Chapter 45
Large Strains of a Spherical Shell with Distributed Dislocations and Disclinations

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Abstract A theory of nonlinear deformation of the elastic Cosserat shells with continuously distributed dislocations and disclinations is formulated. Displacements, rotations, and strains are considered to be arbitrarily large, and the rotation field is kinematically independent of the displacement field. A system of nonlinear differential equations is derived that describes the stress state of an elastic shell with given external loads and given dislocation and disclination densities. This system consists of equilibrium equations and incompatibility equations and contains, as unknown functions, the tensor fields of metric and flexural strains of the elastic shell. The general theory is illustrated by solving a nonlinear problem of the equilibrium of a spherical shell with a spherically symmetric distribution of dislocations and disclinations.

Key words: 6-parameter shell theory · Incompatibility equations · Dislocation and disclination densities · Spherical symmetry

45.1 Introduction

Shell structures of completely different scale are actively used in various industries. Examples include containers for storing and transporting liquid and bulk cargo, and capsules for medicines and cosmetics. Shell-type, or two-dimensional, objects naturally arise in biological systems, as well as in technological processes of various nature. In this connection, crystalline and glassy colloidosomes [1], multielectron

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bubbles on helium films [2], capsules of Janus and patchy particles [3], nematic vesicles [4], and viral capsids [5] deserve mention.

Two-dimensional crystals can be successfully used in nano-design, development of submicron devices and the latest drugs. They are ideal candidates for a range of applications, such as nanocontainers for storing and delivering drugs and therapeutic genes to cells.

Note that many of the two-dimensional objects mentioned above are closed shells, topologically equivalent to a sphere. In this case, new crystallographic patterns arise that are absent in ordinary flat and bulk crystals. One of these features is the mandatory presence of structural defects. It is the presence of certain types of defects that determines the curvature of two-dimensional structures.

Topological defects such as dislocations and disclinations can be found in thin shell structures at different length scales: from the world of carbon allotropes, as in fullerenes, nanotubes, and graphene, to biological systems such as in lipid membranes, and in synthetic structures such as colloidosomes, colloidal particle shells lying at the interface between two fluids [6]-[9].

Most experimental studies have shown that these defects in 2D crystals significantly affect their physical, chemical, and mechanical properties [10]. Dislocation-type defects play an essential role in the mechanical behavior of surface crystals, nanotubes, nanofilms, and other two-dimensional physical systems [11]. Simulation results of the mechanical deformation of colloidal crystalline shells illustrate the role played by geometrically necessary topological defects in controlling plastic yielding and failure and provide general guiding principles to optimize the structural and mechanical stability of curved colloidal crystals [12]. Defects formed on the surface of spherical crystals are a kind of «scaffolding» for the formation of mesomolecules and the occurrence of various chemical reactions [13]. Deeper theoretical understanding of the dislocations influence upon the properties of 2D systems can create background that will open a new direction in science and technology — defect engineering [14].

Many common approaches to studying the effect of a given distribution of structural defects in two-dimensional systems on stress and strain fields are based on non-Euclidean geometry and related methods and concepts [15]. The geometry and energy of disclinated graphene configurations were analyzed with the help of molecular dynamics simulation technique and in the framework of the theory of defects in elastic continuum [14]. Modeling the most topologically regular two-dimensional nanocrystals including various possible polymorphic forms of the HIV viral capsid is performed by minimizing the shell elastic energy in [16]. The studies of viral capsids within the framework of the nonlinear theory of elastic shells [17]-[19] demonstrate good fits to experimentally determined virus shapes and explain many experimental observations in viruses.

This work applies the nonlinear theory of micropolar shells, also called the 6-parameter model. In this theory, the shell is treated as a two-dimensional continuum, i.e., a material surface, each point of which has six degrees of freedom of an absolutely rigid body. Based on the concept of isolated Volterra dislo- cations in a multiply connected two-dimensional elastic body, we build a model of a nonlinearly elastic micropolar shell with distributed dislocations by passing to the limit from a discrete set of dislocations to their continuous distribution. The system of equations describing the nonlinear deformation of a shell with distributed dislocations contains the tensor fields of distortion and rotation as unknown functions. To extend the nonlinear theory of shells to the case of the presence of isolated and distributed disclinations, we transform the indicated system of equations in such a way that the tensor fields of metric and bending strains become unknown functions. To model continuously distributed disclinations, their density function is introduced by analogy with geometrically linear theory as a nonzero right-hand side of the nonlinear compatibility equations for bending strains.

Previously, the theory of continuously distributed dislocations and disclinations was developed in [20]-[23] within the framework of the classical Kirchhoff-Love model of plates and shells (both linear and non-linear). The nonlinear theory of isolated and continuously distributed dislocations in three-dimensional micropolar media is presented in [24]-[27].

45.2 The Model of a Nonlinear Elastic Micropolar Shell

According to the mathematical model of micropolar shells, also called the Cosserat-type theory or the 6-parameter theory, the shell is a two-dimensional continuum, that is, a material surface. Each point (particle) of this continuum has six degrees of freedom of an absolutely rigid body [28]-[35].

Let us denote by σ the surface of the shell in the reference configuration, i. e., in the undeformed state, and define the equation of the surface σ in the form $\boldsymbol{r} = \boldsymbol{r}(q^1, q^2)$, where $\boldsymbol{r}$ is a radius-vector of the particle of σ, and q^1, q^2 are some Gaussian coordinates. The surface Σ of the shell in the current configuration is also referred to the coordinates q^γ ($\gamma = 1, 2$), and the radius-vector $\boldsymbol{R}(q^1, q^2)$ specifies the position of the material point on Σ. The field of rotations, or proper orthogonal tensor field $\boldsymbol{H}(q^1, q^2)$, characterizes the orientation of the shell particles. The tensor field $\boldsymbol{H}$ is kinematically independent of the displacement field of the shell $\boldsymbol{u} = \boldsymbol{R} - \boldsymbol{r}$. The strained state of the Cosserat-type shell is determined by the vector and tensor fields $\boldsymbol{R}(q^1, q^2)$ and $\boldsymbol{H}(q^1, q^2)$, at that $\boldsymbol{H} \cdot \boldsymbol{H}^{\mathrm{T}} = \boldsymbol{I}$, $\det \boldsymbol{H} = 1$, $\boldsymbol{I}$ is three-dimensional identity tensor. The elastic properties of the shell are determined by the function of the specific (per surface σ area unit) potential energy $W(\boldsymbol{E}, \boldsymbol{L})$.

$$\boldsymbol{E} = \boldsymbol{F} \cdot \boldsymbol{H}^{\mathrm{T}}, \ \boldsymbol{L} = \frac{1}{2} \boldsymbol{r}^\gamma \otimes \left(\frac{\partial \boldsymbol{H}}{\partial q^\gamma} \cdot \boldsymbol{H}^{\mathrm{T}} \right)_\times , \tag{45.1}$$

$$\boldsymbol{F} = \operatorname{grad} \boldsymbol{R}. \tag{45.2}$$

Here $\boldsymbol{F}$ is the shell distortion tensor, $\boldsymbol{E}$ is the strain measure, $\boldsymbol{L}$ is the bending strain tensor. The symbol $\boldsymbol{A}_\times = A_{sk} \boldsymbol{e}^s \times \boldsymbol{e}^k$ denotes the vector invariant of the second-rank tensor $\boldsymbol{A} = A_{sk} \boldsymbol{e}^s \otimes \boldsymbol{e}^k$. Gradient and divergence operations on the surface are introduced by the relations [36]:

$$\operatorname{grad}\boldsymbol{\Lambda} = \boldsymbol{r}^{\gamma} \otimes \frac{\partial \boldsymbol{\Lambda}}{\partial q^{\gamma}}, \ \operatorname{div}\boldsymbol{\Lambda} = \boldsymbol{r}^{\gamma} \cdot \frac{\partial \boldsymbol{\Lambda}}{\partial q^{\gamma}},$$
$$\boldsymbol{r}_{\varkappa} = \frac{\partial \boldsymbol{r}}{\partial q^{\varkappa}}, \ \boldsymbol{r}^{\gamma} \cdot \boldsymbol{r}_{\varkappa} = \delta^{\gamma}_{\varkappa}, \ \boldsymbol{r}^{\gamma} \cdot \boldsymbol{n} = 0, \ \gamma, \varkappa = 1,2 \tag{45.3}$$

In (45.3) $\boldsymbol{r}_{\varkappa}$ and $\boldsymbol{r}^{\gamma}$ are main and reciprocal vector bases on σ, $\boldsymbol{n}$ is unit normal to the surface σ, $\delta^{\gamma}_{\varkappa}$ is the Kronecker delta, $\boldsymbol{\Lambda}$ is an arbitrary differentiable tensor field of any rank.

The stress state of the shell is characterized by the surface stress $\boldsymbol{P}$ and couple stress $\boldsymbol{\Pi}$ tensors of Kirchhoff type. These tensors are expressed in terms of strain tensors $\boldsymbol{E}$ and $\boldsymbol{L}$ by using constitutive relations

$$\boldsymbol{P}(\boldsymbol{E},\boldsymbol{L}) = \frac{\partial W}{\partial \boldsymbol{E}}, \ \boldsymbol{\Pi}(\boldsymbol{E},\boldsymbol{L}) = \frac{\partial W}{\partial \boldsymbol{L}}. \tag{45.4}$$

Note that the tensors participating in (45.4) have the property

$$\boldsymbol{n} \cdot \boldsymbol{E} = \boldsymbol{n} \cdot \boldsymbol{L} = \boldsymbol{n} \cdot \boldsymbol{P} = \boldsymbol{n} \cdot \boldsymbol{\Pi} = 0.$$

If the elastic shell is in equilibrium under the given force and moment loads, then the stress and couple stress tensors obey the equations of statics

$$\operatorname{div}(\boldsymbol{P} \cdot \boldsymbol{H}) + \boldsymbol{f} = 0, \ \operatorname{div}(\boldsymbol{\Pi} \cdot \boldsymbol{H}) + \left(\boldsymbol{F}^{\mathrm{T}} \cdot \boldsymbol{P} \cdot \boldsymbol{H}\right)_{\times} + \boldsymbol{l} = 0, \tag{45.5}$$

where $\boldsymbol{f}$ and $\boldsymbol{l}$ are intensities (per surface σ area unit) of external distributed forces and moments.

45.3 Continuously Distributed Dislocations in an Elastic Micropolar Shell

The concept of dislocations in an elastic shell arises naturally when solving the problem of determining the displacement field from a given single-valued differentiable field of the distortion tensor $\boldsymbol{F}(\boldsymbol{r})$. This problem is obviously equivalent to the problem of determining the vector field $\boldsymbol{R}(\boldsymbol{r})$ characterizing the positions of shell particles in the deformed state. Based on (45.2) we have

$$\boldsymbol{R}(\boldsymbol{r}) = \int_{\boldsymbol{r}_0}^{\boldsymbol{r}} d\boldsymbol{r} \cdot \boldsymbol{F} + \boldsymbol{R}(\boldsymbol{r}_0). \tag{45.6}$$

If the initial value $\boldsymbol{R}(\boldsymbol{r}_0)$ is given at some point $\boldsymbol{r}_0$, then under the condition

$$\operatorname{div}(\boldsymbol{d} \cdot \boldsymbol{F}) = 0, \ \boldsymbol{d} = -\boldsymbol{I} \times \boldsymbol{n} \tag{45.7}$$

the expression (45.6)in a simply connected domain defines a single-valued function $\boldsymbol{R}(\boldsymbol{r})$. Tensor $\boldsymbol{d}$ in (45.7) is the surface discriminant tensor [36, 37].

Let us now consider some section σ_0 of the shell surface and assume that the domain σ_0 is multiply-connected and homeomorphic to a circle with N circular holes, and the function $\boldsymbol{F}(\boldsymbol{r})$ is single-valued in the multiply-connected domain. In this case, the property of uniqueness of displacements is, generally speaking, lost. The multivaluedness can be eliminated by making the domain σ_0 simple connected by drawing the required number of cuts (partitions). In this case, the values of the function $\boldsymbol{R}(\boldsymbol{r})$ will differ on different sides of the cut. It follows from the relation(45.6) that the displacement jump at the intersection of each cut is described by the formula

$$\boldsymbol{u}_+ - \boldsymbol{u}_- = \boldsymbol{R}_+ - \boldsymbol{R}_- = \boldsymbol{B}_k, \tag{45.8}$$

where $\boldsymbol{B}_k$ $(k = 1, 2, \ldots N)$ are vectors constant for the given cut, called Burgers vectors. These vectors do not depend on the choice of the cuts system and, according to (45.6), are expressed in terms of the distortion field by the formulas

$$\boldsymbol{B}_k = \oint\limits_{\Gamma_k} d\boldsymbol{r} \cdot \boldsymbol{F}, \tag{45.9}$$

where Γ_k is any closed contour enclosing only one k-th hole. A non-zero value of $\boldsymbol{B}_k$ means that the shell contains isolated dislocations.

If the number of dislocations in a limited part of the shell is considerably high, switching to a continuous distribution of defects is advisable. The total Burgers vector of a discrete set of N isolated dislocations contained in the subregion σ_0 according to (45.9) is given by

$$\boldsymbol{B} = \sum_{k=1}^{N} \boldsymbol{B}_k = \sum_{k=1}^{N} \oint\limits_{\Gamma_k} d\boldsymbol{r} \cdot \boldsymbol{F}. \tag{45.10}$$

Due to the well-known properties of curvilinear integrals and the single-valuedness of the tensor field $\boldsymbol{F}$, the sum of integrals in (45.10) can be replaced by a single integral over the closed contour Γ_0 covering all holes in the domain σ_0:

$$\boldsymbol{B} = \oint\limits_{\Gamma_0} d\boldsymbol{r} \cdot \boldsymbol{F}. \tag{45.11}$$

To pass from a discrete set of dislocations to their continuous distribution, we tend to the hole diameters to zero and transform the contour integral (45.11) by the known [36, 37] formula

$$\iint\limits_{\sigma_0} \operatorname{div}(\boldsymbol{d} \cdot \boldsymbol{\Lambda})\, d\sigma = \oint\limits_{\Gamma_0} d\boldsymbol{r} \cdot \boldsymbol{\Lambda}$$

into a surface integral over the region σ_0 bounded by the contour Γ_0:

$$\boldsymbol{B} = \iint\limits_{\sigma_0} \boldsymbol{\alpha}\, d\sigma, \ \boldsymbol{\alpha} = \operatorname{div}(\boldsymbol{d}\cdot\boldsymbol{F}). \tag{45.12}$$

Since $\boldsymbol{B}$ is the total Burgers vector of all dislocations con- tained in an arbitrary region σ_0, the vector field $\boldsymbol{\alpha}(\boldsymbol{r})$ should be called the dislocation density. In what follows, we will consider the dislocation density to be a given function of Gaussian coordinates, similar to the external loads $\boldsymbol{f}$ and $\boldsymbol{l}$.

In the presence of continuously distributed dislocations in the shell, the vector fields $\boldsymbol{u}(\boldsymbol{r})$ and $\boldsymbol{R}(\boldsymbol{r})$ do not exist, so Eq. (45.2) does not have sense. It is replaced according to (45.12) by the incompatibility equation

$$\operatorname{div}(\boldsymbol{d}\cdot\boldsymbol{F}) = \boldsymbol{\alpha}. \tag{45.13}$$

The complete system of equations describing the equilibrium state of an elastic shell with distributed dislocations consists of relationships (45.1), (45.4), (45.5) and (45.13). This system is easily reduced to equations for two unknown tensors: the distortion tensor $\boldsymbol{F}(\boldsymbol{r})$ and the rotation tensor $\boldsymbol{H}(\boldsymbol{r})$.

45.4 Transformation of Incompatibility Equations and Equilibrium Equations

If the elastic shell in addition to distributed and concentrated dislocations contains isolated disclinations then the distortion $\boldsymbol{F}$ and rotation $\boldsymbol{H}$ tensor fields will be multivalued functions of the coordinates q^1, q^2 whereas in contrast the strain measure $\boldsymbol{E}$ and the bending strain tensor $\boldsymbol{L}$ are single-valued tensor fields.

To analyze the stress state of a shell with isolated disclinations, it is expedient to compose a system of resolving equations in which the multivalued functions $\boldsymbol{F}$ and $\boldsymbol{H}$ are excluded, and the unknowns are the tensor functions $\boldsymbol{E}$ and $\boldsymbol{L}$. Thus, system of equations (45.1), (45.4), (45.5), (45.13) should be transformed by excluding tensors $\boldsymbol{F}$ and $\boldsymbol{H}$ as unknown functions.

First, we transform appropriately expression for the bending strain tensor (45.1). Introducing vectors $\boldsymbol{L}_\varkappa = \boldsymbol{r}_\varkappa \cdot \boldsymbol{L}$, we have a decomposition $\boldsymbol{L} = \boldsymbol{r}^\varkappa \otimes \boldsymbol{L}_\varkappa$. Then, based on (45.1), the following equalities hold ($\varkappa, \gamma = 1, 2$)

$$\frac{\partial \boldsymbol{H}}{\partial q^\varkappa}\cdot\boldsymbol{H}^{\mathrm{T}} = -\boldsymbol{L}_\varkappa\times\boldsymbol{I}, \ \frac{\partial \boldsymbol{H}}{\partial q^\gamma}\cdot\boldsymbol{H}^{\mathrm{T}} = -\boldsymbol{L}_\gamma\times\boldsymbol{I}, \tag{45.14}$$

or

$$\frac{\partial \boldsymbol{H}}{\partial q^\varkappa} = -\boldsymbol{L}_\varkappa\times\boldsymbol{H}, \ \frac{\partial \boldsymbol{H}}{\partial q^\gamma} = -\boldsymbol{L}_\gamma\times\boldsymbol{H}. \tag{45.15}$$

Differentiating the first relation (45.15) with respect to q^γ, and the second one with respect to $q^\varkappa$ we get

$$\frac{\partial^2 \boldsymbol{H}}{\partial q^\gamma \partial q^\varkappa} = -\frac{\partial \boldsymbol{L}_\varkappa}{\partial q^\gamma} \times \boldsymbol{H} - \boldsymbol{L}_\varkappa \times \frac{\partial \boldsymbol{H}}{\partial q^\gamma}, \tag{45.16}$$

$$\frac{\partial^2 \boldsymbol{H}}{\partial q^\varkappa \partial q^\gamma} = -\frac{\partial \boldsymbol{L}_\gamma}{\partial q^\varkappa} \times \boldsymbol{H} - \boldsymbol{L}_\gamma \times \frac{\partial \boldsymbol{H}}{\partial q^\varkappa}. \tag{45.17}$$

Since the left parts of expressions (45.16) and (45.17) are the same, we have

$$\frac{\partial \boldsymbol{L}_\varkappa}{\partial q^\gamma} \times \boldsymbol{H} + \boldsymbol{L}_\varkappa \times \frac{\partial \boldsymbol{H}}{\partial q^\gamma} = \frac{\partial \boldsymbol{L}_\gamma}{\partial q^\varkappa} \times \boldsymbol{H} + \boldsymbol{L}_\gamma \times \frac{\partial \boldsymbol{H}}{\partial q^\varkappa}. \tag{45.18}$$

Multiplying (45.18) by $\boldsymbol{H}^{\mathrm{T}}$ from the right and accounting (45.14) we get

$$\left(\frac{\partial \boldsymbol{L}_\varkappa}{\partial q^\gamma} - \frac{\partial \boldsymbol{L}_\gamma}{\partial q^\varkappa}\right) \times \boldsymbol{I} = \boldsymbol{L}_\varkappa \times \boldsymbol{I} \times \boldsymbol{L}_\gamma - \boldsymbol{L}_\gamma \times \boldsymbol{I} \times \boldsymbol{L}_\varkappa. \tag{45.19}$$

An easily verifiable identity $\boldsymbol{a} \times \boldsymbol{I} \times \boldsymbol{b} = \boldsymbol{b} \otimes \boldsymbol{a} - (\boldsymbol{a} \cdot \boldsymbol{b})\boldsymbol{I}$ and (45.19) implies the equality

$$\left(\frac{\partial \boldsymbol{L}_\varkappa}{\partial q^\gamma} - \frac{\partial \boldsymbol{L}_\gamma}{\partial q^\varkappa}\right) \times \boldsymbol{I} = \boldsymbol{L}_\gamma \otimes \boldsymbol{L}_\varkappa - \boldsymbol{L}_\varkappa \otimes \boldsymbol{L}_\gamma. \tag{45.20}$$

The left and the right parts of expression (45.20) are antisymmetric tensors of the second rank. Their equality is equivalent to the equality of their vector invariants:

$$\frac{\partial \boldsymbol{L}_\varkappa}{\partial q^\gamma} - \frac{\partial \boldsymbol{L}_\gamma}{\partial q^\varkappa} = \boldsymbol{L}_\varkappa \times \boldsymbol{L}_\gamma. \tag{45.21}$$

System (45.21) can be called the compatibility equations for bending deformations. They are the necessary and sufficient conditions for the unique solvability of Eq. (45.14) with respect to the rotation tensor $\boldsymbol{H}$ in a simply connected domain for a given value of this tensor at some point.

For further transformation of system (45.21), we use the directly verifiable identity

$$\operatorname{div}(\boldsymbol{d} \cdot \boldsymbol{L}) = d^{\varkappa\gamma} \frac{\partial \boldsymbol{L}_\gamma}{\partial q^\varkappa}; \; d^{\varkappa\gamma} \triangleq \boldsymbol{r}^\varkappa \cdot \boldsymbol{d} \cdot \boldsymbol{r}^\gamma \tag{45.22}$$

and introduce the tensor $\boldsymbol{L}^\perp$, called the adjugate tensor of the $\boldsymbol{L}$ [36]

$$\boldsymbol{L}^\perp \triangleq \boldsymbol{L}^2 - (\operatorname{tr} \boldsymbol{L})\boldsymbol{L} + \frac{1}{2}\left(\operatorname{tr}^2 \boldsymbol{L} - \operatorname{tr} \boldsymbol{L}^2\right)\boldsymbol{I}. \tag{45.23}$$

Equation (45.23) together with representation $\boldsymbol{L} = \boldsymbol{r}^\varkappa \otimes \boldsymbol{L}_\varkappa$ implies the equality

$$\boldsymbol{L}^\perp = \frac{1}{2}\left(\boldsymbol{L}_\gamma \times \boldsymbol{L}_\varkappa\right) \otimes \left(\boldsymbol{r}^\gamma \times \boldsymbol{r}^\varkappa\right). \tag{45.24}$$

Using the following formula for the unit normal $\boldsymbol{n}$ to the surface σ

$$\boldsymbol{n} d^{\varkappa\gamma} = \boldsymbol{r}^\varkappa \times \boldsymbol{r}^\gamma,$$

and considering (45.24), we get

$$\boldsymbol{L}^{\perp} \cdot \boldsymbol{n} = \frac{1}{2} \left(\boldsymbol{L}_{\gamma} \times \boldsymbol{L}_{\varkappa} \right) d^{\gamma\varkappa}. \tag{45.25}$$

Based on (45.22) and (45.25), the system of compatibility equations for bending strains (45.21) is written as a vector equation

$$\operatorname{div} (\boldsymbol{d} \cdot \boldsymbol{L}) + \boldsymbol{L}^{\perp} \cdot \boldsymbol{n} = 0. \tag{45.26}$$

Turn to the transformation of incompatibility equation (45.13). Given (45.1), we rewrite it as

$$\operatorname{div} (\boldsymbol{d} \cdot \boldsymbol{E} \cdot \boldsymbol{H}) = \boldsymbol{\alpha}. \tag{45.27}$$

Multiplying (45.27) by $\boldsymbol{H}^{\mathrm{T}}$ and bearing in mind that $\boldsymbol{H} \cdot \boldsymbol{H}^{\mathrm{T}} = \boldsymbol{I}$, we get

$$\operatorname{div} (\boldsymbol{d} \cdot \boldsymbol{E}) + \boldsymbol{r}^{\varkappa} \cdot \boldsymbol{d} \cdot \boldsymbol{E} \cdot \frac{\partial \boldsymbol{H}}{\partial q^{\varkappa}} \cdot \boldsymbol{H}^{\mathrm{T}} = \boldsymbol{\alpha}^{*}. \tag{45.28}$$

The vector $\boldsymbol{\alpha}^{*} = \boldsymbol{\alpha} \cdot \boldsymbol{H}^{\mathrm{T}}$ is called the modified dislocation density vector. Referring to (45.14), instead of (45.28) we will have the equation

$$\operatorname{div} (\boldsymbol{d} \cdot \boldsymbol{E}) - \boldsymbol{r}^{\varkappa} \cdot \boldsymbol{d} \cdot \boldsymbol{E} \times \boldsymbol{L}_{\varkappa} = \boldsymbol{\alpha}^{*}. \tag{45.29}$$

Let us prove the identity

$$-\boldsymbol{r}^{\varkappa} \cdot \boldsymbol{d} \cdot \boldsymbol{E} \times \boldsymbol{L}_{\varkappa} = \left(\boldsymbol{E}^{\mathrm{T}} \cdot \boldsymbol{d} \cdot \boldsymbol{L} \right)_{\times}. \tag{45.30}$$

Indeed, since $\boldsymbol{E}^{\mathrm{T}} \cdot \boldsymbol{d} \cdot \boldsymbol{r}^{\varkappa} = -\boldsymbol{r}^{\varkappa} \cdot \boldsymbol{d} \cdot \boldsymbol{E}$, we have

$$\begin{aligned} \left(\boldsymbol{E}^{\mathrm{T}} \cdot \boldsymbol{d} \cdot \boldsymbol{L} \right)_{\times} &= \left(\boldsymbol{E}^{\mathrm{T}} \cdot \boldsymbol{d} \cdot \boldsymbol{r}^{\varkappa} \otimes \boldsymbol{L}_{\varkappa} \right)_{\times} \\ &= \left(\boldsymbol{E}^{\mathrm{T}} \cdot \boldsymbol{d} \cdot \boldsymbol{r}^{\varkappa} \right) \times \boldsymbol{L}_{\varkappa} = -\boldsymbol{r}^{\varkappa} \cdot \boldsymbol{d} \cdot \boldsymbol{E} \times \boldsymbol{L}_{\varkappa}. \end{aligned}$$

So, incompatibility equation (45.13) with respect to the distortion tensor has been transformed into an equation for metric and bending strains, i.e. regarding tensors $\boldsymbol{E}$ and $\boldsymbol{L}$

$$\operatorname{div} (\boldsymbol{d} \cdot \boldsymbol{E}) + \left(\boldsymbol{E}^{\mathrm{T}} \cdot \boldsymbol{d} \cdot \boldsymbol{L} \right)_{\times} = \boldsymbol{\alpha}^{*}. \tag{45.31}$$

Let us now transform equilibrium equations (45.5) in order to exclude the distortion and rotation tensors, $\boldsymbol{F}$ and $\boldsymbol{H}$, as unknown functions. Multiplying the force balance equation by $\boldsymbol{H}^{\mathrm{T}}$ and taking (45.14) into account, we obtain

$$\operatorname{div} \boldsymbol{P} - \boldsymbol{r}^{\varkappa} \cdot \boldsymbol{P} \times \boldsymbol{L}_{\varkappa} + \boldsymbol{f}^{*} = 0; \;\; \boldsymbol{f}^{*} = \boldsymbol{f} \cdot \boldsymbol{H}^{\mathrm{T}}. \tag{45.32}$$

Then we get

$$\boldsymbol{r}^{\varkappa} \cdot \boldsymbol{P} \times \boldsymbol{L}_{\varkappa} = \left(\boldsymbol{P}^{\mathrm{T}} \cdot \boldsymbol{r}^{\varkappa}\right) \times \boldsymbol{L}_{\varkappa} = \left[\left(\boldsymbol{P}^{\mathrm{T}} \cdot \boldsymbol{r}^{\varkappa}\right) \otimes \boldsymbol{L}_{\varkappa}\right]_{\times} = \left(\boldsymbol{P}^{\mathrm{T}} \cdot \boldsymbol{L}\right)_{\times},$$

and Eq. (45.32) is written as

$$\operatorname{div} \boldsymbol{P} - \left(\boldsymbol{P}^{\mathrm{T}} \cdot \boldsymbol{L}\right)_{\times} + \boldsymbol{f}^{*} = 0. \tag{45.33}$$

Moment equilibrium equation (45.5) is transformed in a similar way and takes the form

$$\operatorname{div} \boldsymbol{\Pi} - \left(\boldsymbol{\Pi}^{\mathrm{T}} \cdot \boldsymbol{L} + \boldsymbol{P}^{\mathrm{T}} \cdot \boldsymbol{E}\right)_{\times} + \boldsymbol{l}^{*} = 0; \; \boldsymbol{l}^{*} = \boldsymbol{l} \cdot \boldsymbol{H}^{\mathrm{T}}. \tag{45.34}$$

If we assume that the modified intensities of the force and moment loads $\boldsymbol{f}^{*}$ and $\boldsymbol{l}^{*}$ are known functions, then, by virtue of the constitutive relations (45.4), we see that the Eqs. (45.33) and (45.34) contain as unknown functions the tensor fields of metric and bending strains $\boldsymbol{E}$ and $\boldsymbol{L}$.

Using system of Eqs. (45.26), (45.31), (45.33) and (45.34), one can consider the problem of equilibrium of an elastic shell containing distributed dislocations and isolated disclinations. While the quantitative characteristic of an isolated dislocation is the Burgers vector, then the power of an isolated disclination is determined by the Frank vector [24, 38, 39]. The Frank vector in the nonlinear case, that is at large rotations and strains of the shell, is expressed in terms of a multiplicative curvilinear integral over a closed contour enveloping an isolated disclination [40]. The complex properties of curvilinear multiplicative integrals [24], due to the non-commutativity of finite rotations, do not allow one to explicitly express the total Frank vector of the set of disclinations in terms of the tensor field of bending strains and to carry out the limit transition from a discrete set of isolated disclinations to their continuous distribution. This makes it difficult to rigorously formulate the concept of disclination density in a nonlinear elastic shell. The mentioned transition is possible in the geometrically linear theory of the Cosserat-type shells [41], i.e., for small strains and small rotations. In this case, the Frank vector is expressed in terms of the usual curvilinear integral, and the disclination density is defined as a function of coordinates, the integral of which over the area of an arbitrary region is equal to the total Frank vector of the disclinations contained in this region. The incompatibility equation for bending strains in the geometrically linear case was derived in [41] and has the form

$$\operatorname{div}(\boldsymbol{d} \cdot \boldsymbol{L}) = \boldsymbol{\beta}, \tag{45.35}$$

where $\boldsymbol{\beta}$ is disclination density vector. The left side of (45.35) equation differs from the left side of the (45.26) compatibility equation in that it does not contain the term $\boldsymbol{L}^{\perp} \cdot \boldsymbol{n}$. According to (45.23), this term is nonlinear and is a homogeneous function of the second degree with respect to the tensor $\boldsymbol{L}$.

To study continuously distributed disclinations in nonlinearly elastic shells, we formally, by analogy with geometrically linear theory, introduce the disclination density as a vector function $\boldsymbol{\beta}(q^1, q^2)$ that replaces zero in the right part of compatibility equation (45.26):

$$\operatorname{div}(\boldsymbol{d} \cdot \boldsymbol{L}) + \boldsymbol{L}^{\perp} \cdot \boldsymbol{n} = \boldsymbol{\beta}. \tag{45.36}$$

Equation (45.36) will be called the incompatibility equation for bending strains in the nonlinear theory of elastic shells of the Cosserat type.

45.5 Equilibrium of a Closed Spherical Shell with Distributed Dislocations and Disclinations

In a closed spherical shell of radius r_0, we take the geographic coordinates $0 \leqslant \varphi \leqslant 2\pi$ (longitude) and $-\pi/2 \leqslant \theta \leqslant \pi/2$ (latitude) as Gaussian coordinates. The unit normal to the sphere will be denoted by $\boldsymbol{e}_r$, and the unit vectors tangent to the coordinate lines by $\boldsymbol{e}_\varphi$ and $\boldsymbol{e}_\theta$. The metric $\boldsymbol{g}$ and discriminant $\boldsymbol{d}$ tensors on the sphere have the form

$$\begin{aligned} \boldsymbol{g} &= \boldsymbol{I} - \boldsymbol{e}_r \otimes \boldsymbol{e}_r = \boldsymbol{e}_\varphi \otimes \boldsymbol{e}_\varphi + \boldsymbol{e}_\theta \otimes \boldsymbol{e}_\theta, \\ \boldsymbol{d} &= -\boldsymbol{I} \times \boldsymbol{e}_r = \boldsymbol{e}_\varphi \otimes \boldsymbol{e}_\theta - \boldsymbol{e}_\theta \otimes \boldsymbol{e}_\varphi, \end{aligned} \tag{45.37}$$

and the gradient operator is given by the relation

$$\operatorname{grad} \boldsymbol{\Lambda} = \frac{1}{r_0 \cos\theta} \boldsymbol{e}_\varphi \otimes \frac{\partial \boldsymbol{\Lambda}}{\partial \varphi} + \frac{1}{r_0} \boldsymbol{e}_\theta \otimes \frac{\partial \boldsymbol{\Lambda}}{\partial \theta}. \tag{45.38}$$

Let us assume that the external loads and the densities of dislocations and disclinations are vectors directed along the normal to the sphere:

$$\boldsymbol{f}^* = f_0 \boldsymbol{e}_r, \ \boldsymbol{l}^* = l_0 \boldsymbol{e}_r, \ \boldsymbol{\alpha}^* = \alpha_0 \boldsymbol{e}_r, \ \boldsymbol{\beta} = \beta_0 \boldsymbol{e}_r, \tag{45.39}$$

where f_0, l_0, α_0, β_0 are constant values. Metric and bending strains of the shell will be sought in the form of spherically symmetric tensor fields [42]

$$\boldsymbol{E} = E_1 \boldsymbol{g} + E_2 \boldsymbol{d}, \ \boldsymbol{L} = L_1 \boldsymbol{g} + L_2 \boldsymbol{d}, \tag{45.40}$$

$$E_\mu, L_\mu = \text{const}, \ \mu = 1, 2.$$

We assume that the shell material is isotropic and is described by the following constitutive relations [31]

$$\begin{aligned} \boldsymbol{P} &= a_1 (\operatorname{tr} \boldsymbol{U}) \boldsymbol{g} + a_2 (\boldsymbol{U} \cdot \boldsymbol{g})^{\mathrm{T}} + a_3 (\boldsymbol{U} \cdot \boldsymbol{g}) + a_4 \boldsymbol{U} \cdot \boldsymbol{n} \otimes \boldsymbol{n}, \ \boldsymbol{U} = \boldsymbol{E} - \boldsymbol{g}; \\ \boldsymbol{\Pi} &= b_1 (\operatorname{tr} \boldsymbol{L}) \boldsymbol{g} + b_2 (\boldsymbol{L} \cdot \boldsymbol{g})^{\mathrm{T}} + b_3 (\boldsymbol{L} \cdot \boldsymbol{g}) + b_4 \boldsymbol{L} \cdot \boldsymbol{n} \otimes \boldsymbol{n}, \end{aligned} \tag{45.41}$$

where a_k, b_k $(k = 1, 2, 3, 4)$ are material constants. The relations (45.40) and (45.41) imply that the tensors $\boldsymbol{P}$ and $\boldsymbol{\Pi}$ will also be spherically symmetric

$$\boldsymbol{P} = P_1 \boldsymbol{g} + P_2 \boldsymbol{d}, \ \boldsymbol{\Pi} = \Pi_1 \boldsymbol{g} + \Pi_2 \boldsymbol{d}. \tag{45.42}$$

The external force load in (45.39) is expressed in terms of the given hydrostatic pressure p using (45.40) and the transformation formula for the surface element area under deformation [37] as follows

$$f_0 = \left(E_1^2 + E_2^2\right) p. \tag{45.43}$$

The pressure p is positive if it is internal and negative if it is external.

In view of (45.38)–(45.40) and (45.42) equilibrium equations (45.32), (45.34) and incompatibility equation (45.31), (45.36) in a spherically symmetric problem are reduced to a nonlinear algebraic system of equations for unknown constants E_1, E_2, L_1, L_2

$$P_1 + r_0 \left(P_1 L_2 - P_2 L_1\right) = \frac{r_0}{2} \left(E_1^2 + E_2^2\right) p, \tag{45.44}$$

$$\Pi_1 + r_0 \left(\Pi_1 L_2 - \Pi_2 L_1 + P_1 E_2 - P_2 E_1\right) = \frac{r_0}{2} l_0, \tag{45.45}$$

$$E_2 + r_0 \left(E_1 L_1 + E_2 L_2\right) = \frac{r_0}{2} \alpha_0, \tag{45.46}$$

$$L_2 + \frac{r_0}{2} \left(L_1^2 + L_2^2\right) = \frac{r_0}{2} \beta_0. \tag{45.47}$$

Stress and couple stress components in (45.44), (45.45) are expressed in terms of strain components using constitutive relations (45.41) and have the form

$$\begin{gathered} P_1 = \left(2a_1 + a_2 + a_3\right)\left(E_1 - 1\right),\ P_2 = \left(a_3 - a_2\right) E_2, \\ \Pi_1 = \left(2b_1 + b_2 + b_3\right) L_1,\ \Pi_2 = \left(b_3 - b_2\right) L_2. \end{gathered} \tag{45.48}$$

We present two simple solutions to system (45.44)–(45.47) in a particular case $\alpha_0 = 0$, $\beta_0 = 0$, $l_0 = 0$, $p \neq 0$.

- First solution:

$$E_1 = \frac{A \pm \sqrt{A^2 - 4Ap}}{2p} \quad \text{or} \quad A\left(E_1 - 1\right) = E_1^2 p, \quad A = \frac{2}{r_0}\left(2a_1 + a_2 + a_3\right),$$

$$E_2 = 0,\ L_1 = 0,\ L_2 = 0$$

  The solution exists only for $p < A/4$. The corresponding loading diagram $p(E_1)$ is schematically shown in Fig. 45.1.

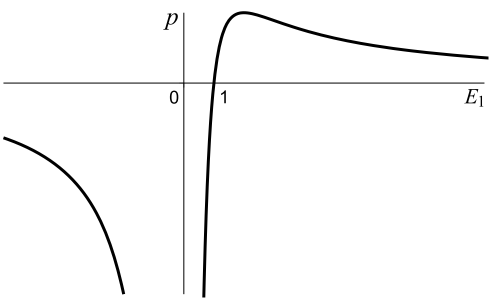

Fig. 45.1 Loading diagram for the shell in the absence of dislocations and disclinations

- Second solution:

$$E_1 = \frac{-A \pm \sqrt{A^2 + 4Ap}}{2p} \quad \text{or} \quad A\,(1 - E_1) = E_1^2 p,$$

$$E_2 = 0,\ L_1 = 0,\ L_2 = -2r_0^{-1}.$$

This solution exists for $p > -A/4$. The loading diagram corresponding to it differs from the previous case only by the sign (Fig. 45.2)

Note the non-uniqueness of the solution of the considered problem even in this simple case. One value of pressure p corresponds to up to four different values of the deformation parameter E_1. Even at zero pressure, system (45.44)–(45.47), in addition to the trivial solution corresponding to the undeformed state, also admits a second solution describing the equilibrium of a spherical shell turned inside out.

45.6 Numerical Results

The quantities r_0, p, l_0, α_0, β_0 and the material shell constants a_k, b_k $(k = 1,2,3)$ are considered to be the given parameters when solving system (45.44)–(45.47). To obtain some numerical results, as the values of the material constants of the shell, we will choose the following values consistent with [30]

$$\begin{aligned} a_1 &= \frac{2\mu h \nu}{1-\nu}, \qquad a_2 = 0, \quad a_3 = 2\mu h, \\ b_1 &= \frac{\mu h^3 \nu}{6(1-\nu)}, \quad b_2 = 0, \quad b_3 = \frac{\mu h^3}{6}. \end{aligned} \tag{45.49}$$

Here μ is the shell material shear modulus, ν is the Poisson's ratio, h is the shell thickness. So six parameters a_k, b_k are replaced by three material parameters. Below, the division by μ will be used to non-dimensionalize the forces, moments, energy, and stress tensors components. Therefore, the parameter μ will not enter the final dimensionless system of equations. Thus the thickness h and Poisson ratio ν of the shell were added to the list of the problem parameters.

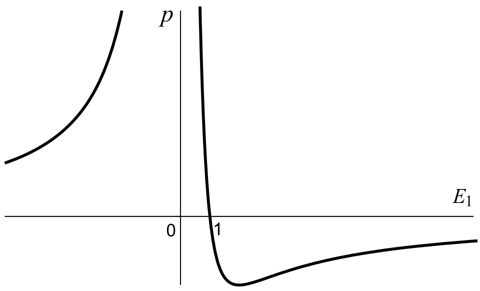

Fig. 45.2 Loading diagram for the everted shell

Let us turn the parameters of the problem, which have the dimension of length, into dimensionless ones, referring them to the radius of the shell. So, for example, the dimensionless shell thickness will take the form

$$\tilde{h} = \frac{h}{r_0}.$$

For non-dimensionalization of the dislocation density α_0 and the disclination density β_0 we also use the value of the radius by the following formulas

$$\tilde{\alpha_0} = \alpha_0 r_0,\ \tilde{\beta_0} = \beta_0 r_0^2.$$

The quantities E_1, E_2 are dimensionless by definition. The non-dimensionalization of the parameters of the bending strain tensor will be carried out according to the scheme

$$\tilde{L}_\gamma = L_\gamma r_0\ (\gamma = 1, 2).$$

Finally, we use the following schemes to make the force and moment quantities included in the equations dimensionless:

$$\tilde{P}_\gamma = \frac{1}{\mu r_0} P_\gamma,\ \tilde{\Pi}_\gamma = \frac{1}{\mu r_0^2} \Pi_\gamma,\ (\gamma = 1, 2)$$

$$\tilde{p} = \frac{1}{\mu} p,\ \tilde{l}_0 = \frac{1}{\mu r_0} l_0.$$

In what follows, the tilde over the dimensionless parameters will be omitted. The examples below consider a shell whose thickness is 5% of the radius, i. e. the ratio $h/r_0 = 1/20$. Poisson's ratio was always taken 1/3. It was noted above that the essentially nonlinear system (45.44)–(45.47) can have a number of solutions depending on the values of the parameters. In the examples given, we confine ourselves to the case of a regular, that is, non-inverted shell. For this, in the calculations, the zero value was chosen as the initial approximation for the parameter L_2.

Figures 45.3-45.5 show the dependences of the dimensionless characteristics E_1, E_2 and L_2 of the deformed state of the unloaded shell ($p = 0, l_0 = 0$) on the dislocation density for different values of the disclination density. As for the L_1 parameter, a direct analysis of system (45.44)–(45.47), taking into account (45.48), (45.44), shows that for any values of the disclination parameter, the following ratio holds up to h^2

$$L_1 = \frac{1}{2} \alpha_0.$$

The important characteristic of the stress-strain state of the shell is its elastic energy. To calculate it, we note that constitutive relations (45.41) correspond to the following form of the function of specific potential energy [34]

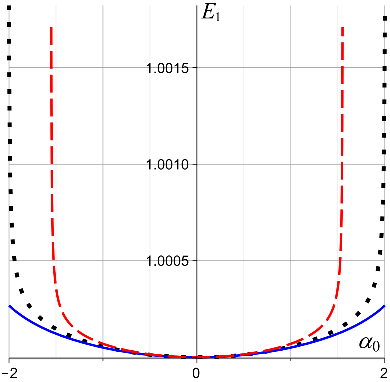

Fig. 45.3 Dependence of the strain parameter E_1 on the dislocation density α_0: $\beta_0 = 0$ — dotted line, $\beta_0 = 0.4$ — solid line, $\beta_0 = -0.4$ — dashed line.

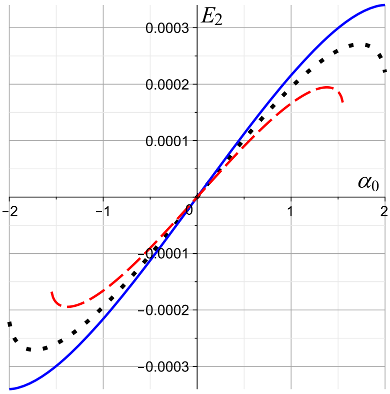

Fig. 45.4 Dependence of the strain parameter E_2 on the dislocation density α_0: $\beta_0 = 0$ — dotted line, $\beta_0 = 0.4$ — solid line, $\beta_0 = -0.4$ — dashed line.

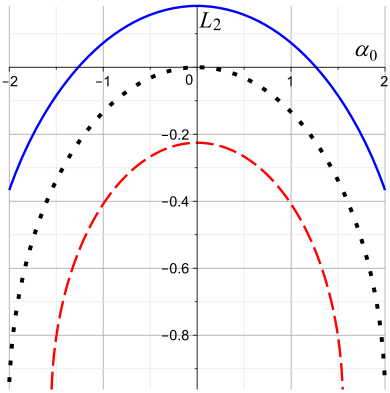

Fig. 45.5 Dependence of the bending strain parameter L_2 on the dislocation density α_0: $\beta_0 = 0$ — dotted line, $\beta_0 = 0.4$ — solid line, $\beta_0 = -0.4$ — dashed line.

$$W = \frac{1}{2}\Big(a_1 \mathrm{tr}^2 \boldsymbol{U} + a_2 \mathrm{tr} \boldsymbol{U}^2 + a_3 \mathrm{tr}\,(\boldsymbol{U}\cdot\boldsymbol{U}^{\mathrm{T}}) + a_4 \boldsymbol{n}\cdot\boldsymbol{E}^{\mathrm{T}}\cdot\boldsymbol{E}\cdot\boldsymbol{n} \\ + b_1 \mathrm{tr}^2 \boldsymbol{L} + b_2 \mathrm{tr} \boldsymbol{L}^2 + b_3 \mathrm{tr}\,(\boldsymbol{L}\cdot\boldsymbol{L}^{\mathrm{T}}) + b_4 \boldsymbol{n}\cdot\boldsymbol{L}^{\mathrm{T}}\cdot\boldsymbol{L}\cdot\boldsymbol{n}\Big). \tag{45.50}$$

Taking (45.40) into account, the specific energy W is a constant value, i.e., it does not depend on the position of the point on the sphere. This means that the total strain energy of the shell S can be found by multiplying W by the surface area of the sphere:

$$S = 4\pi r_0^2 W.$$

The quantity $S_0 = S/(4\pi\mu r_0^3)$ will be further taken as a dimensionless characteristic of the strain potential energy of the sphere. Considering (45.40), (45.49), (45.50) we arrive at the following expression

$$S_0 = (1+\nu)(E_1-1)^2 + (1-\nu)E_2^2 + \frac{\eta^2}{12}\left[(1+\nu)L_1^2 + (1-\nu)L_2^2\right].$$

Figures 45.6 and 45.7 show the dependence of elastic energy on the defect density for an unloaded shell. The dependence of the energy S_0 on the dislocation density α_0 for various disclination densities is shown in Fig. 45.6. It can be seen that the energy is an even function of the parameter α_0. Fig. 45.7 shows the dependence of the energy S_0 on the disclination density β_0 for various dislocation densities. Due to the mentioned above symmetry of the energy as a function of the dislocation density, the graphs are plotted only for zero and positive values of the parameter α_0.

The effect of internal pressure on the energy of the shell is shown in Fig. 45.8, where the solid lines correspond to the level lines of the unloaded shell on the plane of parameters α_0, β_0. The dotted lines are the energy level lines of the shell under internal pressure $p = 0.001$. It can be seen from the figure that the pattern of level lines is not symmetric with respect to the disclination density: as the pressure increases, the surface of the energy function rises and shifts in the direction of positive values of the parameter β_0.

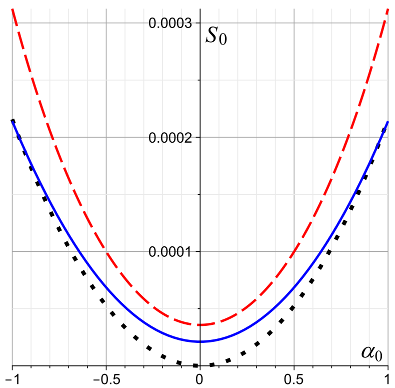

Fig. 45.6 Dependence of the energy on the dislocation density α_0: $\beta_0 = 0$ — dotted line, $\beta_0 = 0.5$ — solid line, $\beta_0 = -0.5$ — dashed line.

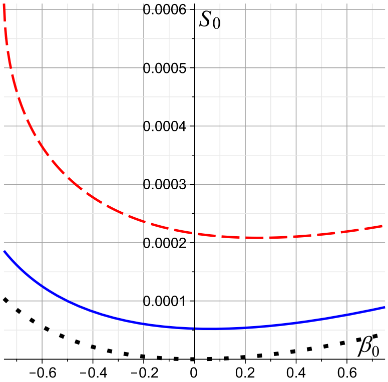

Fig. 45.7 Dependence of the energy on the disclination density β_0: $\alpha_0 = 0$ — dotted line, $\alpha_0 = 0.5$ — solid line, $\alpha_0 = 1$ — dashed line.

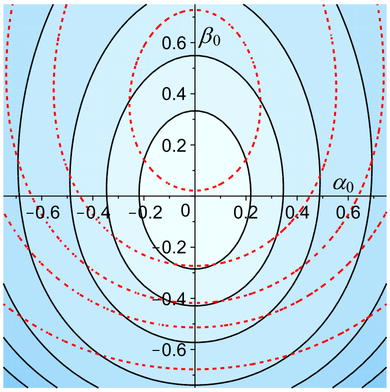

Fig. 45.8 The shell energy level lines as functions of dislocation and disclination density: solid lines — the unloaded shell ($p = 0$), dotted lines — the shell under internal pressure $p_0 = 0.001$.

45.7 Conclusions

This article develops the theory of continuously distributed dislocations and disclinations in nonlinearly elastic shells, described by the Cosserat model with kinematically independent fields of displacements and rotations.

A system of nonlinear equations of incompatibility of metric and bending strains is derived. The vector densities of dislocations and disclinations contained in these equations are considered given, i.e., known functions of the coordinates on the shell surface. Equilibrium equations for forces and moments are transformed in such a way that only metric and bending strain tensors are unknown functions, while distortion and rotation tensors are excluded.

The general theory is illustrated by solving the problem of large strains of a closed spherical shell with a spherically symmetric distribution of dislocations and disclinations. This problem is reduced to a nonlinear algebraic system of equations, which is solved numerically. The effect of dislocations and disclinations on the stress-strain state of a shell loaded with internal pressure is analyzed.

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