocity magnitude of the steady state in branches (4) and (5) at $Ra = 10^5$.

the range of Ra considered in this study. In Figs. 13(c) and 13(d) we observe that the third eigenvalue (plotted in green) crosses zero at $Ra \approx 92\,000$, resulting in a tertiary branch that breaks the remaining symmetry. The branch has been discovered by deflation, but we chose to not report it in the study.

D. Disconnected branches

We now focus on the disconnected branch (11) (see Fig. 3), which comprises an upper and a lower branch, depicted in blue and red in Fig. 14, respectively. At the upper (blue) branch the flow pattern of the velocity magnitude is a three-vortex state with one large tilted vortex spanning the domain and two smaller vortices located at the corners. As $Ra \rightarrow 10^5$ we notice that the state looks similar to branches (1) and (10).

The difference is that branch (10) involves only one smaller vortex at the corner of the domain and branch (1) has no vortices at the corners, while branch (11) has two smaller vortices located at the corners. At $Ra \approx 52\,000$ the branch takes the form of an S-shaped curve with hysteresis, similar to the cusp bifurcation [46].

As the saddle-node bifurcation is approached from below, the growth rate of the most unstable eigenmode decreases toward zero at the critical point [see Fig. 14(c)]. Above the bifurcation point $\mathcal{R}(\lambda)$ increases and seems to saturate as $Ra \rightarrow 10^5$. The frequency corresponding to the growth rate is zero in the whole range of Ra numbers, suggesting that the steady state is unstable to a real eigenmode in this regime. The potential energy of the upper (blue) branch decreases with Ra in contrast to the kinetic energy. As Ra increases the flow pattern of the temperature becomes more efficient

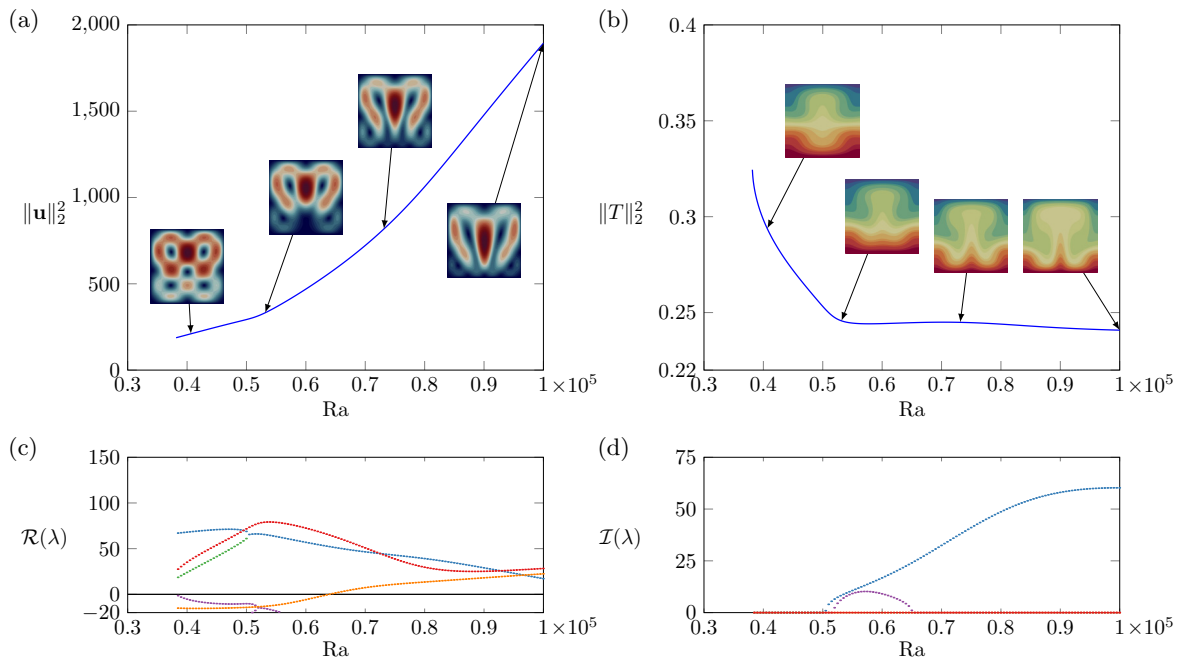


FIG. 12. Evolution of the steady states in branch (6), bifurcating from branch (4) at $Ra \approx 38\,150$, illustrated via (a) the kinetic energy and (b) the potential energy. Also shown are (c) the largest growth rates and (d) the corresponding frequencies.

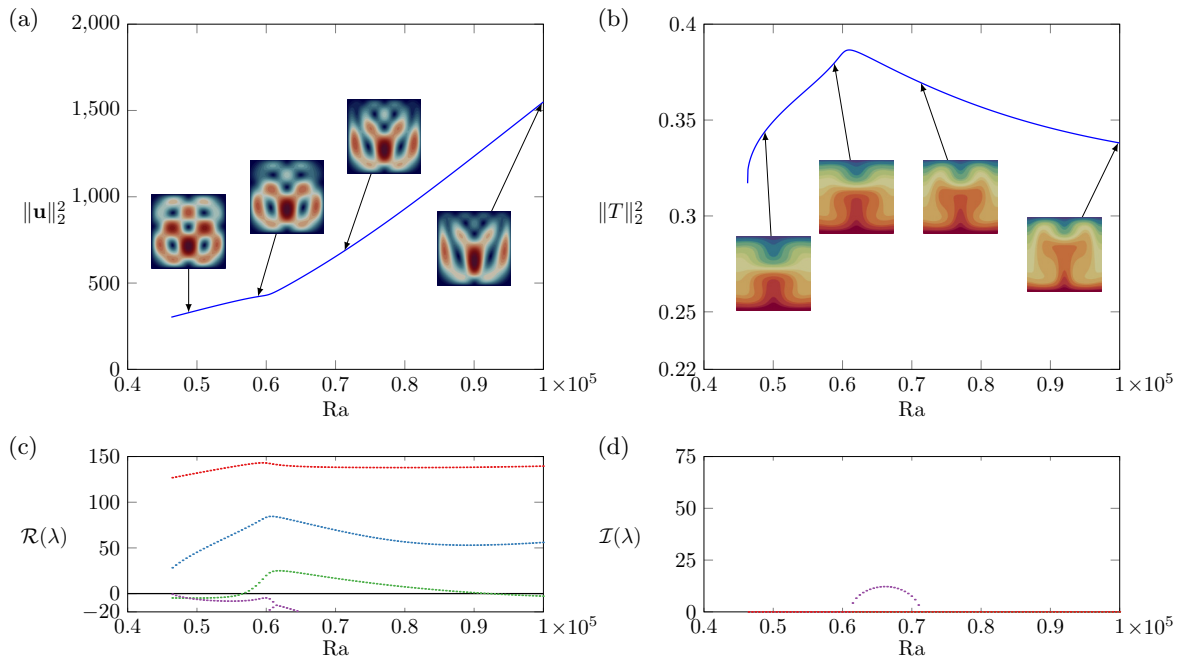


FIG. 13. Evolution of the steady states in branch (7), bifurcating from branch (5) at $Ra \approx 46\,300$, illustrated via (a) the kinetic energy and (b) the potential energy. Also shown are (c) the largest growth rates and (d) the corresponding frequencies.

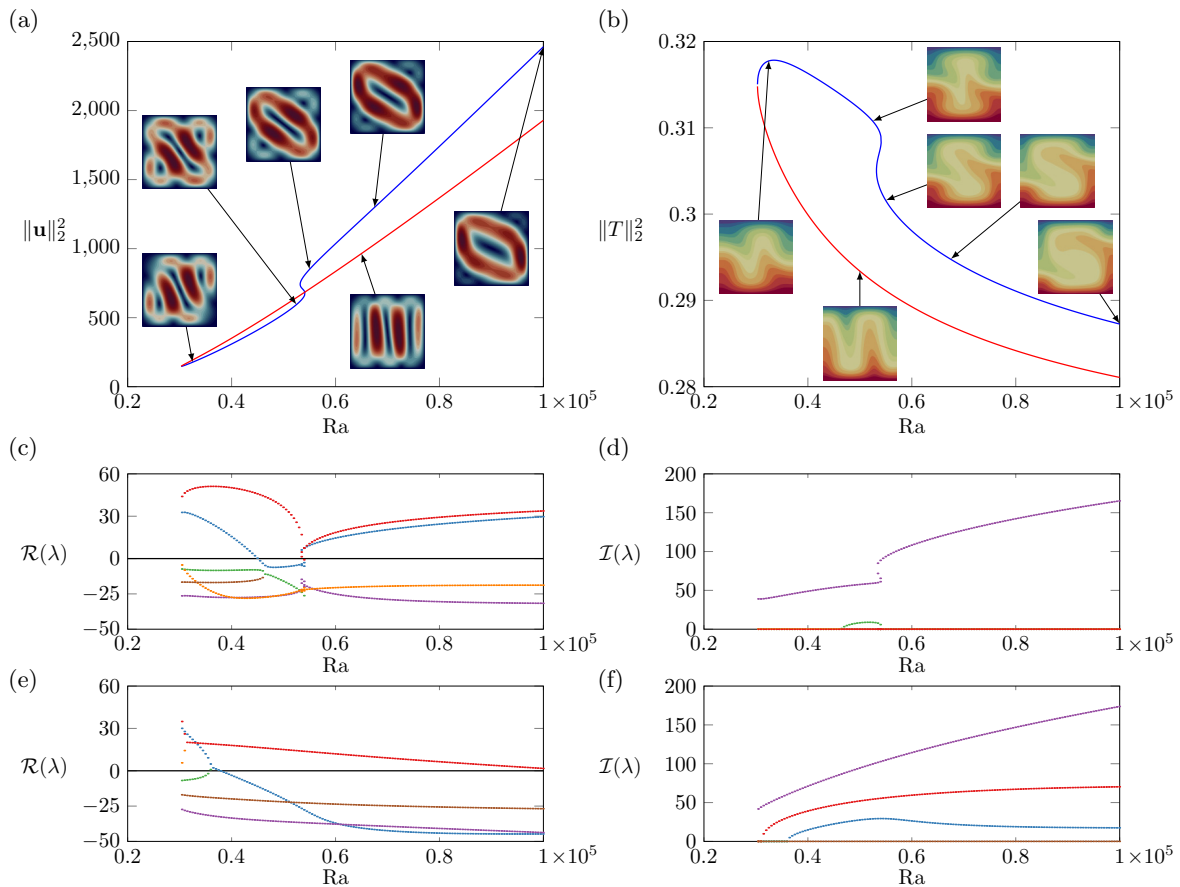


FIG. 14. Evolution of the steady states in the disconnected branch (11), illustrated via (a) the kinetic energy and (b) the potential energy. The upper and lower parts of the branch are colored in blue and red, respectively. Also shown are (c) the largest growth rates and (d) the corresponding frequencies of the upper part of the branch. (e) and (f) Same as (c) and (d) but for the lower part of the branch.

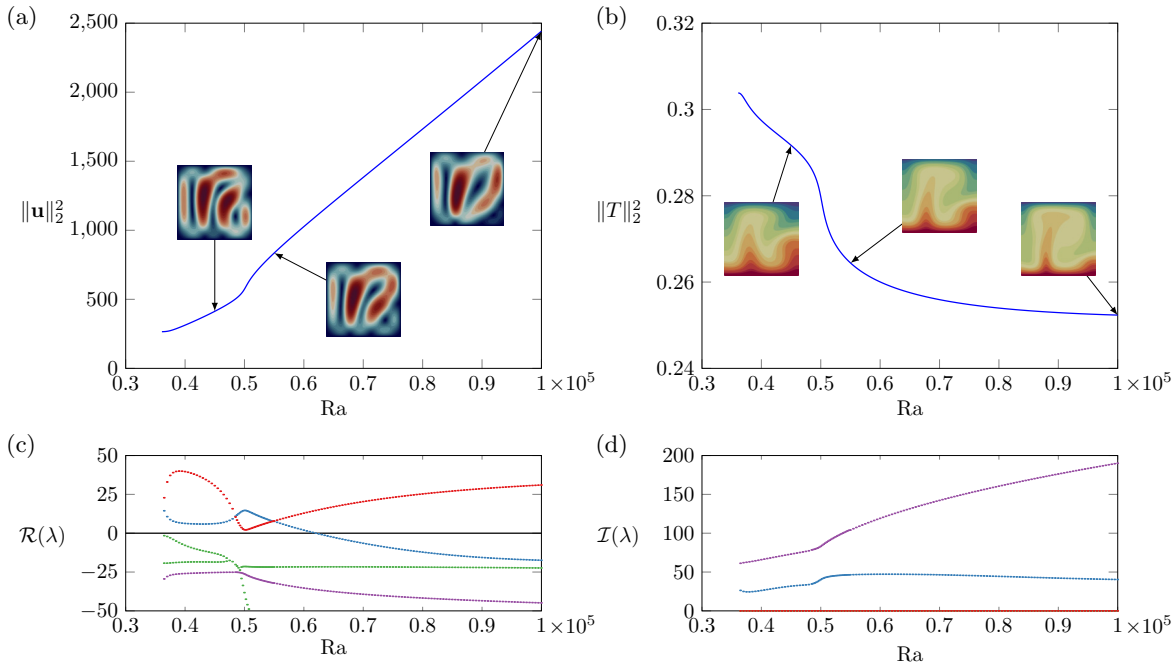


FIG. 15. Evolution of the steady states in branch (8), bifurcating from the lower part of the disconnected branch (11) at $Ra \approx 37\,000$, illustrated via (a) the kinetic energy and (b) the potential energy. Also shown are (c) the largest growth rates and (d) the corresponding frequencies.

at transferring heat due to the large-scale circulation in the flow [see Fig. 3(c)]. The flow pattern of the velocity of the upper (blue) branch, shown for $Ra = 10^5$ [see Fig. 14(a)], exhibits a large-scale vortex and two smaller vortices at the corners of the domain. This is reminiscent of the flow patterns from studies on the dynamics of random-in-time flow reversals [29–31,47]. These reversals in the flow direction of the large-scale circulation at irregular time intervals have been observed in domains with free-slip or no-slip boundaries and in a narrow band of Rayleigh numbers in the range $10^7 \leq Ra \leq 10^9$ depending on the Prandtl number [29–31]. In this regime the system fluctuates in time between essentially the state we show for $Ra = 10^5$ [see Fig. 14(a)] and its mirror symmetric state. These large changes in the dynamics of the flow are caused by bifurcations over a turbulent background [27]. Such bifurcations have been observed in many other types of flows [48–52] and understanding their dynamics is an open question of great interest.

At the lower (red) branch illustrated in Fig. 14(a) we observe the central vortex to be oriented more vertically, giving space to the smaller vortices at the corners to extend along the z axis and almost reach the height of the domain. This flow pattern is an extension of the two-vortex pattern observed in branch (5) (see Fig. 6) and it has similar features to the three-vortex pattern found near the linear limit of branch (3) (see Fig. 7). The patterns of the kinetic and potential energies of this branch are almost invariant within the range $30\,000 \lesssim Ra \leq 10^5$. The flow pattern of the temperature clearly manages to effectively push the hot fluid toward the cold plate at the top and vice versa. This efficiency in convective heat transfer is clearly depicted in Fig. 3(c), where this part of branch (11) has the highest Nusselt number for $Ra > 95\,000$.

Analyzing the stability of the lower (red) branch, we find that the steady solutions become increasingly more stable as the Rayleigh number increases, with $\mathcal{R}(\lambda) \rightarrow 0$ at $Ra \approx 10^5$, leading to a Hopf bifurcation [see Fig. 14(e)]. On the other hand, the frequency corresponding to the growth rate satisfies $\mathcal{I}(\lambda) = 0$ at the threshold of the disconnected branch and as Ra increases the instability becomes progressively oscillatory [see Fig. 14(f)]. The subsequent growth rates presented in Fig. 14(e) remain negative as Ra increases, suggesting that this part of branch (11) is another preferred steady state of the system, particularly for $Ra > 10^5$.

Branch (8) illustrated in Fig. 15 bifurcates from the lower part of the disconnected branch (11) at $Ra \approx 37\,000$ (see also Fig. 3). In this case, the pattern of the velocity transitions into a main bent vortex with a vertically elongated vortex on its left and a smaller vortex at the bottom right corner [see Fig. 15(a)]. From Fig. 3 we can see that even though the kinetic energy of branch (8) is equal to that of the upper part of branch (11) for $Ra > 50\,000$, the potential energy is much smaller and apparently the smallest among the branches we have considered. The pattern of the temperature is essentially a hot plume that rises effectively all the way to the cold plate [see Fig. 15(b)]. This flow pattern becomes increasingly more efficient at transferring heat across the domain as Ra increases [see Fig. 3(c)]. However, it is not as efficient in convecting heat as the pattern of branch (11) [see the lower branch in Fig. 14(b)] because two hot plumes are obviously more effective than one. The steady state of branch (8) is unstable to a real eigenmode over the range $37\,000 \lesssim Ra \leq 10^5$ except for a small range around $Ra = 50\,000$, where it becomes unstable to a complex eigenmode. This can be seen from Figs. 15(c) and 15(d), where the two largest growth rates (colored in red

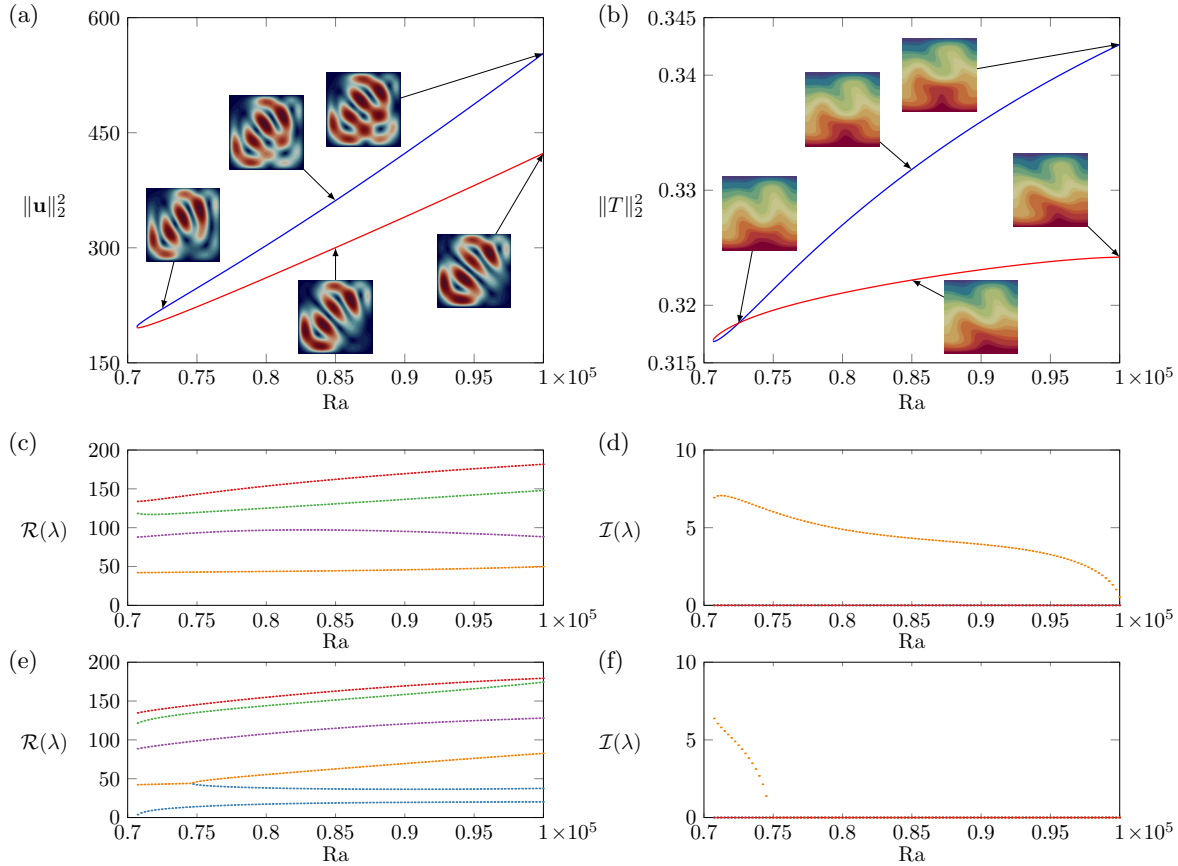


FIG. 16. Evolution of the steady states in the disconnected branch (9), illustrated via (a) the kinetic energy and (b) the potential energy. The upper and lower parts of the branch are colored in blue and red, respectively. Also shown are (c) the largest growth rates and (d) the corresponding frequencies of the upper part of the branch. (e) and (f) Same as (c) and (d) but for the lower part of the branch.

and blue) swap with each other in this small range of Rayleigh numbers. Finally, the real part of the eigenvalue depicted in blue in Figs. 15(c) and 15(d) crosses zero at $Ra \approx 62\,000$, giving birth to a Hopf bifurcation.

The second disconnected branch that we find in this range of Rayleigh numbers is branch (9) and arises at $Ra \approx 70\,000$ (see Fig. 16). From Fig. 16(a) we see that all the symmetries of the flow are broken in this branch and the flow pattern consists of a number of vortices with different orientations. These flow structures are not persistent over the range of parameters that we consider, and hence the heat is not transferred effectively across the domain [see also Fig. 3(c)]. Here Fig. 16 shows that the potential energy of branch (9) increases along with the kinetic energy, unlike in most of the other branches we considered, and from Fig. 3(b) we see that it is significant in comparison to many other branches. Moreover, from the linear stability analysis of the steady states we find that both the upper and lower parts of this disconnected branch are unstable to a real eigenmode, i.e., $\mathcal{R}(\lambda) > 0$ and $\mathcal{I}(\lambda) = 0$, with large growth rates. This suggests that this branch is very unlikely to be observed in a laboratory experiment and highlights the effectiveness of deflated continuation in identifying such unstable disconnected branches and steady states.

V. CONCLUSION

In this work we have computed and analyzed the linear stability of steady states of the two-dimensional Rayleigh-Bénard convection in a square cell with rigid walls. The combination of deflated continuation and a suitable initialization procedure based on the linear stability of the motionless state was revealed to be a powerful numerical technique for finding multiple solutions including disconnected branches, which are not easily accessible by standard bifurcation techniques such as arclength continuation and time-evolution algorithms. A highlight is the success of deflation to discover these branches in an automated manner without any prior knowledge of the dynamics.

We classified the solutions based on the kinetic and potential energies as well as the Nusselt number. Our classification provided a clear view of the steady states of Rayleigh-Bénard convection up to a Rayleigh number of 10^5 . We showed that the steady states of branch (1) (which originated from the conducting state) dictate the dynamics of the flow for $Ra \leq 10^5$, while for $Ra \sim 10^5$ the flow patterns of the disconnected branch (11) start to play a very important role as the steady states become stable. Solutions on branch (11) are reminiscent of the flow pattern that plays a fundamental role in the turbulent dynamics of flow reversals that have been reported

in the literature for Rayleigh-Bénard convection at $Ra \sim 10^7$ [29–31]. This disconnected branch exhibits an S-shaped curve with hysteresis which can be a challenge to discover with other bifurcation techniques.

There are several possible extensions to this work. An interesting but computationally challenging future study is to extend certain solutions of interest to higher values of Ra and determine whether they give the required theoretical scalings in the limit of high Rayleigh number. A first attempt toward this direction has been done in Rayleigh-Bénard convection with periodic boundary conditions in the horizontal direction and no slip in the vertical direction [53,54]. Moreover, the extensions of branch (11) and its stability in the regime where reversals occur are also of great interest. Another extension of interest is to study how the states presented in this study change with respect to other parameters of the system such as the Prandtl number or the aspect ratio of the domain Γ . As observed in Fig. 1(a), the critical Rayleigh number converges to $Ra_c^* \approx 1707.762$ for large aspect ratio. Using alternative formulations of the Rayleigh-Bénard problem, with the aspect ratio playing the role of the bifurcation parameter, it is possible to analyze the evolution of the branches for large aspect ratio and connect them with the solutions of the periodic setup, which has been studied well in the literature, both analytically [42] and numerically [4,5]. This connection will be of great interest to theoreticians and hopefully will spark their interest

to explore analytical solutions on more realistic convection setups with sidewalls.

A different future direction would be to perform bifurcation analysis on Rayleigh-Bénard convection in a three-dimensional rectangular domain. Such an approach will be of interest to experimentalists since direct comparisons with experiments would be possible. However, while the generalization of the bifurcation technique employed in this paper to three dimensions is straightforward, high Rayleigh numbers require an efficient solver to perform the underlying Newton iterations. One possible solution would be to construct an efficient preconditioner robust with respect to the Rayleigh number to be able to reach high- Ra regimes in the spirit of [55,56].

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