Analysis and design of bistable and thermally reversible metamaterials inspired by shape-memory alloys

A. Vasudevan¹, J. A. Rodríguez-Martínez², I. Romero³

¹IMDEA Materials Institute, Eric Kandel 2, Tecnogetafe, Madrid 28906, Spain
²Dept. of Continuum Mechanics and Structural Analysis, University Carlos III of Madrid, Avda. de la Universidad, 30. 28911 Leganés, Madrid, Spain
³Universidad Politécnica de Madrid, José Gutiérrez Abascal, 2, 28006 Madrid, Spain

1 Introduction

Instabilities play an important role in determining the functional capacity of deformable bodies since they can lead to catastrophic failure in the case, for example, of buckling or brittle fracture (see, e.g., [1] and [2] for in-depth introductions to the topic). Generally considered as something to be designed against, recent years have seen a tremendous progress in understanding these instabilities, allowing a change of paradigm where now instead of avoiding them, they can be exploited. Aided by advances in manufacturing, designs have been proposed that harness these instabilities to give structures new and surprising capabilities (see [3, 4] and references therein). In particular, instabilities have been exploited to design mechanical metamaterials, periodic arrays of representative unit cells that when stacked together possess drastically different properties than the base material. Examples of such designs include structures with negative Poisson’s ratio induced by buckling [5, 6, 7], snapping based metamaterials for energy absorption [8, 9, 10, 11, 12, 13, 14, 15], origami or kirigami tessellations with multistability [16, 17, 18, 19, 20], etc.

Instabilities emerge in solids and structures when their potential energy is not (quasi) convex [21]. Interestingly, this property might depend on external factors to the system such as forces and temperature. For example, consider a mechanical system whose potential energy is depicted on the left of Fig. 1 for three different values of the temperature θ. For θ = θ_{ref}, this curve has two local minima and one local maximum where the derivatives of the potential energy

*Corresponding author ignacio.romero@upm.es

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Figure 1: Representative energetic and equilibrium diagrams: (a) shows the potential energy landscape while (b) shows the force-displacement curve for the proposed mechanical system with increasing temperatures. Circles and squares correspond, respectively, to stable and unstable points. At low temperatures (solid and dotted lines, $\theta < \theta_c$) the system has a nonconvex potential energy with two stable and an unstable equilibrium point and changes to convex beyond a critical temperature $\theta_c$ (dashdot line, $\theta > \theta_c$) with a single stable point. For a nonconvex potential, the force-displacement is non-monotonic and exhibits snap-through instabilities that can be exploited for energy absorption as shown by arrows for $\theta = \theta_{ref}$ in (b).

vanish, i.e., where the forces are zero and the system is said to be in equilibrium. The equilibrium point corresponding to the local maximum is unstable since any small perturbation causes the system to jump to one of the local minima. The force-displacement diagram for this system is shown on the right of Fig. 1 and is non-monotonic for $\theta = \theta_{ref}$, passing through zero at three points that correspond to the two stable and one unstable equilibria. This lack of monotonicity is the fundamental mechanism that is used in the design of bistable systems where, beyond a certain load, the structure snaps to another stable point as indicated by arrows in Fig. 1(b). Complete reversibility of the original state is achieved through an unloading cycle by applying a force in the opposite direction as shown in Fig. 1(b).

In this work, we present a theory for the design of bistable and reversible lattice structures. Moreover, reversibility will be achieved through an external stimulus, temperature in our case, that can be controlled at will and can be used to shape the potential energy. Similarly to the system illustrated in Fig. 1, the structures that will be proposed will possess nonconvex potential energies at low temperatures that will become convex beyond a critical temperature. When the temperature is higher than the critical value, the force-displacement relation will become monotonic and this will be exploited to drive the system back to a selected minimum of the original configuration. These controlled transformations are inspired by the thermomechanical cycle characteristic of shape-memory alloys such as Nitinol [22], which exhibit multiple (energetically
equivalent) variants of martensite at low temperature and a single austenite configuration at high temperature. While external loads can favor one particular martensite phase, the original configuration can be recovered employing a heat treatment that transforms first the whole crystal to austenite and back to the original martensite configuration on cooling. Our designed lattices thus mimic the crystallographic phase-transformation mechanisms of shape-memory alloys at the structural lattice scale by means of a judicious choice of geometry and thermomechanical properties.

This research finds resemblance with previous works that sought to design simple atomistic models of shape memory alloys. For instance, [23] developed a one-dimensional model simulating shear in a two-dimensional body described by a discrete system of masses and nonlinear springs with mechanical behavior described by Lennard-Jones potentials. [23] established a link among the energies at different scales (interatomic potential, the double-well potential which is a combination of interatomic potentials, the equilibrium energy, the continuum energy), and identified lattice instabilities that were used to explain the mechanics of solid phase transitions. Similarly, [24] developed an atomistic model to study the stability of thermally-induced martensitic transformations in bi-atomic crystals using a discrete system of point masses with interactions described by Morse potentials. Following [23], the fundamental hypothesis of [24] was that martensitic transformations are manifestations of lattice level instabilities in certain crystals. Equilibrium solutions and their stability were examined as a function of temperature to determine the crystal structures emerging from critical bifurcation points. However, the authors pointed out that their model does not predict any temperature-induced proper martensitic transformations because all the equilibrium paths with low symmetry which are observed in shape-memory alloy martensites were found to be unstable for the range of temperatures investigated. Shortly after, [25, 26] developed a two-dimensional molecular dynamics model for the investigation of crystalline austenite-martensite phase transitions. The discrete model consisted of two types of mass points with interaction functions of Lennard-Jones type which allowed to create stable square crystalline lattices which transformed into sheared variants representative of the martensitic phases as a function of the applied temperature. Unlike previous work of [24], the numerical simulations of [25, 26] were shown to reproduce the fundamental features of the martensitic transformation in shape memory alloys, e.g., the austenite being stable at high temperature and the martensite at lower temperature, unloaded body transforms reversibly between austenite and martensite under temperature control, etc. Additional molecular dynamics simulations were performed by [27] to study post-transformation microstructure and moving austenite–martensite interfaces. The calculations yielded to martensitic morphologies very similar to real materials, including the nucleation of wedge-shaped, twinned martensite plates, plate growth at narrow travelling transformation zones, etc. The molecular dynamics model of [25, 26] was further applied by [28] to study microstructure evolution during cyclic martensitic transformations. The cyclic loading was shown to produce the accumulation of lattice defects so as to establish new microstructural elements which represent a memory of the previous morphologies. These new elements were self-organised and they provided a basis of the reversible shape memory effect in the model material. On the other hand, [29] carried out atomistic calculations using a two-dimensional diatomic lattice
simplest system that exhibits a multi-well macroscopic potential—to study the nucleation and kinetics of shear induced detwinning in shape-memory alloys with interatomic potential described by the Lennard-Jones. The calculations showed that the transformation rate is an increasing function of shear stress and temperature, and that the transverse ledge propagation is the mechanism underlying twin-boundary motion. Moreover, the effect of geometric nonlinearity on the stability of two-dimensional mass-spring lattices was studied by [30], who derived the critical conditions for the mechanical behavior of the springs, and the critical strain in the springs, for which the Cauchy-Born hypothesis fails. More recently, [31] investigated the equilibrium configurations and stability properties of multi-atomic crystalline systems to determine the loading conditions leading to solid-to-solid martensitic phase transformations. Stability criteria with respect to perturbations at the atomic scale (phonon-stability) and at the continuum scale (homogenized-continuum-stability) were reviewed and the so-called Cauchy-Born stability condition was introduced to provide an intermediate criterion by considering perturbations at both the atomistic and continuum scales. [31] provided a unified presentation of these stability criteria for crystalline solids in equilibrium configurations consistent with Cauchy-Born kinematics (uniform deformation and internal shifts of sub-lattices).

In the past, innovative mechanical metamaterial designs have been proposed that exploit thermomechanical coupling to generate interesting functionalities such as thermal cloaking [32], structures with negative or low thermal expansion coefficients [33, 34, 35, 36], shape-morphing structures [37], or materials that can be actuated using shape memory polymers [38, 39]. Our main goal in this work is to guide the design of structural lattices with bars of different materials so that the convexity of the potential energy can be controlled with the temperature in a robust manner. To accomplish this objective rigorously, we emphasize the analytical route and refer to other works where similar ideas have been explored numerically (see, e.g., [40]).

A complete structural analysis of bistable, reversible lattice materials demands tools from nonlinear analysis that can be used to explore the entire design space, both qualitatively and quantitatively. In particular, a rigorous stability analysis is mandatory to identify the main parameters that affect the stability of the structure, their critical values when the stability shifts, and a full characterization of the stability regions. In addition to these preliminary results, a robust design requires the identification of all the physical parameters that affect qualitatively the nature of the stability, for example breaking the symmetry of the solution. For this, we have chosen to employ singularity theory [41, 42, 1], a branch of mathematics that provides a unified methodology to systematically study bifurcation problems, revealing simultaneously all possible perturbations of the governing equations that qualitatively modify the stability of the system. Guided by this theory, the design space is simplified to the maximum and numerical techniques can then be used to identify the numerical values of the critical parameters. Remarkably, this approach guarantees that there remain no hidden parameters that can affect the bifurcation behavior of the system.

Singularity theory provides a complete characterization of the stability and bifurcation diagram of a periodic lattice. Also, it reveals unambiguously the geometrical and/or material parameters that can be modified in order to change the shape of this diagram. This information is critical for the design of bistable,
reversible lattices, since it spares the effort to look for fruitless parameter combinations and reduces the exploration of the design space. After concluding this analysis, we have explored numerically selected examples involving finite lattices that possess the bi-stability and reversibility features. These boundary value problems illustrate that the design is robust enough to carry on even when complete periodicity is loss and hint at potential applications of these lattices.

A summary of the remainder of this work is as follows. In Section 2 we use singularity theory to analyze periodic two-dimensional lattices consisting of thermo-elastic bars, identifying the parameters that guarantee the desired bi-stability and reversibility. One crucial result of this part is the complete characterization of a phase diagram for the structure, one that can be later be used to select the geometry and material properties of the lattices. Numerical examples of this lattice types will be shown in Section 3 that, guided by the previous theoretical results, propose finite size lattices which exhibit the features of bi-stability and reversibility. The analysis of Section 2 is extended to three-dimensional lattices in Section 4. These results are exploited in Section 5 to carry out more complex three-dimensional examples of lattices under full thermo-mechanical loading cycles and reveal some shape-memory-like behavior. Section 6 will close the article with a summary of the most relevant results and some conclusions. For completeness and reference, the key concepts of singularity theory are collected in A.

2 2D unit cell design of thermally reversible metamaterials

2.1 Description and kinematics

In this section, we present a design for two-dimensional, bistable, lattice-based structures that are thermally reversible and use singularity theory as a guide. We use a bottom-up approach and study first a representative unit cell whose behavior, when arranged periodically, will result in a structure with the desired thermomechanical properties.

The unit cell consists of a deformable square frame of sides with length $L$ as depicted in Fig. 2. It is built with elastic springs whose thermoelastic response is known. More specifically, the elastic constant and thermal expansion coefficient of the springs in the outer frame are denoted as $k_{\text{out}}, \alpha_{\text{out}}$, respectively, while the internal springs, in turn, have elastic constant and thermal expansion coefficient $k_{\text{in}}, \alpha_{\text{in}}$, respectively. Boundary conditions are applied on the two bottom vertices as illustrated in Fig. 2.

We study first the solution manifold for this structure and discuss the singularities that might appear due to temperature changes. Motivated by its application to the analysis of periodic lattices, we analyze all possible affine deformations of the frame, namely, those of the form

$$x = FX + c ,$$

where $X \in \mathbb{R}^2$ denotes the undeformed position of a point in the frame, $x$ is its deformed position, and $F, c$ are a constant tensor and vector, respectively. Imposing boundary conditions that preclude any rigid body motion, the vector $c$
Figure 2: Schematic of square 2D unit cell of length $L$ that has diagonal springs with stiffness and coefficient of linear thermal expansion $k_{in}, \alpha_{in}$ (shown in red) and an outer frame with properties $k_{out}, \alpha_{out}$. The system is characterized by displacements $u_1, u_2$ and $u_3$ and to measure the force-displacement response a force $\tilde{F}$ is applied on the top right corner.

must vanish and $F$ must be

$$F = \begin{bmatrix} F_{11} & F_{12} \\ 0 & F_{22} \end{bmatrix},$$

(2)

for some constants $F_{11}, F_{12}, F_{22}$. Under these conditions, the motion of the cell is determined by three displacements, $u_1, u_2$ and $u_3$ (cf. Fig. 2) that satisfy

$$u_1 = F_{12}L, \quad u_2 = (F_{22} - 1)L, \quad u_3 = (F_{11} - 1)L.$$ (3)

2.2 Equilibrium equations

To model the thermoelastic behavior of each spring we choose a free energy with expression

$$\hat{V}(\lambda, \theta) = \frac{k_i}{2} \log^2 \frac{\lambda_i}{\lambda_i^0} - \alpha_i k_i (\theta - \theta_{ref}) \log \frac{\lambda_i}{\lambda_i^0} + \Psi(\theta), \quad \Psi(\theta) = c_0 \left( \theta - \theta_{ref} - \theta \log \frac{\theta}{\theta_{ref}} \right).$$ (4)

where $c_0$ denotes the heat capacity, $\theta, \theta_{ref}$ are the current and reference temperatures of the structure, respectively, $\lambda_i, \lambda_i^0$ are the deformed and natural lengths of the spring and $k_i, \alpha_i$ are its elastic constant and the coefficient of linear thermal expansion and $\Psi$ is a purely thermal contribution to the free energy. We have chosen a specific form for the free energy function which is proportional to the square of the logarithmic strain so that the elastic force softens for large strains and also is non-symmetric for tension and compression. We note, however, that the methodology and analysis shown below can be performed without loss of generality for any other form of the free energy function (see, e.g., [23]).

Expressing the deformed lengths $\lambda_i$ in Eq. (4) as functions of the displacements $\mathbf{u} = (u_1, u_2, u_3)$, and adding the free energy of all the springs, the total
free energy of the system after a change in temperature $\Delta \theta$ reads

$$
\tilde{V}(u, \Delta \theta) = \sum_i \tilde{V}(\lambda_i(u), \theta_{ref} + \Delta \theta),
$$

where $\Delta \theta = \theta - \theta_{ref}$ is the temperature increase with respect to the reference temperature. Defining the normalized temperature $\Theta = \alpha_{out} \Delta \theta$, a normalized free energy $\mathcal{V}$ can be introduced via the relation

$$
\tilde{V}(u, \Delta \theta) = k_{out} \mathcal{V}(u, \Theta; \frac{k_{in}}{k_{out}}, \frac{\alpha_{in}}{\alpha_{out}}).
$$

The equilibrium equations for the frame are obtained by taking the derivatives of the free energy with respect to the displacements and, following the notation of A, they read

$$
g(u, \Theta; \frac{k_{in}}{k_{out}}, \frac{\alpha_{in}}{\alpha_{out}}) = \frac{\partial \mathcal{V}}{\partial u}(u, \Theta; \frac{k_{in}}{k_{out}}, \frac{\alpha_{in}}{\alpha_{out}}) = 0.
$$

This is a system of three nonlinear equations with three unknowns that depend on a control parameter, the nondimensional temperature $\Theta$, and two physical parameters of the structure $k_{in}/k_{out}$ and $\alpha_{in}/\alpha_{out}$.

### 2.3 Bifurcation

We investigate the solutions of Eq. (7) for some fixed values of the parameters while the control variable, the temperature, is varied. In particular, we examine situations where the number of solutions of Eq. (7) changes with temperature. For this purpose, we use singularity theory. The basic parts of this theory are summarized in A, and we refer to the monograph by Golubitsky and Schaeffer [41, 43] for full details and complete proofs of the results presented. Note that similar analysis on bifurcation theory with application of buckling problems can be found, for instance, in [44].

Let us choose, for example, $k_{in}/k_{out} = 0.5$ and $\alpha_{in}/\alpha_{out} = 1000$. Our strategy consists, first, in identifying singular points and then, if they exist, using singularity theory to investigate potential bifurcations. We select the reference temperature $\theta_{ref}$ such that the system is stress-free in its initial configuration and gradually reduce the temperature from $\Theta = \alpha_{out} \Delta \theta = 0$.

To begin the analysis, we first construct the Jacobian, $L = D_1 g$ which is the Hessian of the free energy (6), and use its spectrum to characterize the stability of the equation using the classical Lagrange-Dirichlet criterion. For our particular example, at $\Theta = 0$, i.e. at the stress-free configuration, all the eigenvalues of $L$ are positive and the structure is stable. As the temperature is reduced, we find at a critical temperature that one of the eigenvalues of $L$ turns negative and the point where the eigenvalue vanishes corresponds to the singular point. Interpreting this process physically, as we reduce the temperature, and due to the differences between the coefficient of thermal expansion of the outer frame and the diagonal springs, thermal forces are induced which eventually lead to non-trivial solutions. For this particular example, the point of singularity is at $(u_1, u_2, u_3, \Theta^*) = (0.0, -0.118L, -0.118L, -0.000625)$.

Once the singular point is identified, we apply the Liapunov-Schmidt reduction (cf. A.3). This manipulation allows to obtain, from the system of
equations (7), a scalar equation that characterizes the singularity. We will then test this reduced equation for the recognition conditions (see A.1) to resolve the nature of the bifurcation, if any.

To begin the reduction process, we will first make a translation of the coordinates to $\hat{u} = u - u^s$, $\hat{\Theta} = \Theta - \Theta^s$, so that the point of singularity is now at the origin $(\hat{u}, \hat{\Theta}) = (0, 0)$. The Jacobian $\mathcal{L}$ at $(\hat{u}, \hat{\Theta}) = (0, 0)$ is

$$
\mathcal{L}(0, 0) = \begin{bmatrix}
0 & 0 & 0 \\
0 & 3.214 & 0 \\
0 & 0 & 3.214
\end{bmatrix}. \quad (8)
$$

Clearly, at the point of singularity, rank $\mathcal{L} = 3 - 1 = 2$ and we can follow the procedure of A.3 to reduce the system of equations (7). First, we must choose the vector spaces $\mathcal{M}$ and $\mathcal{N}$ that additively split $\mathbb{R}^3$ into $\ker \mathcal{L} \oplus \mathcal{M}$ and $\mathcal{N} \oplus \text{range } \mathcal{L}$. The choices for $\mathcal{M} = \text{range } \mathcal{L}$ and $\mathcal{N} = \ker \mathcal{L}$ are reasonable choices. Next, we define the maps $E : \mathbb{R}^3 \to \text{range } \mathcal{L}$ and $\mathcal{L}^{-1} : \text{range } \mathcal{L} \to \mathcal{M}$ as

$$
E = \begin{bmatrix}
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix}
\quad \text{and} \quad
\mathcal{L}^{-1} = \begin{bmatrix}
0 & 0 & 0 \\
0 & 0.311 & 0 \\
0 & 0 & 0.311
\end{bmatrix}. \quad (9)
$$

Note that even if $k_{in}/k_{out}, \alpha_{in}/\alpha_{out}$ are changed and provided that singular points still exist, the structure of $\mathcal{L}$ and the above choices do not change. From elementary linear algebra, $\ker \mathcal{L}$ is spanned by the basis vector $(1, 0, 0)$ and $\text{range } \mathcal{L}$ is spanned by the basis vectors $(0, 1, 0)$ and $(0, 0, 1)$. Thus, for the choice $v_0 \in \ker \mathcal{L}$ and $v_0^* \in (\text{range } \mathcal{L})^\perp$ one can select, for example, $v_0 = (1, 0, 0)$ and $v_0^* = (1, 0, 0)$. This completes the definition for the reduction process and we now test directly for the derivatives of Eqs. (49a)-(49e). For the case $k_{in}/k_{out} = 0.5$ and $\alpha_{in}/\alpha_{out} = 1000$, these derivatives evaluate to

$$
g_x(0, 0) = 0, \\
g_{xx}(0, 0) = 0, \\
g_{xxx}(0, 0) = 1.818, \\
g_{\Theta}(0, 0) = 0, \\
g_{\Theta x}(0, 0) = 513.739. \quad (10)
$$

The recognition problem for the pitchfork bifurcation (cf. Eq.(36)) is satisfied by relations (10). Moreover, since $g_{xxx} g_{\Theta x} > 0$, it can be further concluded that the singularity identified corresponds to an inverted pitchfork (see A.1).

Let us now complement the information obtained from singularity theory with numerical solutions. Let $\mathbf{u}$ be the vector of displacements for the structure and consider the application of an external force on the top right corner of the frame of value $\tilde{F} = \Lambda \bar{F}$, where $\Lambda$ is a load scaling factor and $\bar{F}$ is a unit point force in the horizontal direction (cf. Fig. 2). Under these conditions, the free energy of the frame is

$$
\tilde{V}(\mathbf{u}, \Theta; \frac{k_{in}}{k_{out}}, \frac{\alpha_{in}}{\alpha_{out}}) = k_{out} V(\mathbf{u}, \Theta; \frac{k_{in}}{k_{out}}, \frac{\alpha_{in}}{\alpha_{out}}) - \Lambda \mathbf{u}^R, \quad (11)
$$

where $u^R = \hat{u}_1 + \hat{u}_3$ is the horizontal displacement of the top right corner. Note that the first row and column of the Jacobian (8) are zero suggesting that non-trivial solutions might appear in the $u_1$ direction.
Given the lack of convexity of the free energy for arbitrary temperatures, the system is expected to exhibit instabilities. Hence, if we employ a Newton-type solver to trace the equilibrium path of the structure, we might encounter numerical problems when the tangent stiffness becomes singular. The standard remedy for this situation consists in employing a path-following technique based on the arc-length method [45, 46]. The general idea of this approach consists in modifying the Newton solution, appending a new unknown, the generalized arc-length of the solution, and a new equation to the global system of equilibrium equations. The arc-length s is defined over the generalized solution space, and its differential is

\[ ds^2 = d\lambda^2 + |d\mathbf{u}|^2. \]  

(12)

With this definition, at every step of the incremental solution for the structural equilibrium, the following additional equation needs to be added

\[ f(\Delta \mathbf{u}, \Delta \lambda) = |\Delta \mathbf{u}|^2 + \Delta \lambda^2 \psi^2 - \Delta s^2 = 0. \]  

(13)

Here, \( \Delta \mathbf{u} = \mathbf{u} - \mathbf{u}_{i-1} \) and \( \Delta \lambda = \lambda - \Lambda_{i-1} \), and the subscript \((i-1)\) refers to the last converged solution. A scaling factor \( \psi \) is introduced into the constraint \((13)\) to render it dimensionally consistent. In practice, however, \( \psi \) is often chosen to be zero (see, e.g., [47] for more details on the continuation technique).

Fig. 3(a) shows the equilibrium path for a design with \( k_m/k_{out} = 0.5 \) and \( \alpha_m/\alpha_{out} = 1000 \). It can be observed in this figure that when the temperature is
reduced, the force-displacement response turns non-monotonic. Fig. 3(b) plots the bifurcation diagram of the horizontal displacement, $u_1$, as a function of the normalized temperature $\Theta$ which confirms the inverted pitchfork prediction by singularity theory (see Section A.1). Moreover, equilibrium shapes of the cell at temperatures below the bifurcation point are shown in the inset of Fig. 3(b). The solution at the center is unstable and under any perturbation the cell snaps to either of the stable configurations to the left or to the right. Figs. 3(c),(d) plot the bifurcation diagram for the displacements $u_2, u_3$. These have only two branches below the bifurcation point since, due to symmetry, the two stable branches in Fig. 3(b) coincide in Figs. 3(c) and (d).

![Figure 4](image_url)

Figure 4: Phase diagram of the unit cell for different structural parameters $k_{in}/k_{out}$ and $\alpha_{in}/\alpha_{out}$. Gray region corresponds to monostable behavior while colored regions represent bifurcation behavior between a temperature range of $\Theta = 0$ to $\Theta = -1.0 \cdot 10^{-3}$ with the colormap showing the bifurcation temperature. The bifurcation diagrams corresponding to the symbols in different regions of the phase-diagram are shown on the right.

Finally, to study the influence of the ratios $k_{in}/k_{out}$ and $\alpha_{in}/\alpha_{out}$ we systematically vary these parameters and we search for bifurcations between a range of normalized temperatures varying from $\Theta = 0$ to $\Theta = -1.0 \cdot 10^{-3}$. This corresponds to a change in a temperature of 100 °C if $\alpha_{out} \approx 10^{-5}(°C)^{-1}$. Fig. 4 depicts this phase diagram. In the figure, gray regions correspond to points where no bifurcations are observed, while the colored regions represent bifurcation behavior with the colormap indicating the bifurcation temperature. Note that as $k_{in}/k_{out}$ decreases, the minimum value of the ratio $\alpha_{in}/\alpha_{out}$ for which a bifurcation occurs also decreases. In fact, when $k_{out} \gg k_{in}$ the bistable behavior of the structure only takes place for $\alpha_{in}/\alpha_{out} > 600$ (see also Section 2.4.1). A key outcome of the methodology developed in this article is that it simplifies the identification of the range of values for $k_{in}/k_{out}$ and $\alpha_{in}/\alpha_{out}$ for which the structural lattice becomes bistable and thermally reversible.
2.4 Perturbation analysis of the 2D unit cell

One of the central themes of singularity theory is the study of the effect of perturbations on the solution set of an equation. In particular, the universal unfolding of the pitchfork bifurcation is of the form

\[ G(x, \lambda, \alpha_1, \alpha_2) = x^3 - \lambda x + \alpha_1 + \alpha_2 x^2. \]  

(14)

where \( \alpha_1, \alpha_2 \) are auxiliary parameters (see A.2), and thus it contains all the qualitatively possible perturbations of the pitchfork. Based on this result, we proceed now to classify all the possible perturbations of the unit cell, separating those that appear in the unfolding from those whose effects are qualitatively irrelevant.

Considering again the periodic frame of Fig. 2, we study the effect of perturbations on the physical parameters of the system. First, let the stiffness and thermal expansion coefficient of one of the diagonal springs be perturbed as in \( k_{in} \to k_{in}(1 + \delta k_{in}) \) and \( \alpha_{in} \to \alpha_{in}(1 + \delta \alpha_{in}) \), respectively, where both \( \delta k_{in} \) and \( \delta \alpha_{in} \) are non-dimensional parameters (see Fig. 5(a)). In terms of these auxiliary parameters, the free energy of the system can be written as:

\[ \tilde{V}(u, \Delta \theta) = k_{out} \mathcal{V}(u, \Theta, \delta k_{in}, \delta \alpha_{in}; \frac{k_{in}}{k_{out}}, \frac{\alpha_{in}}{\alpha_{out}}). \]  

(15)

The equilibrium equation for the frame depends now on the auxiliary parameters as:

\[ G(u, \Theta, \delta k_{in}, \delta \alpha_{in}; \frac{k_{in}}{k_{out}}, \frac{\alpha_{in}}{\alpha_{out}}) = \frac{\partial \mathcal{V}}{\partial u}(u, \Theta, \delta k_{in}, \delta \alpha_{in}; \frac{k_{in}}{k_{out}}, \frac{\alpha_{in}}{\alpha_{out}}) = 0. \]  

(16)

The main goal now is to investigate the influence of the auxiliary parameters on the bifurcation diagram. This can be tested by examining if the auxiliary parameters generate a universal unfolding of the original bifurcation \( g(u, \Theta) \). To test for universal unfoldings, we must first verify that under the absence of the auxiliary parameters, we recover the original equilibrium equation \( g \). Clearly, for \( \delta k_{in} = \delta \alpha_{in} = 0 \) this is satisfied, since

\[ G(u, \Theta, 0, 0; \frac{k_{in}}{k_{out}}, \frac{\alpha_{in}}{\alpha_{out}}) = g(u, \Theta; \frac{k_{in}}{k_{out}}, \frac{\alpha_{in}}{\alpha_{out}}). \]  

(17)

Next, for the unfolding \( G \) to perturb the bifurcation diagram, for \( \delta k_{in}, \delta \alpha_{in} \neq 0 \), the recognition conditions of the pitchfork (Eqs. (36)), i.e. \( G = G_x = G_{\Theta \theta} = G_{xx} = 0 \) and \( G_{x\Theta}G_{\theta x} \neq 0 \) (where \( G \) is the reduced equation of \( \tilde{G} \) after the Liapunov-Schmidt reduction) must not be valid. If the recognition conditions are satisfied, then by equivalence of Eq. (37), \( G \) can be transformed to the normal form of the pitchfork, and the auxiliary parameters can be replaced by an equivalent single bifurcation parameter, while the bifurcation diagram remains unperturbed. Indeed, for \( \delta k_{in}, \delta \alpha_{in} \neq 0 \) and \( k_{in}/k_{out} = 0.5, \alpha_{in}/\alpha_{out} = 1000 \), and using the formulae of the Liapunov-Schmidt reduction (Eqs. (49a)-(49e)), we find that \( G_x \neq 0 \) and \( G_{\Theta \theta} \neq 0 \), and hence the recognition conditions of the pitchfork bifurcation are not verified. Finally to determine if Eq. (16) is an universal unfolding of \( g \), we test for the recognition problem of the universal unfolding of the pitchfork, i.e.,
Figure 5: Behavior of the structure under perturbation of some parameters of the unit cell. In (a) the stiffness and the coefficient of thermal expansion of one of the diagonal springs is slightly perturbed by $\delta k_{in}$ and $\delta \alpha_{in}$ (shown in green), respectively, while in (b) the same properties but of a member in the outer frame are perturbed (also shown in green) by $\delta k_{out}$ and $\delta \alpha_{out}$, respectively. In (c) the aspect ratio of the unit cell is modified. Moreover, (d), (e) and (f) show the bifurcation diagrams for (a), (b) and (c), respectively. All the numerical examples use $k_{in}/k_{out} = 0.5$ and $\alpha_{in}/\alpha_{out} = 1000$.

\[
\begin{bmatrix}
0 & 0 & g_{x\Theta} & g_{xxx} \\
0 & g_{\Theta x} & g_{\Theta x} & g_{\Theta xx} \\
g_{\Theta k_{in}} & G_{\Theta k_{in}} & G_{\Theta k_{in}} & G_{\Theta k_{in}xx} \\
g_{\Theta \alpha_{in}} & G_{\Theta \alpha_{in}} & G_{\Theta \alpha_{in}} & G_{\Theta \alpha_{in}xx}
\end{bmatrix}
= \begin{bmatrix}
0 & 0 & 513.739 & 1.81813 \\
0 & 513.739 & 0 & 0 \\
0.142 & 0.0321 & -255.01 & -0.164 \\
0.177 & -0.161 & -319.06 & -90.5
\end{bmatrix}
= 3.38 \times 10^6 \neq 0,
\]

where $g$ and $G$ are the reduced equations of $g$ and $G$, respectively, after the Liapunov-Schmidt procedure and the derivatives are evaluated using (Eqs. (49a)-(49g)) at the point of singularity with $\delta k_{in} = \delta \alpha_{in} = 0$. Since the condition for the recognition problem of the universal unfolding for the pitchfork is met, $G(u, \Theta, \delta k_{in}, \delta \alpha_{in}; k_{in}, \alpha_{in})$ is an universal unfolding of $g(u, \Theta, k_{in}, \alpha_{in})$ and it contains all the possible perturbations of the pitchfork. For small changes in $\delta k_{in}$ and $\delta \alpha_{in}$, the bifurcation diagram is expected to change drastically (see also Fig. 20) as confirmed by numerical solutions plotted in Fig. 5(d).

Next, we perturb the stiffness and coefficient of thermal expansion of one of the members in the outer frame (see Fig. 5(b)) or the aspect ratio of the frame (see Fig. 5(c)). For both cases, we can construct the equilibrium equations $G$, the unfolding of $g$, and verify that $G$ satisfies the recognition problem of the pitchfork bifurcation for non-zero perturbation. Thus, doing a change of
coordinates, the auxiliary parameters in this case can be completely replaced to reduce $G$ to the normal form of the pitchfork bifurcation. We can conclude that these perturbations should not change the bifurcation diagram at all as shown by their respective numerical solutions in Figs. 5(e) and 5(f).

Figure 6: A small defect $\delta_0$ is introduced at the support that also perturbs the bifurcation diagram as shown in (b).

Using the idea of universal unfoldings of singularity theory, we have presented a novel strategy where one can directly perform an analytical perturbation analysis to determine the main physical parameters that can affect the bifurcation diagram of the structure. This is a key outcome of this work and it helps in assessing the manufacturability of a lattice, enabling the identification of the critical structural features where defects need to be avoided. In this structure, for example, a defect in a diagonal spring will have a dramatic effect in the mechanical response of the lattice, while defects in the springs of outer frame do not lead to qualitative differences in the bifurcation diagram of the structure. Additionally, while we showed that perturbing the properties of one of the diagonal springs generates a universal unfolding for the problem, it need not be the only parameter that can affect the bifurcation diagram. For instance, a small defect at the support can also perturb the stability of the lattice (see Fig. 6). Singularity theory shows, however, that this additional perturbation can not generate a qualitatively different type of bifurcation from the ones already identified.

2.4.1 Perturbation analysis in the limit $k_{\text{out}} \gg k_{\text{in}}$

Singularity theory proves that there are exactly are four qualitatively different types of perturbations of the pitchfork bifurcation that depend on $\alpha_1$ and $\alpha_2$ in the universal unfolding (see A.2). In Fig. 5(a) we have shown that the auxiliary parameters $\delta k_{\text{in}}$ and $\delta \alpha_{\text{in}}$ generate a universal unfolding of the unperturbed problem. In practice, however, it is hard to relate the physical parameters $\delta k_{\text{in}}, \delta \alpha_{\text{in}}$ to the canonical parameters of the universal unfolding $\alpha_1, \alpha_2$ and thus mostly result in the more commonly observable perturbation of the pitchfork (Fig. 5(d)).

In this section, we pay specific attention to the limit case $k_{\text{out}} \gg k_{\text{in}}$ anticipated in Fig. 4 for which the value $\alpha_{\text{in}}/\alpha_{\text{out}}$ triggering the bistable response of the structure is minimum. In the limit $k_{\text{out}} \gg k_{\text{in}}$, i.e. when the members
The equilibrium equation of the rigid frame is modified to

\[ \bar{u}_1 = u_1/L \]

\[ \Theta = \alpha_{in} \Delta \theta \]

\[ \delta \kappa_{in} = -0.03, \delta \alpha_{in} = 0 \]

\[ \delta \kappa_{in} = 0.03, \delta \alpha_{in} = 0 \]

Stable

Unstable

of the outer frame are almost rigid, the system can be simplified and a single nonlinear equation is required to describe the equilibrium of the lattice. For \( k_{out} \gg k_{in} \), we assume \( u_3 \approx 0 \) and the displacements \( u_1 \) and \( u_2 \) are related by

\[ u_1^2 + (1 - u_2^2) = L^2. \]

In this case, the free energy of the system simplifies to

\[ \mathcal{V}_{\text{rigid}}(u_1, \Theta) = \frac{k_{in}}{2} \left[ \log^2 \left( \frac{1 - u_1}{L} \right) + \log^2 \left( \frac{1 + u_1}{L} \right) \right] - k_{in} \Theta \left[ \log \left( \frac{1 - u_1}{L} \right) + \log \left( \frac{1 + u_1}{L} \right) \right] + \psi(\theta_{ref} + \alpha_{in} \Theta). \]

The equilibrium equation of the rigid frame is

\[ g_{\text{rigid}}(u_1, \Theta) = -\frac{\partial \mathcal{V}_{\text{rigid}}}{\partial u_1}(u_1, \Theta). \]

Eq. (21) has a singular point at \((u_1, \Theta) = (0, -0.5)\). Since Eq. (21) is already a scalar equation, one can apply singularity theory directly to verify that the nature of the bifurcation is indeed a pitchfork (see A.1). In particular, when one of the diagonal springs is perturbed by \( \delta \kappa_{in} \) and \( \delta \alpha_{in} \), the equilibrium equation is modified to

\[ G_{\text{rigid}}(u_1, \Theta, \delta \kappa_{in}, \delta \alpha_{in}) = -\frac{\partial \mathcal{V}_{\text{rigid}}}{\partial u_1}(u_1, \Theta, \delta \kappa_{in}, \delta \alpha_{in}). \]
Approximating Eq. (22) with a third-order Taylor expansion around the point of singularity \((u_1, \Theta) = (0, -1/2)\) we get

\[
G(u_1, \Theta, \delta k_{in}, \delta \alpha_{in}) \approx \frac{1 - (1 + \delta k_{in})(1 + \delta \alpha_{in})}{2} - \frac{(1 + \delta k_{in})(\delta \alpha_{in}) u_1}{L} + (1 + \delta k_{in}) \delta \alpha_{in} (\Theta + 1/2) \\
+ \frac{(3\delta k_{in} + 2)}{2} - 2(1 + \delta k_{in})(1 + \delta \alpha_{in}) \frac{1}{2} \left(\frac{u_1}{L}\right)^2 \\
+ (1 + (1 + \delta k_{in})(1 + \delta \alpha_{in})) \frac{u_1}{L} (\Theta + 1/2) \\
+ 2(1 + \delta k_{in}) \delta \alpha_{in} (\Theta + 1/2) \left(\frac{u_1}{L}\right)^2 \\
+ \frac{5 + 11(1 + \delta k_{in}) - 6(1 + \delta k_{in})(1 + \delta \alpha_{in})}{6} \left(\frac{u_1}{L}\right)^3.
\]

Comparing Eq. (23) with the normal form of the universal unfolding of the pitchfork (Eq. (14)), we can relate the constants \(\delta k_{in}\) and \(\delta \alpha_{in}\) with the parameters \(\alpha_1\) and \(\alpha_2\). This then allows us to probe the perturbed bifurcation diagrams for different values of \(\delta k_{in}\) and \(\delta \alpha_{in}\) as shown in Figs. 7(b)-(e). Thus, when closed-form solutions are available, it is possible to obtain the other two perturbations of the pitchfork that have the kinked shape shown in Figs. 7(c)-(d). For this, one must use specific values of \(\delta k_{in}\) and \(\delta \alpha_{in}\) that are far from one and could not have been guessed, unless guided by singularity theory. This is another novel result of the methodology developed in this paper.

3 Effective macroscopic behavior of 2D lattices

We would like to investigate next if lattices based on the cell designed in Section 2 exhibit a behavior that is similar to the one of the unit cell. Infinite periodic lattices can undergo affine deformation such as the one described in Eq. (1) and therefore certainly share the unit cell behavior. We are interested here, however, in finite lattices that can exhibit complex motions and whose boundary effects might interfere with the stability properties.

Guided by the analysis of the unit cell, we now build macroscopic lattices stacking unit cells and we check using simulations if the response of the unit cell is inherited at the macroscopic scale. We begin by analyzing a one-dimensional array of \(N\) unit cells where the nodes at the bottom are constrained to move in the horizontal direction and the bottom-left corner is completely fixed. We choose parameters \(k_{in}/k_{out} = 0.5\) and \(\alpha_{in}/\alpha_{out} = 1000\) (the same values used in Fig. 5) for which the unit cell exhibits a pitchfork bifurcation. We begin our analysis by ramping down the temperature from \(\Theta = 0\) to \(\Theta_r = -8 \cdot 10^{-4}\) (which is below the bifurcation temperature) employing a quasi-static simulation with Newton’s method. For two lattice structures, \(N = 3\) and \(N = 5\), the deformed structures are shown in Fig. 8(a)(i) and Fig. 8(b)(i), respectively. Then we measure the force-displacement response by applying a point force, \(F\) on the nodes on the top surface using the arc-length method as detailed in Section 2. These curves are shown in Figs. 8(a)-(b), respectively, where (i), (ii) and (iii) are the equilibrium positions. State (i) represents an unstable configuration that can snap to either (ii) or (iii) under small perturbations.
Figure 8: 1D array of $N$ unit cells: (a) and (b) show the force-displacement response for $N = 3$ and $N = 5$, respectively, at $\Theta_r = -8 \cdot 10^{-4}$. The deformed configurations (i), (ii) and (iii) correspond to the equilibrium solutions in panels (a) and (b), respectively. Shown in grey in (i) is the stress-free initial configuration at $\Theta = 0$. The parameters chosen for both panels are $k_{in}/k_{out} = 0.5$, $\alpha_{in}/\alpha_{out} = 1000$.

Next, we analyze a two-dimensional stacking of $N_x \times N_y$ unit cells. To study the whole thermomechanical problem, we use a dynamic relaxation technique designed to simulate structures with complex nonlinearities and instabilities. In this method, the static solution is obtained by determining the steady-state response to the transient dynamic analysis of an ancillary system. Since the transient solution is not necessary, fictitious mass and damping terms are added to accelerate the convergence to the stationary solution (see [48, 49] for details on the fundamentals and implementation of the method).

Fig. 9 shows the complete thermomechanical cycle of a lattice. In its initial state ($\Theta = 0$), the structure is in a stress-free configuration corresponding to Fig. 9(a). When the structure is cooled down to $\Theta = -8 \cdot 10^{-4}$, the symmetric configuration looses its stability, as predicted by the unit cell analysis. As in any numerical computation, round-off errors trigger random perturbation of the equilibrium and hence the cells snap to either the left- or right-tilted (stable) configurations, as depicted in Fig. 9(b). If, still at the same temperature, shearing forces are applied on the lattice, it can deform to either configuration (c) or (d). The colorbar in (b), (c) and (d) is the axial strain and it is interesting to note that both the diagonal strings are in tension while the outer members are in compression which is slightly counter-intuitive. Finally, if the temperature of the structure is raised to its initial value ($\Theta = 0$), the symmetric configuration becomes the only stable one and the system returns to its initial position. Note that all the steps of the thermomechanical cycle of the structure
Figure 9: Shape memory behavior of the lattice: The stress-free configuration (a) is stable at $\Theta = 0$. When the temperature is reduced down to $\Theta = -8 \cdot 10^{-4}$, the structure changes its shape to (b), where some cells buckle to the left and others to the right. Upon shearing at “cold” temperature, the structure can deform from (b) to (c) or (d). Moreover, configuration (a) can be completely recovered using a heat treatment, thus showing shape memory behavior. Data: $20 \times 20$ unit cells and $k_{\text{in}}/k_{\text{out}} = 0.5$, $\alpha_{\text{in}}/\alpha_{\text{out}} = 1000$. The colorbar of the lattice structure is the axial strain in the bars which show both the diagonal members in tension while the outer frame is in compression.

were predicted by the singularity theory, as illustrated by the shaded inverted pitchfork included in the graph behind the contours obtained from the finite element calculations.

This cycle shows that, with the chosen parameters, the behavior of the lattice mimics that of a shape memory material. By tailoring the response of the unit cell, a macroscopic behavior is obtained which exhibits a single stable phase at “high” temperature, and several stable phases at “low” temperature that are energetically equivalent. Remarkably, and similarly to true shape-memory materials, the thermomechanical cycle is completely reversible.

4 3D unit cell design of thermally reversible metamaterials

A natural extension of the two-dimensional lattices studied in Section 3 to three-dimensional geometries can be pursued by considering orthorhombic lattices with a rectangular base ($L_1$ by $L_2$) and height ($L_3$) as shown in Fig. 10. We study two types of such lattices: (a) fcc-type lattices where edges and face diagonals are bars with stiffness and coefficient of thermal expansion $k_{\text{out}}, \alpha_{\text{out}}$
while body diagonals have properties \(k_{\text{in}}, \alpha_{\text{in}}\) respectively; (b) bcc-type lattices that are the same as in (a), but without bars on the face diagonals.

Figure 10: 3D orthorhombic unit cells where (a) is for convenience referred to as an fcc type lattice that has bars along the edges and the face diagonals with properties \(k_{\text{out}}, \alpha_{\text{out}}\) and body diagonals with properties \(k_{\text{in}}, \alpha_{\text{in}}\) while (b) is a bcc type lattice that only has bars along the edges and the body diagonals with properties \((k_{\text{out}}, \alpha_{\text{out}}), (k_{\text{in}}, \alpha_{\text{in}})\) respectively.

Similarly to the analysis of Section 2.4, we consider all possible affine deformations of the frame with expression

\[
x = FX + c,
\]

where \(X \in \mathbb{R}^3\) denotes the undeformed position of a point in the frame, \(x\) is its deformed position, and \(F, c\) are a constant tensor and vector, respectively. Boundary conditions are imposed as shown in Figs. 10(a),(b). Here one vertex is fixed and three vertices on the \(X, Y, Z\) axes are constrained on the \(XZ, XY, YZ\) planes, respectively, to avoid rigid body rotations. Under these conditions, the tensor \(F\) must be of the form:

\[
F = \begin{bmatrix}
F_{11} & F_{12} & 0 \\
0 & F_{22} & F_{23} \\
F_{31} & 0 & F_{33}
\end{bmatrix}.
\]

The motion of the unit cell is thus uniquely determined by six displacements

\[
u_1 = F_{12}L_2, \quad u_4 = F_{23}L_3,
\]
\[
u_2 = (F_{22} - 1)L_2, \quad u_5 = F_{31}L_1,
\]
\[
u_3 = (F_{11} - 1)L_1, \quad u_6 = (F_{33} - 1)L_3,
\]

that can be related to the displacements of the three vertices on the \(X, Y, Z\) axes. By adding the free energy of all the bars, we derive the total free energy:

\[
k_{\text{out}} V(u, \Theta; \lambda_{\text{in}} k_{\text{out}}, \alpha_{\text{in}}) = \sum_i \tilde{V}(\lambda_i(u), \theta_{\text{ref}} + \Delta \theta),
\]

where \(u = (u_1, u_2, u_3, u_4, u_5, u_6), \Theta = \alpha_{\text{out}} \Delta \theta\) is the normalized temperature and \(\tilde{V}(\lambda, \theta)\) is the free energy of each of the individual springs (see Eq. (4)).
The equilibrium equations then follow from the derivative of the free energy as
\[ g(u, \Theta; \frac{k_{\text{in}}}{k_{\text{out}}}, \frac{\alpha_{\text{in}}}{\alpha_{\text{out}}}) = \frac{\partial V}{\partial u}(u, \Theta; \frac{k_{\text{in}}}{k_{\text{out}}}, \frac{\alpha_{\text{in}}}{\alpha_{\text{out}}}) = 0, \tag{28} \]
which is analogous to Eq. (7), now for the three-dimensional cell. Since the kinematics of the unit cell is determined by the solution of six coupled nonlinear equations, the analysis becomes more complex than in the plane case.

We will study next four types of three-dimensional lattices.

4.1 Orthorhombic fcc lattices \((L_1 \neq L_2 \neq L_3)\)

We break the symmetry in fcc-type lattices by choosing all sides of the unit cell to be of different length. This makes the analytical derivations significantly simpler than in the symmetric case. Specifically, we choose \(L_2 = 2, L_3 = 3, \frac{k_{\text{in}}}{k_{\text{out}}} = 1.0\) and \(\frac{\alpha_{\text{in}}}{\alpha_{\text{out}}} = 1000.\) To investigate possible instabilities in the system we look at the eigenvalues of the Jacobian \(L(u, \Theta) = D_{\Theta} g(u, \Theta)\) as we vary the normalized temperature \(\Theta.\) At \(\Theta = 0,\) the stress-free configuration, all the eigenvalues are positive. When \(\Theta = \Theta_s^1 = -0.00188,\) one of the eigenvalues of the Jacobian vanishes and we identify the first singular point \((u_s^1, \Theta_s^1).\) The Jacobian at the point of singularity is
\[ L(u_s^1, \Theta_s^1) = \begin{bmatrix} 0.3073 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3.649 & 0.52 & 0 & 0 & 0 \\ 0 & 0.52 & 5.795 & 0 & 0 & 0.213 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.214 & 0 & 2.782 \end{bmatrix}. \tag{29} \]

Since only one eigenvalue vanishes at the singular point, we can use the Liapunov-Schmidt reduction as presented in A.3 and reduce the six degrees of freedom equation to a scalar equation \(g(x, \bar{\Theta})\) whose derivatives can be directly computed using formulae Eqs. (49a)-(49g). At the singular point \((u_s^1, \Theta_s^1)\) these are:
\[
\begin{align*}
g(u_s^1, \Theta_s^1) &= 0, & g_{\bar{\Theta}}(u_s^1, \Theta_s^1) &= 0, \\
g_x(u_s^1, \Theta_s^1) &= 0, & g_{xx}(u_s^1, \Theta_s^1) &= 0, \tag{30} \\
g_{xx}(u_s^1, \Theta_s^1) &= 0.361, & g_{\bar{\Theta}x}(u_s^1, \Theta_s^1) &= 197.12.
\end{align*}
\]

These equations satisfy the recognition conditions for a pitchfork bifurcation (see A.1) and it can be concluded that there will be such a singularity at \((u_s^1, \Theta_s^1),\) with the bifurcation in displacement \(u_4.\) Note that the fourth row and column of the Jacobian (29) vanish. Moreover \(g_{xx}(u_s^1, \Theta_s^1)g_{\bar{\Theta}x}(u_s^1, \Theta_s^1) > 0,\) hence the bifurcation can be classified as an inverted pitchfork.

Next, we study the effect of reducing the temperature even further. We observe that a second and a third eigenvalue of \(L(u, \Theta)\) vanish at \(\Theta_s^2 = -0.00364\) and \(\Theta_s^3 = -0.00555,\) suggesting that there are two additional points of singularity at \((u_s^2, \Theta_s^2)\) and \((u_s^3, \Theta_s^3),\) respectively. Following the same approach as for the first point of singularity, we can again show that there are inverted pitchforks in the solution at these two points with pitchforks in the direction of \(u_5\) and \(u_1,\) respectively.
Figure 11: Bifurcation diagrams for orthorhombic fcc type lattices with $L_2/L_1 = 2$, $L_3/L_1 = 3$, $k_{in}/k_{out} = 1.0$, $\alpha_{in} = 1000$. One clearly observes three different pitchforks at three different temperatures in the three directions $Y$, $Z$ and $X$ respectively as shown by the respective shear displacements in (a), (b) and (c). Figures (d), (e) and (f) plot the bifurcation diagrams of the axial displacements. Insets in (a), (b) and (c) show the bifurcated lattice in its stable branches of their respective pitchforks. Solid lines are stable solutions while dotted lines are unstable solutions.

We supplement the analytical calculations with numerical solutions using arc-length control. To test the stability of each configuration, we probe each equilibrium with unit forces along each of the displacement directions $u_4, u_5$,
and $u_1$, respectively. The complete bifurcation diagrams are shown in Fig. 11 and the solution path can be interpreted as follows. Starting from the stress free configuration ($\Theta = 0$), the temperature of the lattice is reduced and a first instability occurs at $\Theta_s^1 = -0.00188$, making the $u_4 = 0$ branch unstable thus causing the lattice to snap either in positive or negative Y direction as shown in Fig. 11(a). In real applications, small defects would cause a unit cell to snap into one of the stable branches of the pitchfork of Fig. 11(a). However, numerically we can continue to reduce the temperature while tracing the unstable branch of $u_4$. In this way we can obtain the other stable branches of the pitchfork in directions Z and X, respectively, as show in Figs. 11(b) and 11(c). Finally, Figs. 11 (d)-(f) show the bifurcation diagrams in the axial directions.

4.2 Cubic fcc lattices ($L_1 = L_2 = L_3$)

We consider next the fcc-type lattice with all sides of equal length (i. e. $L_1 = L_2 = L_3$) stiffness ratio $\frac{k_{in}}{k_{out}} = 1.0$ and conductivity ratio $\frac{\alpha_{in}}{\alpha_{out}} = 1000$. In this case, the lattice exhibits full symmetry. Thus as we reduce the temperature $\Theta$, precisely when $\Theta_s = -0.00303$, three eigenvalues of the Jacobian $L(u, \Theta) = D_1 g(u, \Theta)$ simultaneously vanish. In A.3 we described the Liapunov-Schmidt reduction when only one of the eigenvalues becomes zero, but the procedure can be extended for problems with eigenvalues of higher multiplicity. Here, however, we only present numerical results and summarize them in Fig. 12. In this case, and due to the aforementioned symmetries, the pitchforks corresponding to all singularities are identical (see Figs. 12(a)-(c)). Hence, when the singular point is crossed, all six configurations of the buckled lattices are equally favorable.

4.3 Cubic bcc lattices ($L_1 = L_2 = L_3$)

We consider bcc-type lattices that have springs only along the edges and the body diagonals (see Fig. 10(b)). We first consider a symmetric geometry $L_1 = L_2 = L_3$ and $\frac{k_{in}}{k_{out}} = 0.5$, $\frac{\alpha_{in}}{\alpha_{out}} = 1000$. As temperature is reduced, three of the eigenvalues of the Jacobian vanish simultaneously at $\Theta_s = -0.00058$, corresponding to an inverted pitchfork in the three directions as shown in Figs. 13(a)-(c).

4.4 Orthorhombic bcc lattices ($L_1 \neq L_2 \neq L_3$)

Finally, we analyze bcc lattices with the same material parameters as the last case but breaking the geometric symmetry. Remarkably, even when ($L_1 \neq L_2 \neq L_3$) all three instabilities still happen at the same temperature. In this case, the singularity point does not change, although the solutions can considerably differ from those in the symmetric configuration far from the bifurcation (see Figs. 14(a)-(c)). A direct analogy can be made between this case and the two-dimensional analysis where changing the aspect ratio of the frame did not change the bifurcation temperature (see Section 2.4).
Figure 12: Bifurcation diagrams for cubic fcc type lattices with $\frac{L_2}{L_1} = \frac{L_3}{L_1} = 1$, $k_{in}/k_{out} = 1.0$, $\frac{\alpha_{in}}{\alpha_{out}} = 1000$. Due to the symmetry of the cube, the pitchfork in the three directions $Y$, $Z$ and $X$ happens at the same temperature as shown in (a), (b) and (c). (d), (e) and (f) plot the bifurcation diagrams of the axial displacements. Insets in (a), (b) and (c) show the bifurcated lattice in its stable branches of their respective pitchforks. Solid lines are stable solutions while dotted lines are unstable solutions.

4.5 Systematic variation of structural parameters

We finally study the value of the bifurcation temperature as a function of the two structural parameters of the lattice viz. $\frac{k_{in}}{k_{out}}$ and $\frac{\alpha_{in}}{\alpha_{out}}$. Fig. 15 summarizes,
Figure 13: Bifurcation diagrams for cubic bcc type lattices with $\frac{L_2}{L_1} = 1$, $\frac{L_3}{L_1} = 1$, $k_{in}/k_{out} = 0.5$, $\alpha_{in}/\alpha_{out} = 1000$. The pitchforks in the three directions $Y, Z$ and $X$ all happen at the same temperature as shown in (a), (b) and (c). (d), (e) and (f) plot the bifurcation diagrams of the axial displacements. Insets in (a), (b) and (c) show the bifurcated lattice in its stable branches of their respective pitchforks. Solid lines are stable solutions while dotted lines are unstable solutions.

In the form of a phase diagram, the results obtained for a bcc and an fcc lattice, respectively, both with $L_1 = L_2 = L_3$.

The differences between the two types of lattices are noteworthy. To justify this claim, we note that the bottom-left corners of these two phase fields
Figure 14: Bifurcation diagrams for orthorhombic bcc type lattices with $\frac{L_2}{L_1} = 2$, $\frac{L_3}{L_1} = 3$, $\frac{k_{in}}{k_{out}} = 0.5$, $\frac{\alpha_{in}}{\alpha_{out}} = 1000$. The pitchforks in the three directions $Y, Z$ and $X$ all take place at the same temperature despite symmetry being broken as shown in (a), (b) and (c). However, the solutions of the pitchfork are not identical in all the three directions. Shown in red in (a),(b) and (c) is the pitchfork of the cubic bcc lattice ($\frac{L_2}{L_1} = 1$, $\frac{L_3}{L_1} = 1$) with same stiffness and coefficients of thermal expansion for comparison. (d), (e) and (f) plot the bifurcation diagrams of the axial displacements. 

are the most interesting regions of these plot since they refer to lattices where the differences in stiffness and thermal expansion coefficients between the two
types of springs are smallest. By comparing Figs. 15(a) and (b) we conclude that bcc-type lattices in this region buckle at higher temperature than their fcc counterparts. In practice, this means that the temperature difference triggering the buckling of the bcc lattice is, approximately, six times smaller than in the fcc structure.

Figure 15: Phase diagram for (a) fcc type cubic lattices with $L_1 = L_2 = L_3$ and (b) bcc type cubic lattices with $L_1 = L_2 = L_3$ with the colorbar representing the bifurcation temperature.

5 Effective (macroscopic) behavior of 3D lattices

We have already shown in Section 3 that a lattice of $20 \times 20$ unit cells had a structural response and stability behavior dictated, to a certain extent, by the characteristics of the unit cell (see Fig. 9), although boundary effects are noticeable. Motivated again by our interest on the analysis of complex lattices, we study next a periodic three-dimensional lattice of $N_x \times N_y \times N_z$ unit cells. Let $B$ be the periodic macroscopic lattice and $\partial B$ denote its boundary. Periodic boundary conditions are imposed, first, by partitioning $\partial B$ into two disjoint regions $\partial B^+$ and $\partial B^-$. Then, pairs of node positions $X^+_q$ and $X^-_q$ are identified on $\partial B^+$ and $\partial B^-$, respectively, such that the periodicity constraint

$$u^+_q - u^-_q = (F - I)(X^+_q - X^-_q)$$

is imposed [50]. In this equation $F$ is the macroscopic deformation gradient. This constraint is readily implemented using Lagrange multipliers. In practice, for a regular geometry such as a cube, a master node $M_i (i = 1, 2, 3)$ can be defined for each of the pair of opposite faces and the far-field deformation gradient can be imposed on the periodic lattice through the displacement on each of the master nodes according to

$$u(M_i) = (F - I)l_i,$$

where $l_i = l_i e_i$ are orthogonal vectors on the axes of the cube (see, e.g., [51]).

In Figs. 16, 17, and 18, we present numerical examples of large lattices built from different unit cell types and material parameters. We note that, especially
in those situations where structural instabilities arise, there is a dependency of the critical buckling parameter with the size of the representative volume element (RVE) \[52\]. In our numerical simulations, we drive the bifurcation parameter $\Theta$ well beyond the critical value of the unit cell so that we ensure that buckling always takes place.

Figure 16: Buckled configurations of a $20 \times 20 \times 20$ periodic lattice comprising of orthorhombic fcc type unit cells. (a) is the lattice configuration at $\Theta = -0.0021$ beyond the bifurcation point at $\Theta^*_1 = -0.00188$ and is unstable. On application of a small amount of force it buckles to either (b) or (c). The properties of the unit cell are $L_2/L_1 = 2$, $L_3/L_1 = 3$, $k_{\text{in}}/k_{\text{out}} = 1$ and $\alpha_{\text{in}}/\alpha_{\text{out}} = 1000$.

First, in Fig. 16 we consider a periodic $20 \times 20 \times 20$ lattice of orthorhombic fcc-type unit cells with $L_2/L_1 = 2$, $L_3/L_1 = 3$, $k_{\text{in}}/k_{\text{out}} = 1$ and $\alpha_{\text{in}}/\alpha_{\text{out}} = 1000$ whose bifurcation diagrams are plotted in Fig. 11. The lattice exhibits a first bifurcation in the $Y$-direction at $\Theta^*_1$, followed by bifurcations in $Z$ and $X$ directions, respectively, at $\Theta^*_2$ and $\Theta^*_3$. The temperature is reduced from $\Theta = 0$ to $\Theta = -0.0021$ (far below the bifurcation point at $\Theta^*_1 = -0.00188$) where the lattice is still in its non-sheared configuration (see Fig. 16(a)) which is unstable and on an application of a small force buckles to one side or the other (see Figs. 16(b), (c)). Note that, if the temperature is further reduced for this type of unit cell, the lattice can buckle in the other two directions.

Next, in Fig. 17 we consider a periodic $20 \times 20 \times 20$ lattice consisting of cubic bcc-type unit cells with $L_1 = L_2 = L_3$, $k_{\text{in}}/k_{\text{out}} = 1$ and $\alpha_{\text{in}}/\alpha_{\text{out}} = 1000$ whose bifurcation diagrams are plotted in Fig 13. For this unit cell, below the critical $\Theta_x$, bifurcations in all three directions are simultaneously possible and this behavior is shown for our macroscopic lattice in Figs. 17 (b), (c) and (d).

Finally, since defects are unavoidable in real lattices, we simulate a cubic bcc-type lattice where a Gaussian noise is introduced in the stiffness of all the bars. Because of the presence of defects, each of the unit cells buckles slightly below the bifurcation point and can buckle randomly in any of the three directions. The complete thermomechanical cycle is shown in Fig. 18. Starting from a regular lattice depicted in Fig. 18(a), after a reduction of the temperature, some cells buckle in unpredictable directions as shown in Fig. 18(b). On the
Figure 17: Buckled configurations of a $20 \times 20 \times 20$ periodic lattice comprising of cubic bcc type unit cells. (a) is the lattice configuration at $\Theta = -0.0009$ beyond the bifurcation point at $\Theta^* = -0.00058$ and is unstable. As this unit cell buckles symmetrically to any of the three directions below the bifurcation point, on a small application of force, it buckles to (b), (c), or (d). The properties of the unit cell are $L_1 = L_2 = L_3$, $k_{in}/k_{out} = 0.5$ and $\alpha_{in}/\alpha_{out} = 1000$.

application of a shear load, some of the energetically-equivalent buckled configurations are favored and the macroscopic shape of the lattice becomes stable at a tilted configuration, even when the load is removed (see Fig. 18(c)). Finally, when the temperature is raised to the original value, the lattice recovers its undeformed, symmetric configuration.

This complete cycle confirms the theoretical possibility of building lattice metamaterials that can absorb energy (in the low temperature phases) and be healed by simply heating them up. This is the main outcome of the methodology developed in this paper.

6 Concluding remarks

In this article, we have employed singularity theory to guide the design of lattice structures which display bistable and thermally reversible behavior, so that they mimic at the macro-scale the characteristic thermomechanical coupling of shape-memory alloys. In particular, we have investigated structures that possess several energetically equivalent configurations at “low” temperature, all of them accessible when external loading is applied, and a single stable phase at “high” temperature.

Singularity theory has enabled to characterize the stability of these structures at all temperatures and served to identify the main physical material-
related parameters that affect the response of the lattice. A key outcome of this work is that the analytical predictions obtained from singularity theory for unit cells have been compared with numerical simulations of large scale two- and three-dimensional lattices, showing that the bifurcation behaviour of the unit cell determines the macroscopic response of the structures. To the authors’ knowledge, this is the first article that provides a complete structural analysis based on singularity theory of the stability of thermally reversible metamaterials inspired by shape-memory alloys.

One additional outcome of singularity theory is the identification of all the lattices perturbations that can significantly modify their bifurcation diagrams, and hence their stability. Since no real lattice is perfect due to, e.g., manufacturing defects and material uncertainties, the precise characterisation of critical imperfections should be important for guiding inspection campaigns and design constraints. While such practical aspects are not covered in this work, the methodology presented can be useful for these related problems.

The investigation presented in this paper has, as long-term goal, the design of energy absorbing structures that can be healed with a heat treatment after, for example, an impact. A final comment must be added regarding the possibility
of manufacturing real lattices with the proposed features. For the specific lattice geometry investigated in this article, its physical realization is limited by the materials involved in the two types of springs (internal and outer frame springs). As shown in Section 2, the thermal expansion coefficients of these two elements must differ by a factor of 600 so as to provide the lattice with the required bistability and thermal reversibility features in the two-dimensional case. For three-dimensional geometries, however, the ratio is only around 400. These ratios severely restrict the material pairs that could be employed to actually manufacture such lattices. The main result of the article is hence, not the specific lattice design, but the methodology presented, which remains useful to study other lattice configurations in the search of shape-memory metamaterials.

A Singularity theory approach to bifurcation problems

Singularity theory mainly deals with the study of the solution set in equations of the form

\[ g(x, \lambda) = 0 \]  

(33)

where \( g : \mathbb{R} \times \mathbb{R} \to \mathbb{R} \), \( x \) is the state variable and \( \lambda \) is the bifurcation parameter. Bifurcation problems deal specifically with equations where the number of solutions \( x \) that solve Eq. (33) changes with \( \lambda \). The graph of pairs \((x, \lambda)\) that satisfy Eq. (33) is called the bifurcation diagram of the system.

In the simplest problem, and in what follows, the function \( g(x, \lambda) \) is infinitely differentiable. The stability and bifurcation analysis starts by identifying singular points of the solution

\[ g(x_0, \lambda_0) = 0 \quad \text{and} \quad g_x(x_0, \lambda_0) = 0 , \]  

(34)

where \( g_x \) refers, here and below, to the partial derivative \( \partial_x g \). If \( g_x(x_0, \lambda_0) \neq 0 \), sufficiently close to \((x_0, \lambda_0)\), the state variable \( x \) of the solution set can be expressed as a function of \( \lambda \) and hence there cannot be a change in the number of solutions near \( \lambda = \lambda_0 \). In order to have a bifurcation at \((x_0, \lambda_0)\) it is thus necessary, although not sufficient, that this point be singular.

Many types of bifurcations can occur, in general, but the only relevant type for our analysis is the pitchfork bifurcation (see Figs. 3-4). Its defining feature is that the number of solutions changes from one to three when the bifurcation parameter crosses a critical value. The so-called normal form of the pitchfork bifurcation is

\[ g(x, \lambda) = x^3 - \lambda x . \]  

(35)

The number of solutions that satisfy \( g(x, \lambda) = 0 \) changes from one to three as \( \lambda \) varies from negative to positive values (see Fig. 19 for an illustration of the corresponding bifurcation diagram).

The first central issue that singularity theory addresses is the identification of the necessary conditions under which a certain bifurcation problem is qualitatively equivalent to that of a simpler norm form. This is referred to as the recognition problem.
Figure 19: Bifurcation diagram for $g(x, \lambda) = x^3 - \lambda x = 0$.

A.1 The recognition problem

The recognition problem refers to the identification of the nature of a bifurcation using only information from the derivatives of $g$ at the point of singularity. If Eq. (33) has a singularity at $(x_0, \lambda_0)$ and the conditions

$$g = g_x = g_{xx} = g_{x\lambda} = 0, \quad g_{xxx} g_{x\lambda} < 0$$

are satisfied at $(x_0, \lambda_0)$, then $n(\lambda)$, the number of solutions of $g(x, \lambda) = 0$ expressed as a function of the bifurcation parameter, changes from one to three when $\lambda$ changes from small negative values to small positive values, and the problem exhibits a pitchfork bifurcation. Similarly, if the last condition is replaced by $g_{xxx} g_{x\lambda} > 0$, then $n(\lambda)$ changes from three to one and it will correspond to an inverted pitchfork.

Moreover, the theory tells that if conditions in Eq. (36) are satisfied, then $g(x, \lambda)$ is equivalent to the normal form of the pitchfork bifurcation (35) in the sense that there exists a nonlinear transformation of coordinates $(X(x, \lambda), \Lambda(\lambda))$ such that

1. It is a local diffeomorphism of $\mathbb{R}^2$ of the form $(x, \lambda) \rightarrow (X(x, \lambda), \Lambda(\lambda))$ mapping the origin to $(x_0, \lambda_0)$.

2. A nonzero function $S(x, \lambda)$ exists such that

$$S(x, \lambda)g(X(x, \lambda), \Lambda(\lambda)) = x^3 - \lambda x$$

(37)

Since the factor $S(x, \lambda)$ is nonzero, the solutions of $g(x, \lambda) = 0$ differ from those of $x^3 - \lambda x = 0$ only by the diffeomorphism $(X, \Lambda)$.

A.2 Influence of parameters: universal unfoldings

To define the influence of perturbations on the solution set of a given function $g$, let $\alpha = \{\alpha_1, \alpha_2, ..., \alpha_k\}$ be a set of $k$ auxiliary parameters. Then, let us construct a certain family of functions $G(x, \lambda, \alpha)$ such that

$$G(x, \lambda, 0) = g(x, \lambda).$$

(38)
The function $G(x, \lambda, \alpha)$ is called a *perturbation* of $g$. For a given bifurcation problem, singularity theory identifies the minimum set of auxiliary parameters that contains all possible perturbations of $g$, called the *universal unfolding* of $g$. For the pitchfork bifurcation, two auxiliary parameters are required to construct its universal unfolding

$$
G(x, \lambda, \alpha_1, \alpha_2) = x^3 - \lambda x + \alpha_1 + \alpha_2 x^2.
$$

(39)

Thus, the universal unfolding (39) contains all possible perturbations of (35). Moreover, singularity theory calculates how the bifurcation diagram depends on the auxiliary parameters $\alpha_1, \alpha_2$ (see Fig. 20 for the pitchfork bifurcation). The theory predicts four regions in the $(\alpha_1, \alpha_2)$ plane that correspond to qualitatively different perturbations of the pitchfork. The central result is that these are the only possible perturbations for the pitchfork.

In real applications, imperfections may occur in infinitely many ways, but all imperfections can be “lumped together” into two auxiliary parameters that cannot generate bifurcation diagrams that are qualitatively different from the four types mentioned above. The main result that allows this identification is as follows. Let $G(x, \lambda, \alpha_1, \alpha_2)$ be any two-parameter unfolding of $g(x, \lambda)$. Then, $G$ is a *universal unfolding* of $g$ if and only if

$$
\det \begin{pmatrix}
0 & 0 & g_{x\lambda} & g_{xxx} \\
0 & g_{x\lambda} & g_{\lambda\lambda} & g_{\lambda xx} \\
G_{,\alpha_1} & G_{,\alpha_1 x} & G_{,\alpha_1 \lambda} & G_{,\alpha_1 xx} \\
G_{,\alpha_2} & G_{,\alpha_2 x} & G_{,\alpha_2 \lambda} & G_{,\alpha_2 xx}
\end{pmatrix} \neq 0
$$

(40)

at $x = \lambda = \alpha_1 = \alpha_2 = 0$. This is called the *recognition problem for the universal unfolding*. 

Figure 20: Universal unfolding of a pitchfork bifurcation: Regions (1) and (2) are usually perturbations that occur only by a single parameter, while the kinked bifurcation diagrams in (3) and (4) are obtained only under specific imperfection values.
A.3 Liapunov-Schmidt reduction

We have presented heretofore singularity theory for equations where the state variable $x$ is a scalar. In real applications, however, $x$ often belongs to a space of multiple or even infinite dimensions. The Liapunov-Schmidt reduction can reduce a finite or infinite dimensional system of equations to one of a single dimension to which singularity theory can then be applied. Let us consider now an equilibrium equation of the form

$$ g(x, \alpha) = 0 , \quad (41) $$

where $g : \mathbb{R}^n \times \mathbb{R}^{k+1} \to \mathbb{R}^n$, with $n > 1$ is a smooth mapping, $x = (x_1, x_2, \cdots, x_n)$ are the unknowns and $\alpha = (\alpha_0, \alpha_1, \cdots, \alpha_k)$ are auxiliary parameters where $\alpha_0$ can be considered to be the bifurcation parameter. Without loss of generality, we assume that $g(0, 0) = 0$ and define

$$ \mathcal{L} = D_1 g(0, 0) = \left. \frac{\partial g}{\partial x} \right|_{(0,0)} \quad (42) $$

to be the Jacobian matrix. If the Jacobian has full rank, i.e., $\text{rank}(\mathcal{L}) = n$, then by the implicit function theorem $x$ can be uniquely solved as a function of $\alpha$.

Here, we are interested in problems where $\mathcal{L}$ is singular and we focus next on the minimally degenerate case, where the Jacobian has a simple zero eigenvalue and thus $\text{rank}(\mathcal{L}) = n - 1$. The reduction process begins by choosing vector spaces $\mathcal{M}$ and $\mathcal{N}$ that complement the kernel and the range of $\mathcal{L}$, respectively, i.e., $\mathbb{R}^n = \ker \mathcal{L} \oplus \mathcal{M} = \mathcal{N} \oplus \text{range } \mathcal{L}$. Since $\text{rank}(\mathcal{L}) = n - 1$, the dimension of $\ker \mathcal{L}$ is one and $\dim \text{range } \mathcal{L} = n - 1$ which gives $\dim \mathcal{M} = n - 1$ and $\dim \mathcal{N} = 1$. Next, let us define a projection $E : \mathbb{R}^n \to \text{range } \mathcal{L}$. The system of equations Eq. (41) can then be split into an equivalent pair of equations, namely,

$$ Eg(x, \alpha) = 0 \quad (43a) $$
$$ (I - E)g(x, \alpha) = 0 \quad (43b) $$

where $I$ is the identity matrix. Expressing any $x \in \mathbb{R}^n$ as $x = v + w$, with $v \in \ker \mathcal{L}$ and $w \in \mathcal{M}$, we rewrite Eq. (43a) as $F(v, w, \alpha) = 0$ with $F(v, w, \alpha) := Eg(v + w, \alpha)$, where $F : \ker \mathcal{L} \times \mathcal{M} \times \mathbb{R}^{k+1} \to \text{range } \mathcal{L}$. Taking the derivative of the function $F$ with respect to the variable $w$, we have that $D_2 F = ED_1 g = E \mathcal{L} =: \mathcal{L}$ and $\mathcal{L} : \mathcal{M} \times \mathbb{R}^{k+1} \to \text{range } \mathcal{L}$ is invertible. Hence, $w$ can be written uniquely in terms of $v$ and $\alpha$, thus we write $w = W(v, \alpha)$. The map $W : \ker \mathcal{L} \times \mathbb{R}^{k+1} \to \mathcal{M}$ satisfies

$$ Eg(v + W(v, \alpha), \alpha) = 0 \quad \text{and} \quad W(0, 0) = 0 . \quad (44) $$

Replacing $W(v, \alpha)$ in Eq. (43b), we obtain the reduced map $\phi : \ker \mathcal{L} \times \mathbb{R}^{k+1} \to \mathcal{N}$ defined as

$$ \phi(v, \alpha) = (I - E)g(v + W(v, \alpha), \alpha) . \quad (45) $$

The solutions to $\phi(v, \alpha) = 0$ are in one-to-one correspondence with the solutions of Eq. (41), and thus it is the reduced equation we are looking for. By introducing coordinates for the subspaces $\ker \mathcal{L}$, range $\mathcal{L}$, $\mathcal{M}$, $\mathcal{N}$, Eq. (45) can be further simplified to depend only on real numbers. To see this, let $v_0$ and
\( \mathbf{v}_0^* \) be arbitrary nonzero vectors in \( \text{ker } \mathcal{L} \) and \((\text{range } \mathcal{L})^\perp \), respectively. Any vector \( \mathbf{v} \in \text{ker } \mathcal{L} \) can be uniquely written as \( \mathbf{v} = x\mathbf{v}_0 \), with \( x \in \mathbb{R} \). We define \( g : \mathbb{R} \times \mathbb{R}^{k+1} \to \mathbb{R} \) by
\[
g(x, \alpha) = \langle \mathbf{v}_0^*, \phi(x\mathbf{v}_0, \alpha) \rangle ,
\]
where \( \langle , \rangle \) refers to the standard Euclidean inner product. The roots of Eq. (46) are the same as those of Eq. (45) and hence also to the ones of the original Eq. (41). Substituting Eq. (45) in Eq. (46), the operator \((I - \mathcal{E})\) drops out leading to the final reduced equation:
\[
g(x, \alpha) = \langle \mathbf{v}_0^*, g(x\mathbf{v}_0 + \mathbf{W}(x\mathbf{v}_0, \alpha), \alpha) \rangle .
\]

A.4 Recognition conditions for the reduced equation

To investigate the bifurcation behavior of the reduced equation, the partial derivatives of \( g(x, \alpha) \) need to systematically obtained using the chain rule. For that, we introduce an invariant notation for the higher order derivatives of a function of several variables. If \((\mathbf{v}_1, \cdots, \mathbf{v}_n) \in \mathbb{R}^n\), we define
\[
(D^k_n g)_{x,\alpha} (\mathbf{v}_1, \cdots, \mathbf{v}_k) = \frac{\partial}{\partial t_1} \cdots \frac{\partial}{\partial t_k} g \left( x + \sum_{i=1}^{k} t_i \mathbf{v}_i, \alpha \right) \bigg|_{t_1=\cdots=t_k=0} .
\]

Using this definition, the formulae for the first few derivatives of \( g \) evaluated at \((0, 0)\) are
\[
\begin{align*}
g_{,x} &= 0 , \quad & (49a) \\
g_{,xx} &= \langle \mathbf{v}_0^*, D^2_1 g(\mathbf{v}_0, 0) \rangle \quad & (49b) \\
g_{,xxx} &= \langle \mathbf{v}_0^*, D^3_1 g(\mathbf{v}_0, 0, \mathbf{v}_0) + 3D^2_2 g(\mathbf{v}_0, \mathbf{W}_{xx}) \rangle , \quad & (49c) \\
g_{,\alpha} &= \langle \mathbf{v}_0^*, \mathbf{g}_0, \mathbf{g}_{\alpha} \rangle , \quad & (49d) \\
g_{,\alpha x} &= \langle \mathbf{v}_0^*, D_1 g_{,\alpha x}, \mathbf{v}_0 + D^2_1 g(\mathbf{v}_0, \mathbf{W}_{,\alpha x}) \rangle , \quad & (49e) \\
g_{,\alpha \alpha} = \langle \mathbf{v}_0^*, g_{,\alpha \alpha}, \mathbf{W}_{,\alpha} + D_1 g_{,\alpha \alpha} \mathbf{W}_{,\alpha} + D^2_1 g(\mathbf{W}_{,\alpha}, \mathbf{W}_{,\alpha}) \rangle , \quad & (49f) \\
g_{,\alpha \alpha xx} &= \langle \mathbf{v}_0^*, D^2_1 g_{,\alpha x}(\mathbf{v}_0, 0) + D^3_2 g(\mathbf{v}_0, \mathbf{v}_0, \mathbf{W}_{,\alpha x}) + 2D^2_2 g(\mathbf{v}_0, \mathbf{W}_{,\alpha x}) \\
& \quad D_1 g_{,\alpha x}(\mathbf{W}_{,xx}) + D^2_1 g(\mathbf{W}_{,\alpha x}, \mathbf{W}_{,xx}) \rangle . \quad & (49g)
\end{align*}
\]

These derivatives depend themselves on the derivatives of \( \mathbf{W}(x\mathbf{v}_0, \alpha) \) that can be obtained by differentiating Eq. (44) implicitly with respect to \( x \) or \( \alpha \).

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