Elasticity in curved topographies: Exact theories and linear approximations

Siyu Li* and Roya Zandi
Department of Physics and Astronomy, University of California, Riverside, California 92521, USA

Alex Travesset
Department of Physics and Astronomy, Iowa State University and Ames Laboratory, Ames, Iowa 50011, USA

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Almost all available results in elasticity on curved topographies are obtained within either a small curvature expansion or an empirical covariant generalization that accounts for screening between Gaussian curvature and disclinations. In this paper, we present a formulation of elasticity theory in curved geometries that unifies its underlying geometric and topological content with the theory of defects. The two different linear approximations widely used in the literature are shown to arise as systematic expansions in *reference* and *actual* space. Taking the concrete example of a two-dimensional crystal, with and without a central disclination, constrained on a spherical cap, we compare the exact results with different approximations and evaluate their range of validity. We conclude with some general discussion about the universality of nonlinear elasticity.

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I. INTRODUCTION

There are many examples of two-dimensional (2D) crystals on curved spaces, including colloids absorbed on a spherical surface [1,2], negative curvature [3] at an oil-water interface, virus shells [4–6], and colloid mixtures [7], just to name a few. The uniqueness of these problems arises from the subtle but profound relation between geometry and topology.

The equilibrium structure of two-dimensional ordered structures on surfaces with nonzero Gaussian curvature is dictated by the presence and arrangement of defects such as dislocations and disclinations. The energetically forbidden defects in flat surfaces become ubiquitous on curved substrates; nevertheless, their presence gives rise to equilibrium structures that include finite stresses. The standard theory of elasticity [8] is unwieldy to investigate the interplay of the defects and geometry and, often, is not the most suitable starting point for these problems. In fact, in order to satisfy topological constraints, somewhat uncontrolled approximations need to be considered.

In this paper we develop a geometric theory for the elasticity of microscopic crystals that incorporates topological constraints exactly, where disclinations are defined in reference space, thus allowing us to calculate the stress and strain in a curved surface and analyze different approximations employed in the literature. Because the underlying ground state is restricted to a microscopic triangular lattice, disclinations are "quantized" in units of $\frac{\pi}{3}$ and dislocations as multiples of the lattice constant. It is not difficult to generalize to other lattices, but description of the elasticity of amorphous systems, for example, would require a different approach. Cases that will be discussed include fivefold disclinations in a triangular lattice in regions of constant positive Gaussian curvature; see Fig. 1.

*siyu.li@email.ucr.edu

The organization of the paper is as follows: First, in Sec. II we present different approximations employed in literature to solve elasticity equations and provide a conceptual discussion of our approach, which is developed in Sec. III. As an example, the case of a spherical cap, with or without a central disclination and the derivation of all their relevant analytical formulas are presented in Sec. IV. Explicit comparisons between the different approximations and the exact results are presented in Sec. V. Some general conclusions are presented in Sec. VI. More technical and mathematical developments are deferred to the appendices, where we have made a special effort to provide all the detail necessary so that all calculations are fully reproducible.

II. FORMALISM: CONCEPTUAL ASPECTS

The basic quantities in elasticity theory are the displacements $\mathbf{u}(\bar{\mathbf{x}})$ from a reference state $\bar{\mathbf{x}}$,

$$\mathbf{x} \equiv \bar{\mathbf{x}} + \mathbf{u}(\bar{\mathbf{x}}), \tag{1}$$

and the associated strain ($u_{\alpha\beta}$) and stress ($\sigma^{\alpha\beta}$) tensors, which are conjugated variables in the thermodynamic sense [8]. A definition of the strain tensor is given by comparing how a small vector in the *reference* (sometimes denoted as "target" [9,10]) space $d\bar{\mathbf{x}}$ transforms after a mechanical deformation, represented by $d\mathbf{x}$:

$$d\mathbf{x}^2 = d\bar{\mathbf{x}}^2 + 2u_{\alpha\beta} d\bar{\mathbf{x}}^\alpha d\bar{\mathbf{x}}^\beta. \tag{2}$$

The physical interpretation of this equation is that two particles, initially apart by $d\bar{\mathbf{x}}$, after deformation become separated by $d\mathbf{x}$. This equation can be written as a function of two metrics, denoted as reference and actual metrics, as follows,

$$g_{\alpha\beta} = \bar{g}_{\alpha\beta} + 2u_{\alpha\beta}. \tag{3}$$

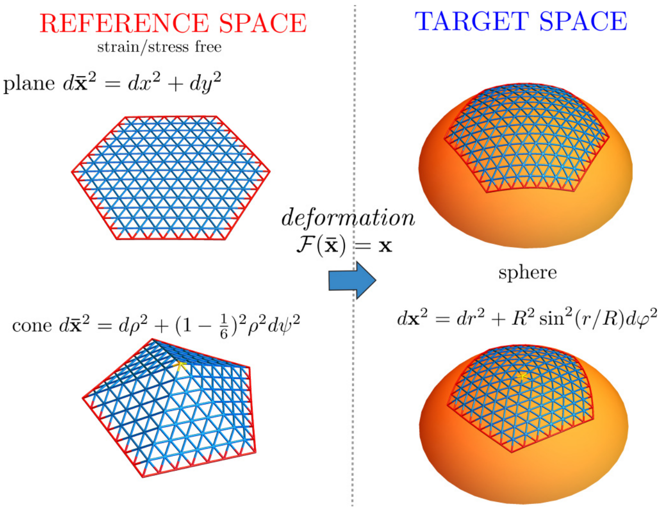

FIG. 1. Illustration of the formalism described in this paper: The reference space may consists of flat surfaces connected by any number of $q_i\frac{\pi}{3}$ disclinations in arbitrary locations, while the actual space is any fixed manifold endowed with its natural metric. The cases of no or single isolated disclination on a spherical cap are solved in Sec. IV.

While the distances in the reference space are measured according to the metric $\bar{g}_{\alpha\beta}$, after deformation, which defines the *actual* space, distances and angles among physical particles change and are determined by the metric $g_{\alpha\beta}$, as illustrated in Fig. 1. The strain tensor is the difference between actual and reference metrics.

The reference state is defined as a strain and stress free configuration, which is typically taken as $\mathbf{x} = (x, y, z)$ in 3D or $\mathbf{x} = (x, y, z = 0)$ in 2D, which implies a Euclidean reference metric

$$d\bar{\mathbf{x}}^2 = dx^2 + dy^2 + dz^2 \text{ (3D)}, \tag{4}$$

$$d\bar{\mathbf{x}}^2 = dx^2 + dy^2 \text{ (2D)}. \tag{5}$$

Physically, the reference state maybe associated with a lattice where all nearest neighbors are at the same distance and form the same angle. In 2D we associate it with the triangular lattice; see Fig. 1. Further below, we will show that the reference state is not unique, as a triangular lattice with topological defects such as disclinations and dislocations is also allowed. We mention, in passing, that in 3D a lattice where all nearest neighbors are at the same distance and form the same angle would consist of a tiling with regular tetrahedra, which is not possible [11] and leads to several consequences that have been discussed elsewhere [12,13].

Our goal in this paper is to develop a formalism to obtain the stress and strain in a curved surface. In particular, we focus on how an initially flat monolayer, whose reference state is given by $\bar{\mathbf{x}}$, consisting of a plane with additional defects, deforms into a given topography $\vec{r}(\bar{\mathbf{x}})$ embedded in 3D space, as illustrated in Fig. 1. Note that both the reference metric $d\bar{\mathbf{x}}^2$ and actual metric $d\vec{r}^2$ (which, for simplicity, will be denoted as $d\mathbf{x}^2$ in what is, certainly, an abuse of notation) are known beforehand. We aim at finding the transformation

$$\mathbf{x} = \mathcal{F}(\bar{\mathbf{x}}), \tag{6}$$

which will be obtained by solving the equations of elasticity theory. How this transformation is related to the more familiar quantities in elasticity theory—the stress tensor $\sigma^{\alpha\beta}$, the Airy function (χ) [14], etc.—will be discussed extensively later in the paper.

The problem of finding the transformation given in Eq. (6) is quite subtle because of the interplay of curvature, topology, and defects such as disclinations or dislocations [14,15]. Disclinations, for example, lead to long-range effects that forbid many putative configurations; e.g., in a boundary free crystal, where the sum of all disclination charges is related to the Euler characteristic χ_E through the Gauss Bonnet theorem [16]

$$\sum_{i=1}^{M} s_i = \int d^2\mathbf{x}\sqrt{g}K(\mathbf{x}) = 2\pi\chi_E, \tag{7}$$

where $K(\mathbf{x})$ is the Gaussian curvature, g is the determinant of the surface metric, and for a triangular lattice $s_i = \frac{\pi}{3}q_i$ ($q_i = \pm 1$). In the case of a spherical surface, $\chi_E = 2$, leading to the well known result that a spherical crystal has an excess of twelve $q_i = 1$ disclinations (pentamers) in the absence of heptamers ($q_i = -1$).

Solutions to the theory of elasticity are obtained mostly within the Foppl–von Karman theory of elastic plates, which amounts to small displacements from equilibrium positions, an approach we denote as the Euler framework (EF). A useful quantity to calculate the free energy and stress of a curved object is the Airy stress function. For a crystal consisting of M disclinations at positions $\mathbf{x}_i$ and with charge s_i, the equation for the Airy function is

$$\frac{1}{Y}\Delta^2\chi(\mathbf{x}) = \sum_{i=1}^{M} s_i\delta(\mathbf{x}_i - \mathbf{x}) - K(\mathbf{x}), \tag{8}$$

where Δ is the 2D Laplacian on a plane and Y is the Young modulus [8,17]. Note that the Gaussian curvature of the surface acts as an external field. Relevant solutions to Eq. (8) are available for a buckled disclination or dislocation [17], a spherical cap with and without a central disclination [18,19], and also for a spherical cap with an off-center disclination [20–22]. We emphasize again that the EF is exact in the limit of small curvature only. More precisely, if r_m is the dimension of the crystal and R some "average" curvature of the surface, the small curvature limit is defined by

$$\alpha \equiv \frac{r_m}{R} = \theta_m \ll 1. \tag{9}$$

In a spherical cap (with constant curvature radius R), a major problem arises as $\alpha \to \pi$, that is, as the spherical cap becomes a full sphere. Because within EF the solution of Eq. (8) is defined on a plane for a disk of area $A = \pi r_m^2$, the constraint (7),

$$\int d^2\mathbf{x}\, K(\mathbf{x}) = \int \frac{d^2\mathbf{x}}{R^2} = \frac{A}{R^2} = \pi\alpha^2 \neq 4\pi, \tag{10}$$

breaks down.

For a full sphere [23], the topological constraint (10) cannot be satisfied within the EF. The failure to exactly satisfy a topological constraint is a serious conceptual problem that typically results in very significant computational errors. In Refs. [24–26] a generalization of Eq. (8), which we denote as the Laplace formalism (LF), was proposed:

$$\frac{1}{Y}\Delta_g^2\chi(\mathbf{x}) = \frac{1}{\sqrt{g(\mathbf{x})}}\sum_{i=1}^{M} s_i\delta(\mathbf{x}_i - \mathbf{x}) - K(\mathbf{x}), \tag{11}$$

where the Laplacian Δ_g is computed with the actual metric, i.e., on the curved surface. Now, for a full sphere, the topological constraint Eq. (7) is satisfied identically. Although very successful and highly accurate in many applications [27], the LF appears as an uncontrolled approximation: It is not obvious how to compute next orders so that eventually the exact solution will be recovered. Furthermore, for a crystal with boundaries, like a crystal spanning a spherical cap, it is not immediately apparent what additional boundary conditions must supplement Eq. (11).

For the reasons stated, neither the EF nor the LF are entirely satisfactory, despite their many successes. There is a clear need for a more rigorous formalism able to develop the LF as a systematic expansion, from which the EF appears as a low curvature expansion. A first insight on how to develop this formalism is provided by the fact that physical quantities (energies, stresses, strains, etc.) should be independent of surface parametrizations, that is, expressed in terms of geometric invariants, an approach pioneered by Kondo [28] in 1955 and Koiter as early as 1966 [29]. An elegant formulation with numerous new insights has been provided in Ref. [30] and extended further in Ref. [31]. In previous papers (see Refs. [32,33]) we anticipated some aspects of the formalism fully elaborated here.

Before delving into the actual formalism, it is worth describing the main ideas and concepts, which are very intuitive despite the significant amount of differential geometry [16] necessary for its rigorous development. As already discussed, both the actual metric $g_{\mu\nu}(\mathbf{x})$ and the reference $\bar{g}_{\mu\nu}(\bar{\mathbf{x}})$ are known; what is therefore needed is the transformation Eq. (6) that enables us to express the two metrics either as $g_{\mu\nu}(\bar{\mathbf{x}})$ or $\bar{g}_{\mu\nu}(\mathbf{x})$.

A simple counting of the number of variables helps one understand the problem better. A general metric has three degrees of freedom, g_{11}, g_{22}, g_{12}, so in order to exactly map $\bar{g}_{\mu\nu}$ into $g_{\mu\nu}$ three functions are necessary. The solution of elasticity theory, Eq. (6), provides only two of them as $\mathcal{F}$ is a 2D mapping. The third function is associated with the Gaussian curvature. If the curvatures of the reference and actual metrics are not the same, a situation that is called *geometric frustration* or *metric incompatibility*, then it is not possible to make the two metrics $\bar{g}_{\mu\nu}$ and $g_{\mu\nu}$ coincide by Eq. (6). Since the Gaussian curvature is a scalar invariant under reparametrizations, metric incompatibility immediately leads to nonzero strains (and stresses), as is obvious from Eq. (2).

A few more clarifications are pertinent. First of all, as discussed above, the reference metric represents a strain and stress free configuration. This is different from other descriptions in which the reference metric is flat but under stress and strain; see Ref. [34]. We emphasize that the reference metric in our formalism does not have any residual strains or stresses. This is mainly due to the fact that it consists of patches of a flat metric joined by point disclinations (called quasiflat), where elasticity theory is not defined at the core. The metric of a plane, representing a triangular lattice, is an example of a reference metric that can be embedded into the actual space without any stresses. However, there are others: a cone with the appropriate aperture angle and $q = 1, 2, 3$ disclination charge at its tip and $q = 0$ (hexamers) everywhere else is also a stress and strain free configuration in the actual space. In the same way, one can consider a reference metric that contains an arbitrary number of defects, and hence the associated curvature will be given by the disclination density $s(\bar{\mathbf{x}})$:

$$\begin{aligned}\bar{K}(\bar{\mathbf{x}}) &= s(\bar{\mathbf{x}})\\ &= \frac{1}{\sqrt{\bar{g}}}\sum_{j=1}^{M} s_j\delta(\bar{\mathbf{x}} - \bar{\mathbf{x}}^j)\\ &= \frac{1}{\sqrt{\bar{g}}}\left(\sum_{j=1}^{N_D} s_j\delta(\bar{\mathbf{x}} - \bar{\mathbf{x}}^j) + \sum_{i=1}^{N_d}\epsilon^{\alpha\beta}b_\alpha^i\partial_\mu\left(e_\beta^\mu\delta(\bar{\mathbf{x}} - \bar{\mathbf{x}}^i)\right)\right),\end{aligned} \tag{12}$$

where use has been made of vielbeins e_β^μ; see Appendix B. The second equality follows by separating the M disclinations as N_D isolated disclinations and N_d dislocations, that is, considering tightly bound disclinations as dipoles characterized by a Burgers vector $\vec{b}$. Only for a few cases, such as $N_D = 0, N_d = 0$ (plane), $N_D = 1, N_d = 0$ (cone), or $N_D = k, N_d = 0$ (with $12 \geqslant k \geqslant 2$, icosahedral sections)—see also the limiting case $N_D = 0, N_d = 1$ [35] as well as others—is it possible to embed explicit solutions in actual space such that $K = \bar{K}$ and therefore they are strain and stress free. In this form, elasticity solutions amount to expressing a given metric $g_{\alpha\beta}$ as its optimal approximate in terms of "quanta" of disclinations of charge $\frac{\pi}{3}q$ and dislocations of Burgers vector $\mathbf{b}$. In fact, the geometric content of this "quanta" becomes even more explicit by noting that isolated disclinations are "quanta" of Gaussian curvature while dislocations are of geometrical torsion [32,36].

In this paper, we will not further discuss the role of dislocations; however, it is worth noting that it is possible to approximate any metric by Eq. (12) if $N_d \to \infty$, as demonstrated in Ref. [32]. This corresponds to the limit where Burgers vectors $\mathbf{b}$ are infinitesimally small, i.e., mean field solutions, also discussed in Refs. [37,38]. In this limit, the *perfect curvature condition* (PCC)

$$K(\mathbf{x}) = s(\mathbf{x}) \tag{13}$$

is satisfied. As pointed out in Ref. [3], it has the electrostatic analogy of a continuum of charge $K(\mathbf{x})$ being represented by N_D isolated charges and a continuum of polarization, i.e., $N_d \to \infty$ dipoles. More generally, the quantity

$$\eta(\mathbf{x}) = K(\mathbf{x}) - s(\mathbf{x}) \tag{14}$$

is a measure of the geometric frustration or metric incompatibility. The PCC $\eta(\mathbf{x}) = 0$ is the necessary and sufficient condition for a stress and strain free state to exist in actual space. We next develop these ideas in precise mathematical form.

III. FORMALISM: DEVELOPMENT

A. Exact formulas

As introduced previously, we will consider two metrics, $g_{\mu\nu}(\mathbf{x})$ (actual metric) and $\bar{g}_{\mu\nu}(\mathbf{x})$ (reference metric). The reference domain $\mathcal{B}_r$ represents the rest frame where the elastic energy is zero. The actual metric is defined over $\mathcal{B}_t$, which we denote as the *actual* domain. Consistent with our discussion in Sec. II, we will denote as $\mathbf{x}$ the actual coordinates and as $\bar{\mathbf{x}}$ the reference coordinates. The solution of the problem is then to determine $\mathcal{F}$ in Eq. (6) [$\mathbf{x} = \mathcal{F}(\bar{\mathbf{x}})$].

The most general elastic free energy has the form

$$F = \frac{1}{2}\int_{\mathcal{B}} W(g(\mathbf{x}), \bar{g}(\mathbf{x}))dV_g. \qquad (15)$$

We now show that an appropriate choice of W leads to the familiar expression for the elastic energy [8]; see also Ref. [31]. Using Y as the Young modulus and ν_P as the Poisson ratio, we define the quantities

$$A^{\alpha\beta\gamma\delta} = \frac{Y}{1-\nu_P^2}[\nu_P g^{\alpha\beta}g^{\gamma\delta} + (1-\nu_P)g^{\alpha\gamma}g^{\beta\delta}],$$
$$A_{\alpha\beta\gamma\delta} = \frac{1}{Y}[(1+\nu_P)g_{\alpha\gamma}g_{\beta\delta} - \nu_P g_{\alpha\beta}g_{\gamma\delta}] \qquad (16)$$

in such a way that $A^{\alpha\beta\gamma\delta}A_{\gamma\delta\alpha'\beta'} = g^{\alpha}_{\alpha'}g^{\beta}_{\beta'}$. Then the functional $W(g(\mathbf{x}), \bar{g}(\mathbf{x}))$ is defined so that it reduces to the standard elastic energy for an isotropic medium, that is

$$W(g(\mathbf{x}), \bar{g}(\mathbf{x})) = A^{\alpha\beta\gamma\delta}u_{\alpha\beta}u_{\gamma\delta}, \qquad (17)$$

where the strain tensor [see Eq. (2)] is

$$2u_{\alpha\beta}(\mathbf{x}) = g_{\alpha\beta}(\mathbf{x}) - \bar{g}_{\alpha\beta}(\mathbf{x}). \qquad (18)$$

Note that the free energy Eq. (15) is invariant under general reparametrizations. Working in the actual frame, the metric $g_{\alpha\beta}(\mathbf{x})$ is known, so we will derive the equilibrium equations in order to determine the reference metric $\bar{g}_{\mu\nu}(\mathbf{x})$, which, expressed in the actual coordinates, is not known. The stress tensor is given by

$$\sigma^{\alpha\beta} = \frac{1}{\sqrt{g}}\frac{\delta F}{\delta u_{\alpha\beta}} = A^{\alpha\beta\gamma\delta}u_{\gamma\delta}. \qquad (19)$$

Variations of Eq. (15) under reparametrizations (ξ_β) of the reference metric $\delta\bar{g}_{\alpha\beta} = -\bar{\nabla}_\alpha\xi_\beta - \bar{\nabla}_\beta\xi_\alpha$, leaving the actual metric invariant, give

$$\begin{aligned}\delta F &= -\frac{1}{2}\int_{\mathcal{B}} d^2\mathbf{x}\sqrt{g}\sigma^{\alpha\beta}\delta\bar{g}_{\alpha\beta}\\ &= \int_{\mathcal{B}} d^2\mathbf{x}\sqrt{g}\sigma^{\alpha\beta}\bar{\nabla}_\alpha\xi_\beta\\ &= \int_{\mathcal{B}} d^2\mathbf{x}\left[\frac{\partial}{\partial x_\alpha}(\sqrt{g}\sigma^{\alpha\beta}\xi_\beta) - \sqrt{\bar{g}}\bar{\nabla}_\alpha\left(\left(\frac{g}{\bar{g}}\right)^{1/2}\sigma^{\alpha\beta}\right)\xi_\beta\right].\end{aligned} \qquad (20)$$

The first term is a total derivative, and it can be converted to an integral along the boundary

$$\int_{\mathcal{B}} d^2\mathbf{x}\frac{\partial}{\partial x_\alpha}(\sqrt{g}\sigma^{\alpha\beta}\xi_\beta) = \int_{\partial\mathcal{B}} dx^\rho\sqrt{g}\epsilon_{\rho\gamma}\sigma^{\gamma\beta}\xi_\beta. \qquad (21)$$

Should the boundary contain a line tension term

$$F_l = \gamma\int_{\partial\mathcal{B}} ds, \qquad (22)$$

then

$$\delta F_l = -\gamma\int_{\partial\mathcal{B}} dx^\mu\nabla_\mu t^\nu\xi_\nu, \qquad (23)$$

where t^μ is the unit tangent to the boundary. We take into account the geometric formula

$$t^\mu\nabla_\mu t^\nu = \frac{1}{r_{\mathcal{B}}}e^\nu_\alpha n^\alpha, \qquad (24)$$

with $r_{\mathcal{B}}$ the radius of curvature, n^α the normal, and e^ν_α the vielbeins; see Appendix B. The correct boundary condition is

$$n_\gamma\hat{\sigma}^{\gamma\nu} = -\frac{\gamma}{r_{\mathcal{B}}}n^\nu, \qquad (25)$$

where $\hat{\sigma}^{\alpha\beta} = e^\alpha_\mu e^\beta_\nu\sigma^{\mu\nu}$; see Appendix B for the different expressions of the stress tensor and some additional details on the derivation of these formulas. This boundary condition reduces to the one derived for the EF in Ref. [19].

From the definition of the covariant derivative, we have

$$\nabla_\alpha\sigma^{\alpha\beta} = \frac{\partial\sigma^{\alpha\beta}}{\partial x_\alpha} + \Gamma^\alpha_{\alpha\gamma}\sigma^{\gamma\beta} + \Gamma^\beta_{\alpha\gamma}\sigma^{\alpha\gamma}. \qquad (26)$$

Therefore, the equations determining equilibrium are

$$\bar{\nabla}_\alpha\left(\left(\frac{g}{\bar{g}}\right)^{1/2}\sigma^{\alpha\beta}\right) = \bar{\nabla}_\alpha\sigma^{\alpha\beta} + \left(\Gamma^\alpha_{\alpha\gamma} - \bar{\Gamma}^\alpha_{\alpha\gamma}\right)\sigma^{\gamma\beta} = 0, \qquad (27)$$

which can also be written as

$$\nabla_\alpha\sigma^{\alpha\beta} + \left(\bar{\Gamma}^\beta_{\alpha\gamma} - \Gamma^\beta_{\alpha\gamma}\right)\sigma^{\alpha\gamma} = 0, \qquad (28)$$

derived first in Ref. [30]. The appropriate boundary conditions as defined by Eq. (25). Here, we have used the Christoffel symbols that are symmetric, $\Gamma^\beta_{\alpha\gamma} = \Gamma^\beta_{\gamma\alpha}$.

A general solution to Eq. (27) is given by the following ansatz [31]:

$$\sigma^{\alpha\beta} = \frac{1}{\sqrt{g}}\frac{1}{\sqrt{\bar{g}}}\epsilon^{\alpha\rho}\epsilon^{\beta\gamma}\bar{\nabla}_\rho\bar{\nabla}_\gamma\chi, \qquad (29)$$

where $\epsilon^{12} = -\epsilon^{21} = 1$, and zero otherwise, and χ is the Airy function. Using the identity

$$\frac{1}{g}\epsilon^{\alpha\rho}\epsilon^{\mu\nu} = g^{\alpha\mu}g^{\rho\nu} - g^{\alpha\nu}g^{\rho\mu}, \qquad (30)$$

Eq. (29) can be written as

$$\sigma^{\alpha\beta} = \left(\frac{\bar{g}}{g}\right)^{1/2}(\bar{g}^{\alpha\beta}\bar{g}^{\rho\gamma} - \bar{g}^{\alpha\gamma}\bar{g}^{\beta\rho})\bar{\nabla}_\rho\bar{\nabla}_\gamma\chi. \qquad (31)$$

Using the formula $g^{\rho\gamma}\Gamma^\nu_{\rho\gamma} = -\frac{1}{\sqrt{g}}\partial_\gamma(\sqrt{g}g^{\gamma\nu})$ and the fact that the covariant derivative of the metric is zero, i.e., $\bar{\nabla}_\alpha\bar{g}_{\mu\nu} = 0$, we find

$$\bar{\nabla}_\alpha \sigma^{\alpha\beta} + \left(\Gamma^\alpha_{\alpha\gamma} - \bar{\Gamma}^\alpha_{\alpha\gamma}\right)\sigma^{\gamma\beta} = \frac{1}{\sqrt{g\bar{g}}}\epsilon^{\alpha\rho}\epsilon^{\beta\gamma}\bar{\nabla}_\alpha\bar{\nabla}_\rho\bar{\nabla}_\gamma\chi. \quad (32)$$

The right-hand side of the above equation can be expressed in terms of the Riemann tensor [see Eq. (E4)] as

$$\begin{aligned}\epsilon^{\alpha\rho}\epsilon^{\beta\gamma}\bar{\nabla}_\alpha\bar{\nabla}_\rho\bar{\nabla}_\gamma\chi &= \tfrac{1}{2}\epsilon^{\alpha\rho}\epsilon^{\beta\gamma}[\bar{\nabla}_\alpha, \bar{\nabla}_\rho]\bar{\nabla}_\gamma\chi \\ &= \tfrac{1}{2}\epsilon^{\alpha\rho}\epsilon^{\beta\gamma}\bar{R}^\mu_{\gamma\alpha\rho}\bar{\nabla}_\mu\chi = 0, \end{aligned} \quad (33)$$

where the last identity follows since the Riemann tensor of the reference metric is zero outside the defect cores, that is, almost everywhere; see Eq. (12). Thus, Eq. (29) provides a general solution of Eq. (27) in terms of the Airy function.

Substituting the solution of Eq. (29) into the definition of the strain (18) gives

$$\frac{1}{\sqrt{g}}\frac{1}{\sqrt{\bar{g}}}\epsilon^{\alpha\rho}\epsilon^{\beta\gamma}\bar{\nabla}_\rho\bar{\nabla}_\gamma\chi = \frac{1}{2}A^{\alpha\beta\gamma\delta}(g_{\gamma\delta} - \bar{g}_{\gamma\delta}) \quad (34)$$

or

$$\begin{aligned}\bar{g}_{\alpha\beta} &= g_{\alpha\beta} - \frac{2}{\sqrt{g\bar{g}}}A_{\mu\lambda\alpha\beta}\epsilon^{\mu\rho}\epsilon^{\lambda\gamma}\bar{\nabla}_\rho\bar{\nabla}_\gamma\chi, \\ \bar{g}_{\alpha\beta} &= g_{\alpha\beta} - \frac{2}{Y}\left(\frac{g}{\bar{g}}\right)^{1/2}\left[g_{\alpha\beta}g^{\rho\gamma} - (1+\nu_P)g^\gamma_\alpha g^\rho_\beta\right]\bar{\nabla}_\rho\bar{\nabla}_\gamma\chi.\end{aligned} \quad (35)$$

Thus $\bar{g}_{\mu\nu}(\chi(\mathbf{x}))$ can be obtained from the above equation. Note, however, that among all possible functions χ, there is only a unique family that has the right curvature $\bar{K}$, so the equation above needs to be supplemented with the additional constraint

$$2\bar{K} = \bar{R} = \bar{g}^{\mu\nu}\bar{R}_{\mu\nu} = \bar{g}^{\mu\nu}\bar{R}^\rho_{\mu\rho\nu} = 0, \quad (36)$$

which uniquely determines the family of solutions χ. Here $\bar{K} = s(\mathbf{x})$ is the Gaussian curvature, $\bar{R}$ the scalar curvature, $\bar{R}_{\mu\nu}$ the Ricci tensor, and $\bar{R}^\rho_{\mu\gamma\nu}$ the Riemann tensor. That is, the solution consists of, among all possible functions of χ, selecting the one that makes $\bar{g}_{\mu\nu}$ a quasiflat metric. Thus, Eqs. (18), (19), (29), and (36) define a complete system of equations whose solution provides $\bar{g}(x)$ or $g(\bar{x})$, $\sigma^{\mu\nu}$, and χ. In general, such a solution is complicated as $\bar{g}_{\mu\nu}$ appears on both sides of the equation, and the right-hand includes its derivatives. Explicit solutions are possible in some cases that are discussed further below.

Using Eqs. (17)–(19) and (35), the expression for the elastic energy [Eq. (15)] without any approximations is

$$F = \frac{1}{2}\int_{\mathcal{B}}\sigma^{\alpha\beta}A_{\alpha\beta\rho\sigma}\sigma^{\rho\sigma}d\mathrm{Vol}_g \quad (37)$$

$$= \frac{1}{2Y}\int_{\mathcal{B}}d\mathrm{Vol}_g\frac{g}{\bar{g}}((1+\nu_p)g^{\alpha\rho}g^{\beta\sigma} - \nu_p g^{\alpha\beta}g^{\rho\sigma}) \times \bar{\nabla}_\alpha\bar{\nabla}_\beta\chi\bar{\nabla}_\rho\bar{\nabla}_\sigma\chi. \quad (38)$$

Note that up to this point all formulas are exact. We now discuss some common approximations.

B. Incompatibility metric approximation

1. Actual frame

Since the actual metric $g_{\mu\nu}(\mathbf{x})$ is known, the goal is to compute the reference metric $\bar{g}_{\mu\nu}(\mathbf{x})$, and from there one can obtain the transformation (6). If one assumes that η [see Eq. (14)] is somehow small, the Airy function and the metric are

$$\chi = \chi^{(1)} + \chi^{(2)} + \cdots, \quad (39)$$

$$\bar{g} = g + g^{(1)} + g^{(2)} + \cdots, \quad (40)$$

where each term contains increasing powers of η. Obviously the Airy function is at least linear with η, as, for $\eta = 0$, $\chi = 0$, and $g = \bar{g}$. Plugging this expansion into the Airy equation (35) provides the explicit orders in the expansion. The first order is

$$g^{(1)}_{\alpha\beta} = -\frac{2}{Y}(g_{\alpha\beta}\Delta\chi^{(1)} - (1+\nu_P)\nabla_\alpha\nabla_\beta\chi^{(1)}), \quad (41)$$

where $\Delta = g^{\alpha\beta}\nabla_\alpha\nabla_\beta = \frac{1}{\sqrt{g}}\partial_\alpha(g^{\alpha\beta}\sqrt{g}\partial_\beta)$ is the Laplace-Beltrami operator. Higher orders are discussed in Appendix C. The goal is now to derive an explicit equation for $\chi^{(i)}$, as discussed below.

2. First-order expressions for energy and stress: Actual frame

With the metric expressed linearly in terms of the Airy function, the next step is to enforce the constraint (36). For this purpose, it is necessary to compute the scalar curvature. This calculation is relegated to Appendix C, and gives

$$\bar{K} = K + \frac{1}{Y}(\Delta^2\chi^{(1)} + 2K\Delta\chi^{(1)} + (1+\nu_p) \times g^{\mu\lambda}\nabla_\mu K\nabla_\lambda\chi^{(1)}). \quad (42)$$

In addition to the square of Laplacian in the above equation, there are additional terms that will be explored further below. The stress tensor within this order is

$$\sigma^{\alpha\beta} = g^{\alpha\beta}\Delta\chi^{(1)} - g^{\alpha\mu}g^{\beta\nu}\nabla_\mu\nabla_\nu\chi^{(1)}, \quad (43)$$

and the energy

$$F = \frac{1}{2Y}\int d^2u\sqrt{g}\left[(\Delta\chi^{(1)})^2 + \frac{(1+\nu_P)}{g}\epsilon^{\alpha\sigma}\epsilon^{\rho\beta}\nabla_\alpha\nabla_\beta\chi^{(1)}\nabla_\rho\nabla_\sigma\chi^{(1)}\right]. \quad (44)$$

As elaborated in Appendix D, it may be expressed as

$$\begin{aligned}F &= \frac{1}{2Y}\int d^2u\sqrt{g}(\Delta\chi^{(1)})^2 \\ &\quad - \frac{1+\nu_p}{2Y}\int d^2u\sqrt{g}Kg^{\alpha\beta}\nabla_\alpha\chi^{(1)}\nabla_\beta\chi^{(1)} \\ &\quad - \frac{1+\nu_p}{2Y}\oint dx^\rho\sqrt{g}\epsilon_{\rho\alpha}\sigma^{\alpha\beta}\nabla_\beta\chi^{(1)}.\end{aligned} \quad (45)$$

A variation on the previous expansion consists in dropping the cross terms involving $K\chi$ in Eq. (42). The resulting equations are

$$\bar{K} = K + \frac{1}{Y}\Delta^2\chi^{(1)}, \quad (46)$$

with corresponding energy

$$F = \frac{1}{2Y}\int d^2u\sqrt{g}(\Delta\chi^{(1)})^2 - \frac{1+\nu_p}{2Y}\oint dx^\rho\sqrt{g}\epsilon_{\rho\alpha}\sigma^{\alpha\beta}\nabla_\beta\chi^{(1)}, \quad (47)$$

which we recognize as the LF discussed in Sec. II. Note that, in the absence of line tension or external stress, the boundary conditions determine that the second term vanishes identically. Henceforth, we will refer the approximation Eq. (42) as the incompatibility framework (IF) in order to differentiate it from the LF.

3. Reference frame

The expansions for the metric and the Airy function are

$$\chi = \chi^{(I)} + \chi^{(II)} + \cdots, \tag{48}$$

$$g = \bar{g} + \bar{g}^{(I)} + \bar{g}^{(II)} + \cdots. \tag{49}$$

Similarly to the actual approximation (41), the first order is

$$\bar{g}^{(I)}_{\alpha\beta} = \frac{2}{Y}(\bar{g}_{\alpha\beta}\bar{\Delta}\chi^{(I)} - (1+\nu_P)\bar{\nabla}_\alpha\bar{\nabla}_\beta\chi^{(I)}), \tag{50}$$

with $\bar{\Delta}$ being the Laplace-Beltrami operator of the reference metric. Higher orders are discussed in Appendix C.

4. First-order expressions for energy and stress: Reference frame

The formulas derived in the previous case automatically translate into the reference frame by replacing $g_{\alpha\beta} \leftrightarrow \bar{g}_{\alpha\beta}$ and $\chi^{(1)} \to -\chi^{(I)}$, leading to

$$K = \bar{K} - \frac{1}{Y}(\bar{\Delta}^2\chi^{(I)} + 2\bar{K}\bar{\Delta}\chi^{(I)} + (1+\nu_p)\bar{g}^{\mu\lambda}\bar{\nabla}_\mu\bar{K}\bar{\nabla}_\lambda\chi^{(I)}). \tag{51}$$

The stress tensor within this order is

$$\sigma^{\alpha\beta} = \bar{g}^{\alpha\beta}\bar{\Delta}\chi^{(I)} - \bar{g}^{\alpha\mu}\bar{g}^{\beta\nu}\bar{\nabla}_\mu\bar{\nabla}_\nu\chi^{(I)}, \tag{52}$$

and the energy

$$F = \frac{1}{2Y}\int d^2u\sqrt{\bar{g}}\bigg[(\bar{\Delta}\chi^{(I)})^2 + \frac{(1+\nu_P)}{\bar{g}}\epsilon^{\alpha\sigma}\epsilon^{\rho\beta}\bar{\nabla}_\alpha\bar{\nabla}_\beta\chi^{(I)}\bar{\nabla}_\rho\bar{\nabla}_\sigma\chi^{(I)}\bigg]. \tag{53}$$

Given the assumptions about the reference metric [see Eq. (12)], the above equations simplify to

$$\frac{1}{Y}\bar{\Delta}^2\chi^{(I)} = \bar{K} - K \tag{54}$$

and energy

$$F = \frac{1}{2Y}\int d^2u\sqrt{\bar{g}}(\bar{\Delta}\chi^{(I)})^2, \tag{55}$$

where $\bar{\Delta}$ is the Laplacian on the plane. Thus, the reference frame expansion coincides with the EF discussed in Sec. II. The singular terms in Eq. (12) can be dropped from the second term in Eq. (53) as they only contribute within the defect cores. These contributions are accounted for by an empirical core energy term E_{core} as linear elasticity breaks down.

IV. RESULTS

As a concrete example, we will solve the case of a crystal on a sphere of radius R, as illustrated in Fig. 1. The extent of the crystal is parametrized by its aperture angle θ_M. This problem has been described previously within the EF by Schneider and Gommper [18] as well as Morozov and Bruinsma [19] and Grason [21]. In the current notation, the Gaussian curvature is $K = \frac{1}{R^2}$ and $\bar{K}$ the disclination density $\bar{K} = s(\mathbf{r})$. The reference frame metric is Euclidean and is defined over a disk of radius ρ_0 by

$$ds^2 = d\rho^2 + \rho^2\left(1 - \frac{s}{2\pi}\right)^2 d\psi^2 \equiv \bar{g}_{\mu\nu}d\bar{x}^\mu d\bar{x}^\nu. \tag{56}$$

The case $s = \frac{\pi}{3}q_i$ corresponds to a disclination of positive charge placed at the center of the disk. The actual metric is

$$ds^2 = dr^2 + R^2\sin^2(r/R)d\varphi^2 \equiv g_{\mu\nu}dx^\mu dx^\nu. \tag{57}$$

The problem then consists in finding the function $\mathcal{F}$ such that

$$x^\mu = \mathcal{F}(\bar{x}^\mu), \tag{58}$$

where $x^\mu = (r, \varphi)$ and $\bar{x}^\mu = (\rho, \psi)$. We will investigate symmetric solutions where $\psi = \varphi$,

$$r \equiv r(\rho) = F(\rho), \tag{59}$$

so that the problem becomes one dimensional.

A. Exact solution

We first summarize the steps necessary to reach the exact solutions. As emphasized, $\bar{g}_{\mu\nu}(\bar{x})$ (metric of quasi-flat geometry with disinclinations in reference space) and $g_{\mu\nu}(x)$ (metric of curved geometry in actual space) are known. The goal is to find $g_{\mu\nu}(\bar{x})$ or $\bar{g}_{\mu\nu}(x)$, which is equivalent to finding $\bar{x}(x)$ [by solving, for example $g_{\mu\nu}(\bar{x}) = \frac{\partial\bar{x}^\alpha}{\partial x_\mu}\frac{\partial\bar{x}^\beta}{\partial x_\nu}g_{\alpha\beta}(x)$]. Note that we consider both reference and actual metrics with azimuthal symmetry, thus the problem reduces to finding the one-dimensional function $\rho(r)$. Combining Eqs. (18), (19), and (27) allows us to find $\bar{g}(x)$. Further below, using Eqs. (60)–(65), ρ as a function of r is finally obtained.

We start with presenting the reference metric in actual coordinates,

$$ds^2 = d\rho^2 + \rho^2 d\psi^2 \equiv [\rho'(r)]^2dr^2 + w^2\rho^2(r)d\varphi^2, \tag{60}$$

where $\rho' = d\rho/dr$, $w \equiv 1 - \frac{s}{2\pi}$. The nonzero Christoffel symbols are

symbol	Γ^r_{rr}	$\Gamma^r_{\varphi\varphi}$	$\Gamma^\varphi_{\varphi r}$
reference	$\frac{\rho''(r)}{\rho'(r)}$	$-w^2\frac{\rho(r)}{\rho'(r)}$	$\frac{\rho'(r)}{\rho(r)}$
actual	0	$-R\sin(r/R)\cos(r/R)$	$\frac{\cot(r/R)}{R}$

(61)

The components of the stress tensor (19) are the difference between the actual and reference metric, that is

$$\sigma^{rr} = \frac{Y}{2(1-\nu_p^2)}\left[1 - \rho'(r)^2 + \nu_p\left(1 - \left(\frac{w\rho(r)}{R\sin(r/R)}\right)^2\right)\right],$$

$$\sigma^{r\varphi} = 0,$$

$$\sigma^{\varphi\varphi} = \frac{Y}{2(1-\nu_p^2)R^2\sin^2(r/R)} \times \left[1 - \left(\frac{w\rho(r)}{R\sin(r/R)}\right)^2 + \nu_p(1-\rho'(r)^2)\right]. \tag{62}$$

Inserting Eq. (61) into Eq. (27), we obtain

$$\frac{d\sigma^{rr}}{dr} + \Gamma^{\varphi}_{\varphi r}\sigma^{rr} + \bar{\Gamma}^{r}_{rr}\sigma^{rr} + \bar{\Gamma}^{r}_{\varphi\varphi}\sigma^{\varphi\varphi} = 0, \tag{63}$$

which becomes

$$\frac{d\sigma^{rr}}{dr} + \left(\frac{\cot\left(\frac{r}{R}\right)}{R} + \frac{\rho''(r)}{\rho'(r)}\right)\sigma^{rr} - \frac{w^2\rho(r)}{\rho'(r)}\sigma^{\varphi\varphi} = 0. \tag{64}$$

Introducing Eq. (62) into Eq. (64) yields a nonlinear ordinary differential equation for $\rho(r)$,

$$\begin{aligned}
&\frac{2vw^2}{R^2\sin\left(\frac{r}{R}\right)^2}\rho(r)^2\left(\frac{\cot\left(\frac{r}{R}\right)}{R} - \frac{\rho'(r)}{\rho(r)}\right) - 2\rho'(r)\rho''(r)\\
&+\left(\frac{\cot\left(\frac{r}{R}\right)}{R} + \frac{\rho''(r)}{\rho'(r)}\right)\\
&\times\left[1 - \rho'(r)^2 + v\left(1 - \frac{w^2\rho(r)^2}{R^2\sin\left(\frac{r}{R}\right)^2}\right)\right]\\
&- w^2\frac{\rho(r)}{\rho'(r)}\frac{1}{R^2\sin\left(\frac{r}{R}\right)^2}\\
&\times\left[1 - \frac{w^2\rho(r)^2}{R^2\sin\left(\frac{r}{R}\right)^2} + v - v\rho'(r)^2\right] = 0,
\end{aligned} \tag{65}$$

with boundary conditions $\rho(0) = 0$ and $\sigma^{rr}(\theta_m R) = \frac{Y}{1-\nu_p^2}[1 - \rho'(\theta_m R)^2 + v(1 - \frac{w^2\rho(\theta_m R)^2}{R^2\sin(\theta_m)^2})] = 0$. Although within this formalism the Airy function is not necessary to calculate the stress, its actual form is valuable as a comparison with its approximations. It is given as

$$\begin{aligned}
\sigma^{rr} &= \frac{1}{R\sin(r/R)w\rho(r)\rho'(r)}\bar{\nabla}^2_{\varphi}\chi = \frac{w}{R\sin(r/R)\rho'(r)^2}\frac{d\chi}{dr},\\
\sigma^{\varphi\varphi} &= \frac{1}{R\sin(r/R)w\rho'(r)\rho(r)}\left(\frac{d^2\chi}{dr^2} - \frac{\rho''(r)}{\rho'(r)}\frac{d\chi}{dr}\right),
\end{aligned} \tag{66}$$

where $\sigma^{r\varphi} = 0$ is satisfied identically. Note that only one of the equations needs to be satisfied, as the other becomes then an identity.

B. Incompatibility metric approximation solutions

1. Reference frame

The equations describing the Airy function for a disclination of charge s in the reference frame have been described above, namely

$$\bar{\Delta}^2\chi^{(I)} + Y(K - s(\mathbf{r})) = 0. \tag{67}$$

The solution can be read directly from Ref. [19], and it is given by

$$\chi^{(I)}(\rho) = \frac{Y}{64R^2}\left(2\rho_0^2\rho^2 - \rho^4\right) + \frac{Ys}{8\pi}\rho^2\left(\ln(\rho/\rho_0) - \frac{1}{2}\right), \tag{68}$$

where $\rho_0 = R\theta_m$ is the radius of the crystal. This is a double expansion in the small parameters ρ_0^2/R^2 and $s/(2\pi)$.

Substitution of Eq. (68) into Eq. (50) gives

$$\begin{aligned}
\bar{g}^{(I)}_{rr} &= \frac{1}{8R^2}\left[\rho_0^2 - \rho^2 + \nu_p\left(3\rho^2 - \rho_0^2\right)\right] - \frac{s}{2\pi}\nu_p\\
&\quad+\frac{s}{2\pi}(1-\nu_p)\ln\left(\frac{\rho}{\rho_0}\right),\\
\bar{g}^{(I)}_{\phi\phi} &= w^2\rho^2\left(\frac{1}{8R^2}\left[\rho_0^2 - 3\rho^2 + \nu_p\left(\rho^2 - \rho_0^2\right)\right]\right.\\
&\quad\left.+\frac{s}{2\pi} + \frac{s}{2\pi}(1-\nu_p)\ln\left(\frac{\rho}{\rho_0}\right)\right).
\end{aligned} \tag{69}$$

The actual frame metric becomes

$$\begin{aligned}
g_{rr} &= \bar{g} + \bar{g}^{(I)}_{rr}\\
&= 1 + \frac{1}{8R^2}\left[\rho_0^2 - \rho^2 + \nu_p\left(3\rho^2 - \rho_0^2\right)\right]\\
&\quad-\frac{s}{2\pi}\nu_p + \frac{s}{2\pi}(1-\nu_p)\ln\left(\frac{\rho}{\rho_0}\right) \equiv r'(\rho)^2,\\
g_{\phi\phi} &= \bar{g}_{\phi\phi} + \bar{g}^{(I)}_{\phi\phi}\\
&= w^2\rho^2 + w^2\rho^2\left(\frac{1}{8R^2}\left[\rho_0^2 - 3\rho^2 + \nu_p\left(\rho^2 - \rho_0^2\right)\right]\right.\\
&\quad\left.+\frac{s}{2\pi} + \frac{s}{2\pi}(1-\nu_p)\ln\left(\frac{\rho}{\rho_0}\right)\right) \equiv \sin^2[r(\rho)].
\end{aligned} \tag{70}$$

Using the transformation properties of $g(\bar{x})_{\mu\nu}$ in terms of $\mathcal{F}$ in Eq. (6), we obtain

$$\begin{aligned}
r(\rho) &= \rho\left(1 + \frac{1}{16R^2}\left[\rho_0^2 - \frac{\rho^2}{3} + \nu_p\left(\rho^2 - \rho_0^2\right)\right]\right.\\
&\quad\left.-\frac{s}{4\pi} + \frac{s}{4\pi}(1-\nu_p)\ln\left(\frac{\rho}{\rho_0}\right)\right),
\end{aligned} \tag{71}$$

which is inverted to give the complete solution,

$$\begin{aligned}
\rho(r) &= r\left(1 - \frac{1}{16R^2}\left[(\theta_m R)^2 - \frac{r^2}{3} + \nu_p[r^2 - (\theta_m R)^2]\right]\right.\\
&\quad\left.+\frac{s}{4\pi} - \frac{s}{4\pi}(1-\nu_p)\ln\left(\frac{r}{\theta_m R}\right)\right).
\end{aligned} \tag{72}$$

The stresses are then found using Eq. (52),

$$\begin{aligned}
\sigma^{\rho\rho} &= \frac{Y}{16R^2}\left(\rho_0^2 - \rho^2\right) + \frac{Ys}{4\pi}\ln\left(\frac{\rho}{\rho_0}\right),\\
\rho^2\sigma^{\psi\psi} &= \frac{Y}{16R^2}\left(\rho_0^2 - 3\rho^2\right) + \frac{Ys}{4\pi}\left(1 + \ln\left(\frac{\rho}{\rho_0}\right)\right),
\end{aligned} \tag{73}$$

and the free energy from Eq. (55) becomes

$$\begin{aligned}
\frac{F}{\pi\rho_0^2 Y} &= \frac{\theta_m^4}{384} + \frac{1}{32}\left(\frac{s^2}{\pi^2} - \frac{s}{2\pi}\theta_m^2\right),\\
\frac{F}{AY} &= \frac{\theta_m^4}{1536} + \frac{1}{32}\left(\frac{s}{\pi} - \frac{\theta_m^2}{4}\right)^2,
\end{aligned} \tag{74}$$

where A is the area of the crystal. The limit $\theta_m \to 0$ (flat limit) agrees with previous results [17].

2. Actual frame

With the assumptions that $\psi=\varphi$, the actual metric becomes

$$ds^2=[\mathcal{F}'(\rho)]^2 d\rho^2+\sin^2[\mathcal{F}(\rho)]d\psi^2. \tag{75}$$

The equations for the Airy function are either Eq. (42) (IF) or Eq. (46) (LF), namely

$$\Delta^2\chi_{IF}^{(1)}+\frac{2}{R^2}\Delta\chi_{IF}^{(1)}=s(\mathbf{x})-\frac{1}{R^2}\ (\mathrm{IF}),\quad \Delta^2\chi_{LF}^{(1)}=s(\mathbf{x})-\frac{1}{R^2}\ (\mathrm{LF}), \tag{76}$$

where $s(\mathbf{x})$ is the disclination density.

The solutions to Eq. (76) are

$$\begin{aligned}\chi_{IF}^{(1)}(r)/(YR^2)=&\ln\left[\cos\left(\frac{r}{2R}\right)\right]-\ln\left[\cos\left(\frac{\theta_m}{2}\right)\right]-\frac{1}{2}\cos\left(\frac{r}{R}\right)\csc(\theta_m)\tan\left(\frac{\theta_m}{2}\right)+\frac{1}{2}\cot(\theta_m)\tan\left(\frac{\theta_m}{2}\right)\\&+\frac{s}{2\pi}\left[\sin^2\left(\frac{r}{2R}\right)\ln\left(\frac{\tan\left(\frac{r}{2R}\right)}{\tan\left(\frac{\theta_m}{2}\right)}\right)-\frac{1}{2}\sin^2\left(\frac{r}{2R}\right)\sec^2\left(\frac{\theta_m}{2}\right)+\frac{1}{2}\tan^2\left(\frac{\theta_m}{2}\right)\right]\end{aligned} \tag{77}$$

and also

$$\begin{aligned}\chi_{LF}^{(1)}(r)/(YR^2)=&\mathrm{Li}_2\left[\sin^2\left(\frac{r}{2R}\right)\right]-\mathrm{Li}_2\left[\sin^2\left(\frac{\theta_m}{2}\right)\right]-\cot^2\left(\frac{\theta_m}{2}\right)\ln\left(\frac{1+\tan^2\left(\frac{r}{2R}\right)}{1+\tan^2\left(\frac{\theta_m}{2}\right)}\right)\ln\left[1+\tan^2\left(\frac{\theta_m}{2}\right)\right]\\&+\frac{s}{2\pi}\left\{\mathrm{Li}_2\left(-\tan^2\left(\frac{r}{2R}\right)\right)-\mathrm{Li}_2\left(-\tan^2\left(\frac{\theta_m}{2}\right)\right)+\ln\left(\tan\left(\frac{r}{2R}\right)\right)\ln\left(1+\tan^2\left(\frac{r}{2R}\right)\right)\right.\\&-\ln\left(\tan\left(\frac{\theta_m}{2}\right)\right)\ln\left(1+\tan^2\left(\frac{\theta_m}{2}\right)\right)+2\ln\left(\cos\left(\frac{r}{2R}\right)\right)\\&\times\left[\cot^2\left(\frac{\theta_m}{2}\right)\ln\left(\cos\left(\frac{\theta_m}{2}\right)\right)+\ln\left(\sin\left(\frac{\theta_m}{2}\right)\right)\right]\\&\left.-2\ln\left(\cos\left(\frac{\theta_m}{2}\right)\right)\left[\cot^2\left(\frac{\theta_m}{2}\right)\ln\left(\cos\left(\frac{\theta_m}{2}\right)\right)+\ln\left(\sin\left(\frac{\theta_m}{2}\right)\right)\right]\right\},\end{aligned} \tag{78}$$

with Li_2 the dilogarithmic function. It is relevant at this point to compare the Airy function in actual space with the one in reference space; the difference between then gives an idea of the errors involved in the corresponding approximations. Using Eq. (68) by expanding Eq. (78) to the next orders gives

$$\begin{aligned}\chi_{IF}^{(1)}(x)/(YR^2)=&-\frac{1}{64}(x^2-\theta_m^2)^2+\frac{s}{16\pi}\left[\theta_m^2-x^2+2x^2\ln\left(\frac{x}{\theta_m}\right)\right]-\frac{1}{384}(\theta_m^6-2x^2\theta_m^4+x^4\theta_m^2)\\&+\frac{s}{192\pi}\left[3x^4+2\theta_m^4-5x^2\theta_m^2-2x^4\ln\left(\frac{x}{\theta_m}\right)\right]\\\chi_{LF}^{(1)}(x)/(YR^2)=&-\frac{1}{64}(x^2-\theta_m^2)^2+\frac{s}{16\pi}\left[\theta_m^2-x^2+2x^2\ln\left(\frac{x}{\theta_m}\right)\right],\\&-\frac{1}{2304}(\theta_m^6+2x^6-3x^4\theta_m^2)+\frac{s}{384\pi}\left[\theta_m^4-x^2\theta_m^2+2x^4\ln\left(\frac{x}{\theta_m}\right)\right],\end{aligned} \tag{79}$$

with $x=r/R$. It is important to note that there are only linear terms in disclination charge s, but higher orders in x and θ_M. This is basically due to the fact that defects in both IF and LF appear linearly, but the displacements do not need to be small. The explicit form of the stresses can be found using Eq. (43):

$$\begin{aligned}\sigma_{IF}^{rr}(r)Y=&\frac{1}{4}\cos\left(\frac{r}{R}\right)\left[-\sec^2\left(\frac{r}{2R}\right)+\sec^2\left(\frac{\theta_m}{2}\right)+\frac{s}{2\pi}\left(2\ln\left(\frac{\tan\left(\frac{r}{2R}\right)}{\tan\left(\frac{\theta_m}{2}\right)}\right)+\sec^2\left(\frac{r}{2R}\right)-\sec^2\left(\frac{\theta_m}{2}\right)\right)\right],\\R^2\sin^2\left(\frac{r}{R}\right)\sigma_{IF}^{\phi\phi}(r)/Y=&\frac{1}{4}\cos\left(\frac{r}{R}\right)\left[\sec^2\left(\frac{r}{2R}\right)+\sec^2\left(\frac{\theta_m}{2}\right)+\frac{s}{2\pi}\left(2\ln\left(\frac{\tan\left(\frac{r}{2R}\right)}{\tan\left(\frac{\theta_m}{2}\right)}\right)-\sec^2\left(\frac{r}{2R}\right)-\sec^2\left(\frac{\theta_m}{2}\right)\right)\right]\\&+\frac{s}{2\pi}-\frac{1}{2}\end{aligned} \tag{80}$$

and

$$\begin{aligned}
\sigma^{rr}_{LF}(r)/Y &= \frac{1}{2}\sec^2\left(\frac{r}{2R}\right)\cos\left(\frac{r}{R}\right)\Bigg[-\cot^2\left(\frac{r}{2R}\right)\ln\left(\cos^2\left(\frac{r}{2R}\right)\right)+\cot^2\left(\frac{\theta_m}{2}\right)\ln\left(\cos^2\left(\frac{\theta_m}{2}\right)\right)\\
&\quad+\frac{s}{2\pi}\left(\ln\left(\frac{\tan\left(\frac{r}{2R}\right)}{\tan\left(\frac{\theta_m}{2}\right)}\right)+\csc^2\left(\frac{r}{2R}\right)\ln\left(\cos\left(\frac{r}{2R}\right)\right)-\csc^2\left(\frac{\theta_m}{2}\right)\ln\left(\cos\left(\frac{\theta_m}{2}\right)\right)\right)\Bigg],\\
R^2\sin^2\left(\frac{r}{R}\right)\sigma^{\phi\phi}_{LF}(r)/Y &= 1+\frac{1}{2}\sec^2\left(\frac{r}{2R}\right)\Bigg[\cot^2\left(\frac{r}{2R}\right)\ln\left(\cos^2\left(\frac{r}{2R}\right)\right)+\cot^2\left(\frac{\theta_m}{2}\right)\ln\left(\cos^2\left(\frac{\theta_m}{2}\right)\right)\\
&\quad+\frac{s}{2\pi}\left(\ln\left(\frac{\tan\left(\frac{r}{2R}\right)}{\tan\left(\frac{\theta_m}{2}\right)}\right)-\cos\left(\frac{r}{R}\right)\csc^2\left(\frac{r}{2R}\right)\ln\left(\cos\left(\frac{r}{2R}\right)\right)-\csc^2\left(\frac{\theta_m}{2}\right)\ln\left(\cos\left(\frac{\theta_m}{2}\right)\right)\right)\Bigg],
\end{aligned}\tag{81}$$

which we thoroughly analyze in the next section.

V. DISCUSSION

We now present approximate solutions and compare them to those of the exact equations, and analyze each quantity in turn.

A. The function $\mathcal{F}$

This function defines how distances between particles in reference frame are transformed in actual space. We have not been able to find an analytical expression for the exact equation (65), which we could nevertheless solve numerically. In Fig. 2 we compare it to the EF solution defined by Eq. (72). In order to visualize the difference, the figures are shown as a function of $r - \rho(r)$. Quite interestingly, the EF mapping shows very small errors, certainly for $\theta_m < 0.1$, which corresponds to an aperture angle of 60 degrees. Even for $\theta_m \sim 1.5$ (half the sphere), the linear approximation does extremely well when a disclination is present, which is expected as the disclination charge screens the Gaussian curvature, so that the geometric frustration parameter η [see Eq. (14)] is small, and subsequent corrections to the linear contribution become very small.

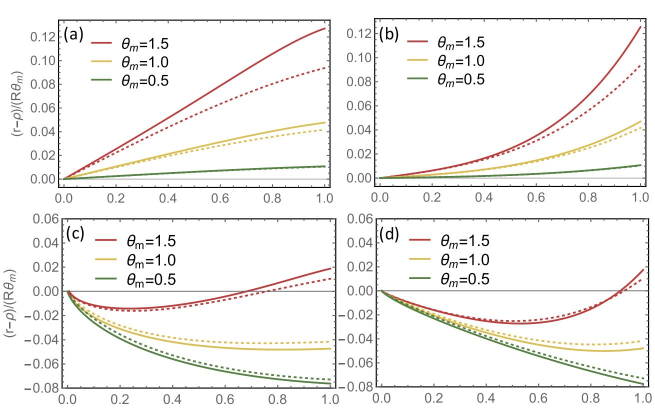

FIG. 2. The difference between actual and reference coordinate $[r - \rho(r)]$ as a function of the actual coordinate (r) for different values of disclination charge s and Poisson ratio ν_p: (a) [$s = 0$, $\nu_p = 0.2$], (b) [$s = 0$, $\nu_p = 0.8$], (c) [$s = \frac{\pi}{3}$, $\nu_p = 0.2$], and (d) [$s = \frac{\pi}{3}$, $\nu_p = 0.8$]. The solid lines correspond to the exact result, Eq. (65), while the dotted lines denote the EF solution, Eq. (72).

B. Airy function and stresses

The Airy function, computed with the different approximations, namely EF [Eq. (68)], IF [Eq. (77)] and LF [Eq. (78)] is shown in Fig. 3 for two different values of the aperture angle (cap size). Small but significant differences are observed for larger caps.

The stresses show similar trends, as observed for the Airy function illustrated in Fig. 4. As expected, for large values of the aperture angle the exact result is in much better agreement with the case of a disclination at the center (note the different scales in the plot).

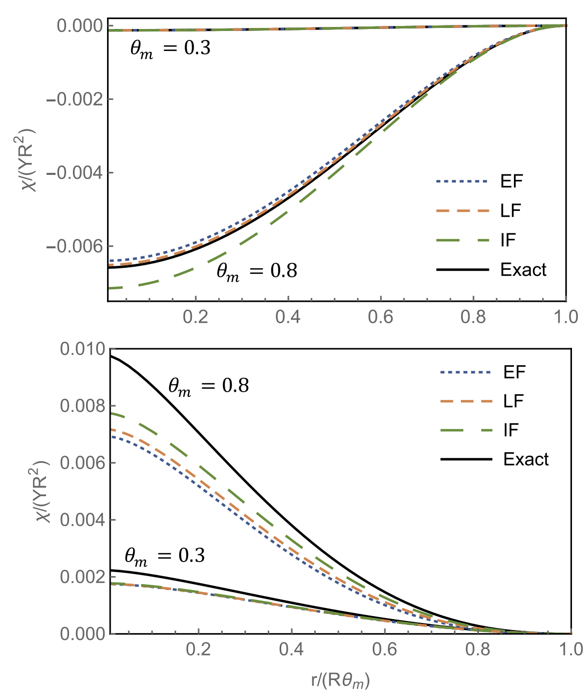

FIG. 3. χ as function of r (actual frame) or ρ (reference frame) corresponding to cap sizes $\theta_m = 0.8$ and $\theta_m = 0.3$. The upper figure corresponds to $s = 0$ and lower one to $s = \pi/3$.

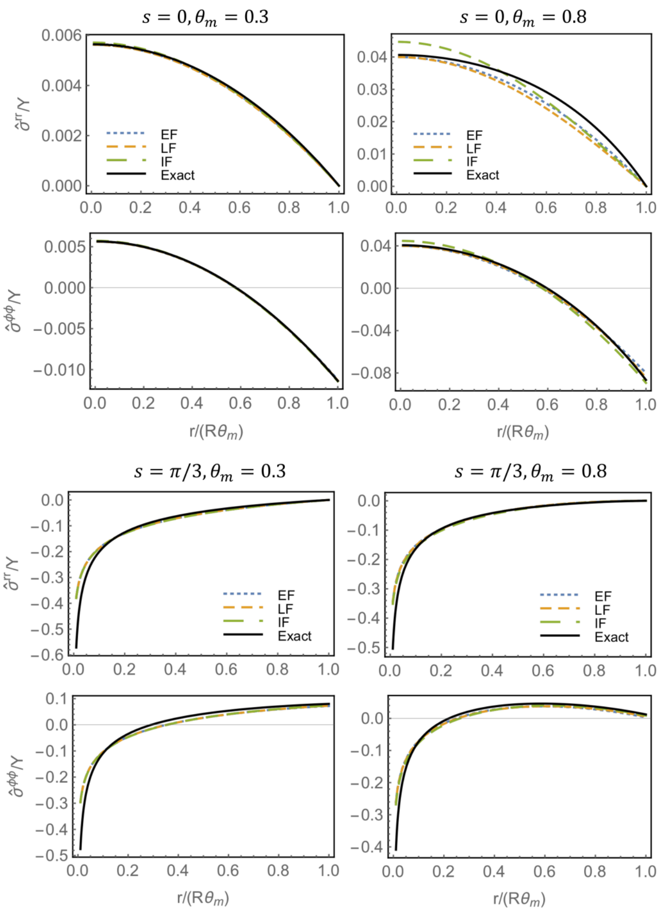

FIG. 4. Stress $\hat{\sigma}^{rr}$ and $\hat{\sigma}^{\phi\phi}$ with small cap size ($\theta_m = 0.3$, left column) and large cap size ($\theta_m = 0.8$, right column). The top four plots of stress correspond to zero disclination and four bottom plots to a single disclination at the center.

C. Energy

The values for the total free energy are shown in Fig. 5 as a function of the aperture angle θ_m. As expected, in the flat limit $\theta_m \to 0$, the EF, LF, and IF all converge to a value that is different from the exact result, which is also slightly different from another exact result obtained by Seung and Nelson (SN) [17] (see the discussion in conclusions and Appendixes),

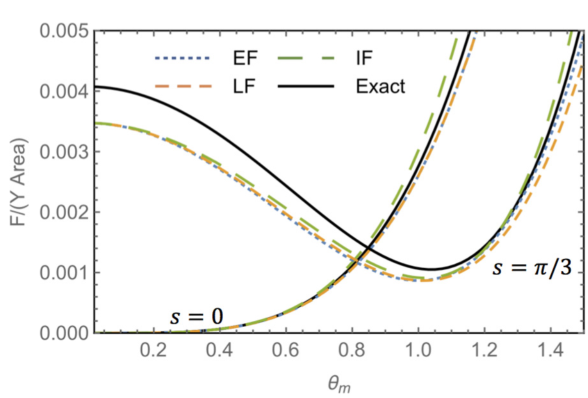

FIG. 5. Free energy per unit area for $s = 0$ and $s = \frac{\pi}{3}$ for different models presented in the paper.

namely

$$\begin{aligned} \frac{F}{YA} &= \frac{1}{288} \\ &= 0.0035 \text{ (EF, LF, IF)} \\ &= 0.0041 \text{ (exact)} \\ &= 0.0040 \text{ (exact SN).} \end{aligned} \tag{82}$$

The (small) disagreement between EF, LF, and IF with the exact result is a consequence of large displacements near the core of a disclination on a flat topography [39]. The small disagreement with SN results also reflects the intrinsic ambiguity of what is meant by an "exact" elastic theory, as terms with higher powers of the strain tensor, for example, may be included in the definition of the elastic energy, Eq. (15), a point which we will elaborate in the conclusions.

For the case of a central disclination, at finite and increasing values of the aperture angle θ_m, the different linear approximations gradually converge to the exact result. Note that the free energy goes through a minimum at around $\theta_m \approx 1.05$, which maybe interpreted as the point where the disclination optimally screens the Gaussian curvature. It seems reasonable that this point maybe calculated when the PCC equation (13) is satisfied on average, namely

$$\int d^2\mathbf{x}\, s(\mathbf{x}) = \int d^2\mathbf{x}\, K(\mathbf{x}) \to \frac{\pi}{3} = 2\pi[1 - \cos(\theta_c)], \tag{83}$$

that is, at $\theta_M = \theta_c = \arccos(5/6) = 0.59$, which is significantly lower and reflects the role of the boundary conditions. It is also important to note that, when $\theta_M > \theta_c$, the approximation to the energy for the disclination free monolayer starts to deviate from the exact result.

VI. CONCLUSIONS

In this paper we have presented a general fully covariant elastic theory, as defined by the energy equations (15) and (17), anticipated in Refs. [30,31]. In particular, we have considered the reference metric, which consists of patches of flat manifolds, connected by quanta of $\pi/3$ charges (for a triangular lattice), so that the reference space is not necessarily flat everywhere. The actual metric is the induced metric from ambient (3D) space on the given curved surface. The continuum formalism presented in the paper is identical to the limit of vanishing lattice constant of a discrete model consisting of equilateral triangles (or squares). Therefore, the disclination charges are quantized as $\pi/3$ ($\pi/2$), and the dislocation charges are quantized in units of the lattice constant a, the Burgers vector.

We have discussed three different linear approximations (EF, LF, IF) from which all analytical results quoted in the literature have been derived. Quite unexpectedly, the differences are quantitatively very small, but the ones in actual space (LF, IF) have the advantage that satisfy topological relations [see Eq. (7)] exactly. It is possible to compute orders beyond linear and, in this way, obtain the exact result, although for general problems the calculations are quite demanding.

The actual meaning of the "exact solution," however, appears as an ambiguous concept. While our exact result of a single disclination on a flat monolayer as $\theta_m \to 0$ is almost the same as the value [see Eq. (82)] obtained by Seung and Nelson [17], it is not obvious that the energies obtained by the two methods match for all values of θ_m. The Seung and Nelson energy is given as

$$F_D = \frac{\epsilon}{2}\sum_{\langle i,j\rangle}(d_{ij} - \bar{d}_{ij})^2 = \frac{\epsilon}{2}\sum_{\langle i,j\rangle}(|\vec{r}_i - \vec{r}_j| - a)^2, \tag{84}$$

where $\langle i, j\rangle$ are the nearest neighbors defined by a triangulation $\mathcal{T}$. This energy is conceptually the same as the one defined by Eqs. (15) and (17), since $\bar{d}_{ij} = a$ is the distance in reference and d_{ij} in actual space, and, expanding in small displacements, both energies coincide for the choices of elastic constants $Y = 2\epsilon/\sqrt{3}$ and $\nu_p = 1/3$ [17]. However, these two approaches differ beyond linear order. It is possible to make them agree at higher orders by adding higher powers of $|d_{ij} - \bar{d}_{ij}|$ in

$$F = F_D + \sum_{l=2}^{M}\frac{\epsilon_l}{2}(d_{ij} - \bar{d}_{ij})^{2l} \tag{85}$$

so that, for appropriately chosen values ϵ_l, higher orders of the displacement beyond linear will agree with the energy equation (17). Additional powers of $u_{\alpha\beta}$ can also be added to Eq. (17), to make it agree with Eq. (84). In either case, it serves to make the point that Eqs. (17) and (84) represent two different nonlinear elastic theories, and therefore it is expected that the exact results for a single disclination will differ. It should be noted, however, that both exact results are close, thus highlighting that nonlinear corrections are small. The natural question becomes, then, which one is the "correct" model? A satisfactory answer can be given if the underlying microscopic potential among particles is known. Then it is possible to impose that the higher orders of elasticity theory [see Eq. (85)] match the same orders of the energy of the crystal in powers of the displacement, as discussed in Ref. [26], where exceedingly accurate predictions for energies were obtained for any geometry.

Another fundamental aspect of the geometric theory of elasticity discussed in this paper is the choice of the reference metric, which corresponds to a configuration where all nearest neighbor distances and angles are the same. In some cases, such as for a defect free disk or a cone with a single disclination, it is possible to optimize the geometry, resulting in strain and stress free configurations in actual space. For other, more complex defect distributions, such actual space configurations do not exist. A conspicuous property of the model in Eq. (84), however, is that it involves nearest neighbor distances only, and the condition that the angles are the same does not need to be satisfied. Thus, general Archimedean tiling configurations, such as the one shown in Fig. 6, are strain and stress free for an actual space consisting of a plane. It is interesting to note that it is possible to build dodecagonal quasicrystals out of $(3^3.4^2)$ Archimedean tiling, which have been observed in nanocrystal systems [40]. Within elasticity theory, those Archimedean tilings require a Poisson ratio $\nu_p = 1/3$, as is clear from the discussion following Eq. (84); see also Ref. [39].

We have shown that the "exact" equations of elasticity theory amount to minimizing the difference between the actual

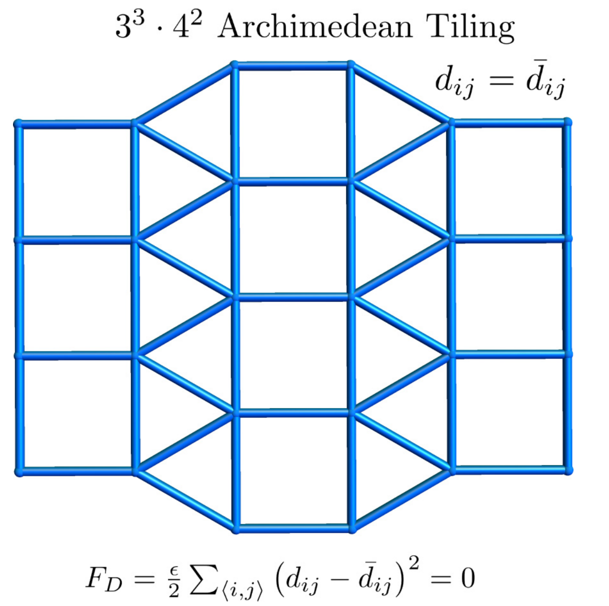

FIG. 6. Example of the $(3^3 \cdot 4^2)$ Archimedean tiling with zero elastic energy. Such a configuration, however, has zero energy modes and requires additional constraints to be stable.

and the reference metric,

$$g(\text{actual metric}) - \bar{g}(\text{reference metric}) = 2u_{\alpha\beta},$$

where the actual metric is fixed by the topography (the surface; see Fig. 1), and the reference metric is such that its curvature $\bar{K}$ is a sum of disclinations and dislocations,

$$\begin{aligned}\bar{K} &= \text{disclinations} + \text{dislocations}\\ &= \text{“quanta” of curvature} + \text{“quanta” of torsion},\end{aligned}$$

where the disclinations are quantized in units of $\frac{\pi}{3}$ and the dislocations in units of the Burgers vector $\vec{b}$. These equations summarize the geometric content of the equations in elasticity theory as applied to arbitrary topographies. For boundary free crystals, they also satisfy topological constraints, for example Eq. (7).

There are a number of issues that we have not discussed. For example, the free energy, Eq. (17), is invariant under general parametrizations, which in turn, through the Noether theorem, gives rise to conservation laws that relate to the stress tensor. Also, the IF includes a term [see Eq. (42)] that has a derivative of the Gaussian curvature. In those cases where the Gaussian curvature is not constant and varies rapidly, this term may become important or even dominant.

In summary, we presented a covariant formulation of elasticity that unifies geometric and topological concepts with the theory of defects. All available results in the literature maybe recovered from this formulation as suitable approximations, thus providing a rigorous justification on their validity, and providing the necessary framework for our recent studies of icosahedral order in virus shells [33]. Throughout this paper, the geometry has been fixed. There are obviously many fascinating problems when the geometry is allowed to fluctuate (see, for example Ref. [41]), but those problems will be discussed elsewhere.

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APPENDIX A: THE SEUNG-NELSON RESULT AS A FUNCTION OF AREA

Seung and Nelson [17] quote, for a flat disclination,

$$\frac{F}{Ys^2R^2} = 0.008. \tag{A1}$$

The radius is given by $R = na$, where n is an integer and a is the lattice constant. A more precise calculation computes this coefficient as 0.00785 [39]. This is a numerical calculation considering a pentagonal shape crystal containing $5n^2$ triangles. Each triangle has an area $\frac{\sqrt{3}}{4}a^2$, hence

$$\frac{F}{YA} = 0.008\left(\frac{\pi}{3}\right)^2 \Big/ (5\sqrt{3}/4) \approx 0.00405, \tag{A2}$$

or 0.00400 with the more precise value [39]. This is the coefficient used in Eq. (82).

APPENDIX B: GEOMETRY, CURVATURE, VIELBEINS, AND THE DEFINITION OF THE STRESS TENSOR

It should be noticed that the stress tensor, defined by Eq. (19) is in general different than the one defined in standard textbooks, such as Landau and Lifshitz, which we denote as $\hat{\sigma}^{\alpha\beta}$. We now show the relation between both tensors. For that purpose, we introduce the vielbeins e^{α}_{μ}, defined as

$$\begin{aligned} g_{\mu\nu} &= e^{\alpha}_{\mu} e^{\beta}_{\mu} \delta_{\alpha\beta}, \\ \delta_{\alpha\beta} &= e^{\mu}_{\alpha} e^{\mu}_{\beta} g_{\mu\nu}. \end{aligned} \tag{B1}$$

Then, there is the relation

$$\hat{\sigma}^{\alpha\beta} = e^{\alpha}_{\mu} e^{\beta}_{\nu} \sigma^{\mu\nu}. \tag{B2}$$

The advantage of $\hat{\sigma}^{\alpha\beta}$ is that the units of all the components are the same. This is not the case for $\sigma^{\mu\nu}$. Obviously, all physical quantities have the same dimensions in either form.

Also, the line tension term (22) is simplified by

$$\int_{\partial\mathcal{B}} ds = \int_{\partial\mathcal{B}} \sqrt{g} dl = \int_{\partial\mathcal{B}} dx^{\mu} g_{\mu\nu} t^{\nu}, \tag{B3}$$

where $t^{\nu} = \frac{1}{\sqrt{g}}\frac{dx^{\mu}}{dl}$ for any parametrization $x^{\mu}(l)$. Here t^{μ} is the unit tangent vector to the curve defining the boundary. Note that

$$g = g_{\mu\nu}\frac{dx^{\mu}}{dl}\frac{dx^{\nu}}{dl} \tag{B4}$$

and $dx^{\mu} = \sqrt{g} t^{\mu} dl$. The variation of this term gives

$$\begin{aligned} \int_{\partial\mathcal{B}} dx^{\mu} \delta g_{\mu\nu} t^{\nu} &= -\int_{\partial\mathcal{B}} dx^{\mu} (\nabla_{\nu}\xi_{\mu} + \nabla_{\mu}\xi_{\nu}) t^{\nu} \\ &= \int_{\partial\mathcal{B}} dx^{\mu} (\xi_{\mu}\nabla_{\nu} + \xi_{\nu}\nabla_{\mu}) t^{\nu} \\ &= \int_{\partial\mathcal{B}} dx^{\mu} \nabla_{\mu} t^{\nu} \xi_{\nu}, \end{aligned} \tag{B5}$$

where $dx^{\mu}\xi_{\mu} = 0$, as the vector ξ^{μ} is perpendicular to t^{μ}. Note that the vector

$$n_{\rho} = \sqrt{g}\epsilon_{\mu\rho} t^{\mu}, \tag{B6}$$

is a unit vector, perpendicular to t^{μ}.

The variation in Eq. (B5) refers to $\delta g_{\alpha\beta}$ with the implicit condition $\delta \bar{g}_{\alpha\beta} = 0$, while the variation leading to Eq. (20) is with respect to $\delta \bar{g}_{\alpha\beta}$ with $\delta g_{\alpha\beta} = 0$. One notes, however, that the general transformation

$$\begin{aligned} \delta g_{\alpha\beta} &= \nabla_{\alpha}\xi_{\beta} + \nabla_{\beta}\xi_{\alpha}, \\ \delta \bar{g}_{\alpha\beta} &= \bar{\nabla}_{\alpha}\xi_{\beta} + \bar{\nabla}_{\beta}\xi_{\alpha}, \end{aligned} \tag{B7}$$

encodes a simple reparametrization and, therefore, under this transformation any term F_a appearing in the energy should satisfy

$$\delta F_a = \delta_g F_a + \delta_{\bar{g}} F_a = 0, \tag{B8}$$

hence the correct variation with respect to $\bar{g}_{\alpha\beta}$ picks up a minus sign as compared with Eq. (B5),

$$\delta F_l = -\int_{\partial\mathcal{B}} dx^{\mu} \nabla_{\mu} t^{\nu} \xi_{\nu}, \tag{B9}$$

as used in the main text.

APPENDIX C: INCOMPATIBILITY METRIC APPROXIMATIONS

1. Incompatibility metric approximation: Actual frame

The second order in the expansion (39) is given by

$$\begin{aligned} g^{(2)}_{\alpha\beta} = &-\frac{2}{Y}(g_{\alpha\beta}\Delta\chi^{(2)} - (1+\nu_P)\nabla_{\alpha}\nabla_{\beta}\chi^{(2)}) \\ &-\frac{2}{Y}\big(g_{\alpha\beta}g^{\rho\gamma}\Gamma^{\mu(1)}_{\rho\gamma} - (1+\nu_P)\Gamma^{\mu(1)}_{\alpha\beta}\big)\nabla_{\mu}\chi^{(1)} \\ &-\frac{1}{2}g^{(1)}_{\alpha\beta}g^{\gamma\sigma}g^{(1)}_{\gamma\sigma}. \end{aligned} \tag{C1}$$

Obviously, the expansion can be continued to all orders, and in this way a perturbative solution to Eqs. (35) and (36) can be found. The goal is now to derive an explicit equation for $\chi^{(i)}$, as shown below.

2. Incompatibility metric approximation: Reference frame

The second order in Eq. (50) can also be computed as

$$\begin{aligned} \bar{g}^{(II)}_{\alpha\beta} = &\frac{2}{Y}(\bar{g}_{\alpha\beta}\bar{\Delta}\chi^{(II)} - (1+\nu_P)\bar{\nabla}_{\alpha}\bar{\nabla}_{\beta}\chi^{(II)}) \\ &+\frac{1}{2}\bar{g}^{(I)}_{\alpha\beta}\bar{g}^{\gamma\sigma}\bar{g}^{(I)}_{\gamma\sigma}. \end{aligned} \tag{C2}$$

3. First-order solution: Actual frame

We will compute the Ricci tensor $\bar{R}_{\sigma\nu} = \bar{R}^{\rho}_{\sigma\rho\nu}$, which from Eq. (E18) is

$$\bar{R}_{\sigma\nu} = R_{\sigma\nu} + \nabla_{\mu}\Gamma^{\mu(1)}_{\nu\sigma} - \nabla_{\nu}\Gamma^{\mu(1)}_{\mu\sigma}. \tag{C3}$$

The first term is obtained from Eqs. (41), (E16), and (E18), leading to

$$
\begin{aligned}
-Y\nabla_\mu\Gamma^{\mu(1)}_{\nu\sigma} = {}& \nabla_\sigma\nabla_\nu\Delta\chi^{(1)} - (1+\nu_P)g^{\mu\gamma}\nabla_\mu\nabla_\nu\nabla_\sigma\nabla_\gamma\chi^{(1)} \\
&+ \nabla_\nu\nabla_\sigma\Delta\chi^{(1)} - (1+\nu_P)g^{\mu\gamma}\nabla_\mu\nabla_\sigma\nabla_\nu\nabla_\gamma\chi^{(1)} \\
&- g_{\sigma\nu}\Delta^2\chi^{(1)} + (1+\nu_P)g^{\mu\gamma}\nabla_\mu\nabla_\gamma\nabla_\nu\nabla_\sigma\chi^{(1)}
\end{aligned}
\tag{C4}
$$

This is simplified by using Eqs. (E3) and (E4):

$$
\begin{aligned}
&g^{\mu\gamma}\nabla_\mu\nabla_\gamma\nabla_\nu\nabla_\sigma\chi^{(1)} \\
&\quad = g^{\mu\gamma}\nabla_\mu\nabla_\nu\nabla_\gamma\nabla_\sigma\chi^{(1)} - g^{\mu\gamma}\nabla_\mu\big(R^\lambda_{\sigma\gamma\nu}\nabla_\lambda\chi^{(1)}\big)
\end{aligned}
\tag{C5}
$$

and

$$
\begin{aligned}
&g^{\mu\gamma}\nabla_\mu\nabla_\sigma\nabla_\nu\nabla_\gamma\chi^{(1)} \\
&\quad = g^{\mu\gamma}\nabla_\sigma\nabla_\mu\nabla_\nu\nabla_\gamma\chi^{(1)} - g^{\mu\gamma}R^\lambda_{\nu\mu\sigma}\nabla_\lambda\nabla_\gamma\chi^{(1)} \\
&\quad\quad - g^{\mu\gamma}R^\lambda_{\gamma\mu\sigma}\nabla_\nu\nabla_\lambda\chi^{(1)}.
\end{aligned}
\tag{C6}
$$

One more application of Eq. (E4) converts Eq. (C6) into

$$
\begin{aligned}
&g^{\mu\gamma}\nabla_\mu\nabla_\sigma\nabla_\nu\nabla_\gamma\chi^{(1)} \\
&\quad = g^{\mu\gamma}\nabla_\sigma\nabla_\nu\nabla_\mu\nabla_\gamma\chi^{(1)} - g^{\mu\gamma}\nabla_\sigma\big(R^\lambda_{\gamma\mu\nu}\nabla_\lambda\chi^{(1)}\big) \\
&\quad\quad - g^{\mu\gamma}R^\lambda_{\nu\mu\sigma}\nabla_\lambda\nabla_\gamma\chi^{(1)} - g^{\mu\gamma}R^\lambda_{\gamma\mu\sigma}\nabla_\nu\nabla_\lambda\chi^{(1)}.
\end{aligned}
\tag{C7}
$$

Using the expression of the Riemann tensor in two dimensions, Eq. (E9), we obtain

$$
\begin{aligned}
&g^{\mu\gamma}R^\lambda_{\nu\mu\sigma}\nabla_\lambda\nabla_\gamma\chi^{(1)} = Kg_{\nu\sigma}\Delta\chi^{(1)} - K\nabla_\sigma\nabla_\nu\chi^{(1)}, \\
&g^{\mu\gamma}R^\lambda_{\gamma\mu\sigma}\nabla_\nu\nabla_\lambda\chi^{(1)} = -K\nabla_\nu\nabla_\sigma\chi^{(1)}
\end{aligned}
\tag{C8}
$$

and

$$
g^{\mu\gamma}\nabla_\sigma\big(R^\lambda_{\gamma\mu\nu}\nabla_\lambda\chi^{(1)}\big) = -\nabla_\sigma K\nabla_\nu\chi^{(1)} - K\nabla_\sigma\nabla_\nu\chi^{(1)}. \tag{C9}
$$

Also

$$
\begin{aligned}
&g^{\mu\gamma}\nabla_\mu\big(R^\lambda_{\sigma\gamma\nu}\nabla_\lambda\chi^{(1)}\big) \\
&\quad = g_{\sigma\nu}g^{\mu\lambda}\nabla_\mu K\nabla_\lambda\chi^{(1)} - \nabla_\sigma K\nabla_\nu\chi^{(1)} + g_{\sigma\nu}K\Delta\chi^{(1)} \\
&\quad\quad - K\nabla_\sigma\nabla_\nu\chi^{(1)}.
\end{aligned}
\tag{C10}
$$

Collecting all these terms, Eq. (C4) becomes

$$
\begin{aligned}
-Y\nabla_\mu\Gamma^{\mu(1)}_{\nu\sigma} = {}& 2\nabla_\sigma\nabla_\nu\chi^{(1)} - g_{\sigma\nu}\Delta^2\chi^{(1)} \\
&- (1+\nu_P)\big[\nabla_\sigma\nabla_\nu\Delta\chi^{(1)} + 2K\nabla_\sigma\nabla_\nu\chi^{(1)} \\
&+ g_{\sigma\nu}g^{\mu\lambda}\nabla_\mu K\nabla_\lambda\chi^{(1)}\big].
\end{aligned}
\tag{C11}
$$

The next quantity to compute is

$$
\begin{aligned}
-Y\nabla_\nu\Gamma^{\mu(1)}_{\mu\sigma} = {}& \nabla_\nu\nabla_\sigma\Delta\chi^{(1)} - (1+\nu_P)g^{\mu\gamma}\nabla_\nu\nabla_\mu\nabla_\sigma\nabla_\gamma\chi^{(1)} \\
&+ 2\nabla_\nu\nabla_\sigma\Delta\chi^{(1)} - (1+\nu_P)g^{\mu\gamma}\nabla_\nu\nabla_\sigma\nabla_\mu\nabla_\gamma\chi^{(1)} \\
&- \nabla_\nu\nabla_\sigma\Delta\chi^{(1)} + (1+\nu_P)g^{\mu\gamma}\nabla_\nu\nabla_\mu\nabla_\gamma\nabla_\sigma\chi^{(1)},
\end{aligned}
\tag{C12}
$$

that immediately leads to

$$
-Y\nabla_\nu\Gamma^{\mu(1)}_{\mu\sigma} = 2\nabla_\sigma\nabla_\nu\Delta\chi^{(1)} - (1+\nu_P)\nabla_\nu\nabla_\sigma\chi^{(1)}. \tag{C13}
$$

Therefore, the Ricci tensor is

$$
\begin{aligned}
\bar{R}_{\sigma\nu} = {}& R_{\sigma\nu} + \frac{1}{Y}(g_{\sigma\nu}\Delta^2\chi^{(1)} + (1+\nu_P)[2K\nabla_\sigma\nabla_\nu\chi^{(1)} \\
&+ g_{\sigma\nu}g^{\mu\lambda}\nabla_\mu\chi^{(1)}\nabla_\lambda K]).
\end{aligned}
\tag{C14}
$$

Finally, the scalar curvature is obtained as the trace of the Ricci tensor, hence

$$
\bar{K} = K + \frac{1}{Y}(\Delta^2\chi^{(1)} + 2K\Delta\chi^{(1)} + (1+\nu_p)g^{\mu\lambda}\nabla_\mu K\nabla_\lambda\chi^{(1)}). \tag{C15}
$$

APPENDIX D: ELASTIC ENERGY IN THE ACTUAL FRAME

Our starting point is Eq. (44), which for the sake of convenience we repeat here:

$$
\begin{aligned}
F = {}& \frac{1}{2Y}\int d^2u\sqrt{g}\bigg[(\Delta\chi^{(1)})^2 \\
&+ \frac{(1+\nu_P)}{g}\epsilon^{\alpha\sigma}\epsilon^{\rho\beta}\nabla_\alpha\nabla_\beta\chi^{(1)}\nabla_\rho\nabla_\sigma\chi^{(1)}\bigg].
\end{aligned}
\tag{D1}
$$

We now focus on the second term. Using Eq. (30), this term becomes

$$
\begin{aligned}
&\epsilon^{\alpha\sigma}\epsilon^{\rho\beta}\nabla_\alpha\nabla_\beta\chi^{(1)}\nabla_\rho\nabla_\sigma\chi^{(1)} \\
&\quad = g[\nabla_\alpha\nabla_\beta\chi^{(1)}\nabla^\alpha\nabla^\beta\chi^{(1)} - (\Delta\chi^{(1)})^2].
\end{aligned}
\tag{D2}
$$

Making further use of Eq. (E1) allows us to prove the following identity:

$$
\begin{aligned}
&\sqrt{g}T^{\alpha\beta}\nabla_\alpha\nabla_\beta\chi^{(1)} \\
&\quad = \partial_\alpha(\sqrt{g}T^{\alpha\beta}\nabla_\beta\chi^{(1)}) - \sqrt{g}\nabla_\alpha T^{\alpha\beta}\nabla_\beta\chi^{(1)} \\
&\quad = \partial_\alpha(\sqrt{g}T^{\alpha\beta}\nabla_\beta\chi^{(1)}) - \sqrt{g}\nabla_\alpha(g^{\alpha\beta}\Delta\chi^{(1)})\nabla_\beta\chi^{(1)} \\
&\quad\quad - \sqrt{g}Kg^{\beta\alpha}\nabla_\alpha\chi^{(1)}\nabla_\beta\chi^{(1)}
\end{aligned}
\tag{D3}
$$

where $T^{\alpha\beta} = \nabla^\alpha\nabla^\beta\chi^{(1)}$. Note that

$$
\begin{aligned}
\nabla_\alpha T^{\alpha\beta} &= \nabla_\alpha g^{\alpha\rho}g^{\beta\nu}\nabla_\rho\nabla_\nu\chi^{(1)} \\
&= g^{\beta\nu}g^{\alpha\rho}\nabla_\alpha\nabla_\rho\nabla_\nu\chi^{(1)} \\
&= g^{\beta\nu}g^{\alpha\rho}\nabla_\nu\nabla_\alpha\nabla_\rho\chi^{(1)} - g^{\beta\nu}g^{\alpha\rho}R^\lambda_{\rho\alpha\nu}\nabla_\lambda\chi^{(1)} \\
&= g^{\beta\alpha}\nabla_\alpha\Delta\chi^{(1)} + Kg^{\beta\alpha}\nabla_\alpha\chi^{(1)}.
\end{aligned}
\tag{D4}
$$

Here, we have used the identity (E5).

Using the same operations, it is

$$
\begin{aligned}
&\sqrt{g}\nabla_\alpha(g^{\alpha\beta}\Delta\chi^{(1)})\nabla_\beta\chi^{(1)} \\
&\quad = \partial_\alpha(\sqrt{g}\Delta\chi^{(1)}g^{\alpha\beta}\nabla_\beta\chi^{(1)}) - \sqrt{g}(\Delta\chi^{(1)})^2.
\end{aligned}
\tag{D5}
$$

Hence, the second term in Eq. (D1) becomes

$$
-\frac{1+\nu_p}{2Y}\int d^2u\sqrt{g}Kg^{\alpha\beta}\nabla_\alpha\chi^{(1)}\nabla_\beta\chi^{(1)} \tag{D6}
$$

plus a total derivative

$$
\begin{aligned}
&\frac{1+\nu_p}{2Y}\int d^2u\,\partial_\alpha[\sqrt{g}(T^{\alpha\beta}\nabla_\beta - \Delta\chi^{(1)}g^{\alpha\beta}\nabla_\beta)\chi^{(1)}] \\
&\quad = -\frac{1+\nu_p}{2Y}\int d^2u\,\partial_\alpha[\sqrt{g}\sigma^{\alpha\beta}\nabla_\beta\chi^{(1)}],
\end{aligned}
\tag{D7}
$$

where use has been made of the definition of the stress tensor; see Eq. (43). The above integral contributes only at the boundary, leading to the contribution

$$-\frac{1+\nu_p}{2Y}\oint dx^\rho\sqrt{g}\epsilon_{\rho\alpha}\sigma^{\alpha\beta}\nabla_\beta\chi^{(1)}. \tag{D8}$$

For a spherical cap, the above equation is

$$\frac{1+\nu_p}{2Y}\oint d\theta\sqrt{g}\sigma^{r\beta}\nabla_\beta\chi^{(1)} \tag{D9}$$

and therefore, in the absence of line tension, vanishes by the boundary condition $\sigma^{r\beta}=0,\ \beta=r,\theta$ at the boundary.

APPENDIX E: GENERAL FORMULAS IN RIEMANNIAN GEOMETRY

1. Useful identities

The following results apply for any metric $g_{\mu\nu}$ in any dimension, unless further restrictions are stated:

$$\tfrac{1}{2}\partial_\mu(\ln g)=\Gamma^\rho_{\mu\rho}. \tag{E1}$$

The last equation can be written also as

$$\frac{1}{\sqrt{g}}\partial_\mu(\sqrt{g})=\Gamma^\rho_{\mu\rho}. \tag{E2}$$

Another relation involving Christoffel symbols is

$$g^{\rho\gamma}\Gamma^\nu_{\rho\gamma}=-\frac{1}{\sqrt{g}}\partial_\gamma(\sqrt{g}g^{\gamma\nu}). \tag{E3}$$

The following relation involves the Riemann tensor:

$$[\nabla_\mu,\nabla_\nu]V^\rho=R^\rho_{\lambda\mu\nu}V^\lambda. \tag{E4}$$

The same relation exists for forms as well, namely

$$[\nabla_\mu,\nabla_\nu]W_{\rho\gamma}=-R^\lambda_{\rho\mu\nu}W_{\lambda\gamma}-R^\lambda_{\gamma\mu\nu}W_{\rho\lambda}. \tag{E5}$$

Finally, the Ricci and scalar curvatures are defined as

$$R_{\mu\nu}=R^\lambda_{\mu\lambda\nu},\quad R=g^{\mu\nu}R_{\mu\nu} \tag{E6}$$

The equations from here onwards are valid in two dimensions only:

$$\frac{1}{g}\epsilon^{\alpha\rho}\epsilon^{\mu\nu}=g^{\alpha\mu}g^{\rho\nu}-g^{\alpha\nu}g^{\rho\mu}, \tag{E7}$$

$$g^{\alpha\beta}=\frac{1}{g}\epsilon^{\alpha\rho}\epsilon^{\beta\sigma}g_{\rho\sigma}. \tag{E8}$$

And, the Riemann tensor is

$$R_{\rho\lambda\mu\nu}=K(g_{\rho\mu}g_{\lambda\nu}-g_{\rho\nu}g_{\lambda\mu}), \tag{E9}$$

where $K=R/2$ is the Gaussian curvature.

2. Expansion around a given metric

From the incompatibility expansion (39) we have

$$\bar{\Gamma}^\rho_{\mu\alpha}=\Gamma^\rho_{\mu\alpha}+\eta\Gamma^{\rho(1)}_{\mu\alpha}+\eta^2\Gamma^{\rho(2)}_{\mu\alpha}+\cdots. \tag{E10}$$

Here, the η value is just a formal quantity that allows to keep track of the different orders in the expansion.

The compatibility of the connection with the metric implies

$$\begin{aligned}\nabla_\mu g_{\alpha\beta}&=0,\\ \bar{\nabla}_\mu\bar{g}_{\alpha\beta}&=0.\end{aligned} \tag{E11}$$

This last equation, in explicit terms, is

$$\bar{\nabla}_\mu\bar{g}_{\alpha\beta}=\frac{\partial\bar{g}_{\alpha\beta}}{\partial x_\mu}-\bar{\Gamma}^\rho_{\mu\alpha}\bar{g}_{\rho\beta}-\bar{\Gamma}^\rho_{\mu\beta}\bar{g}_{\alpha\rho}=0. \tag{E12}$$

Introducing the expansion (E10) into the previous equation leads to

$$\begin{aligned}&\nabla_\mu g_{\alpha\beta}+\eta\big(\nabla_\mu g^{(1)}_{\alpha\beta}-\Gamma^{\rho(1)}_{\mu\alpha}g_{\rho\beta}-\Gamma^{\rho(1)}_{\mu\beta}g_{\alpha\rho}\big)\\&\quad+\eta^2\big(\nabla_\mu g^{(2)}_{\alpha\beta}-\Gamma^{\rho(2)}_{\mu\alpha}g_{\rho\beta}-\Gamma^{\rho(2)}_{\mu\beta}g_{\alpha\rho}\\&\quad-\Gamma^{\rho(1)}_{\mu\alpha}g^{(1)}_{\rho\beta}-\Gamma^{\rho(1)}_{\mu\beta}g^{(1)}_{\alpha\rho}\big),\end{aligned} \tag{E13}$$

which immediately leads to the identities

$$\begin{aligned}&\nabla_\mu g^{(1)}_{\alpha\beta}-\Gamma^{\rho(1)}_{\mu\alpha}g_{\rho\beta}-\Gamma^{\rho(1)}_{\mu\beta}g_{\alpha\rho}=0,\\&\nabla_\mu g^{(2)}_{\alpha\beta}-\Gamma^{\rho(2)}_{\mu\alpha}g_{\rho\beta}-\Gamma^{\rho(2)}_{\mu\beta}g_{\alpha\rho}-\Gamma^{\rho(1)}_{\mu\alpha}g^{(1)}_{\rho\beta}-\Gamma^{\rho(1)}_{\mu\beta}g^{(1)}_{\alpha\rho}=0\end{aligned} \tag{E14}$$

with solutions

$$\Gamma^{\rho(1)}_{\mu\alpha}=\frac{g^{\rho\beta}}{2}\big(\nabla_\mu g^{(1)}_{\alpha\beta}+\nabla_\alpha g^{(1)}_{\beta\mu}-\nabla_\beta g^{(1)}_{\mu\alpha}\big) \tag{E15}$$

and

$$\Gamma^{\rho(2)}_{\mu\alpha}=\frac{g^{\rho\beta}}{2}\big(\nabla_\mu g^{(2)}_{\alpha\beta}+\nabla_\alpha g^{(2)}_{\beta\mu}-\nabla_\beta g^{(2)}_{\mu\alpha}\big)-g^{\rho\beta}\Gamma^{\gamma(1)}_{\mu\alpha}g^{(1)}_{\gamma\beta}. \tag{E16}$$

These expressions allow us to compute the Riemann tensor, defined from

$$\bar{R}^\rho{}_{\sigma\mu\nu}=\partial_\mu\bar{\Gamma}^\rho_{\nu\sigma}-\partial_\nu\bar{\Gamma}^\rho_{\mu\sigma}+\bar{\Gamma}^\rho_{\mu\lambda}\bar{\Gamma}^\lambda_{\nu\sigma}-\bar{\Gamma}^\rho_{\nu\lambda}\bar{\Gamma}^\lambda_{\mu\sigma}. \tag{E17}$$

Inserting the terms in Eqs. (E15) and (E16), after some algebra it leads to

$$\begin{aligned}\bar{R}^\rho_{\sigma\mu\nu}&=R^\rho_{\sigma\mu\nu}+\eta\big(\nabla_\mu\Gamma^{\rho(1)}_{\nu\sigma}-\nabla_\nu\Gamma^{\rho(1)}_{\mu\sigma}\big)\\&\quad+\eta^2\big(\nabla_\mu\Gamma^{\rho(2)}_{\nu\sigma}-\nabla_\nu\Gamma^{\rho(2)}_{\mu\sigma}+\Gamma^{\rho(1)}_{\mu\lambda}\Gamma^{\lambda(1)}_{\nu\sigma}-\Gamma^{\rho(1)}_{\nu\lambda}\Gamma^{\lambda(1)}_{\mu\sigma}\big).\end{aligned} \tag{E18}$$

The Ricci tensor is

$$\begin{aligned}\bar{R}_{\sigma\nu}&=R_{\sigma\nu}+\eta\big(\nabla_\mu\Gamma^{\mu(1)}_{\nu\sigma}-\nabla_\nu\Gamma^{\mu(1)}_{\mu\sigma}\big)\\&\quad+\eta^2\big(\nabla_\mu\Gamma^{\mu(2)}_{\nu\sigma}-\nabla_\nu\Gamma^{\mu(2)}_{\mu\sigma}+\Gamma^{\mu(1)}_{\mu\lambda}\Gamma^{\lambda(1)}_{\nu\sigma}-\Gamma^{\mu(1)}_{\nu\lambda}\Gamma^{\lambda(1)}_{\mu\sigma}\big).\end{aligned} \tag{E19}$$

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