Geometric Theory of Defects

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Notations

$\mathbb{R}^3$ - continuous elastic media = Euclidean three-dimensional space

$x^i, y^i \quad i=1,2,3$ - Cartesian coordinates

δ_{ij} - Euclidean metric

$u^i(x)$ - displacement vector field

$\varepsilon_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i)$ - strain tensor

σ^{ij} - stress tensor

Elasticity theory of small deformations

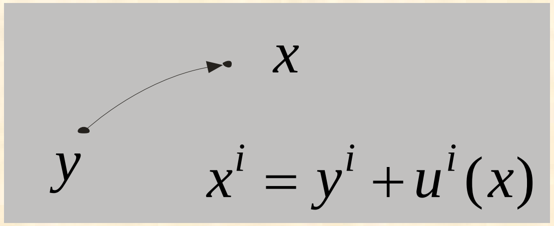
$\partial_i \sigma^{ij} + f^j = 0$ - Newton's law

$\sigma^{ij} = \lambda \delta^{ij} \varepsilon_k{}^k + 2\mu\varepsilon^{ij}$ - Hooke's law

$f^i(x)$ - density of nonelastic forces $(f^i = 0)$

λ, μ - Lame coefficients

Differential geometry of elastic deformations



$$x^i = y^i + u^i(x)$$

$y^i \to x^i(y)$ - diffeomorphism: $\mathbb{R}^3 \to \mathbb{R}^3$

$$y^i \mapsto x^i$$

$$\delta_{ij} \qquad g_{ij}$$

$$g_{ij}(x) = \frac{\partial y^k}{\partial x^i}\frac{\partial y^l}{\partial x^j}\delta_{kl} \approx \delta_{ij} - \partial_i u_j - \partial_j u_i = \delta_{ij} - 2\varepsilon_{ij}$$ - induced metric

$$\tilde{\Gamma}_{ijk} = \tfrac{1}{2}(\partial_i g_{jk} + \partial_j g_{ik} - \partial_k g_{ij}) \neq 0$$ - Christoffel's symbols

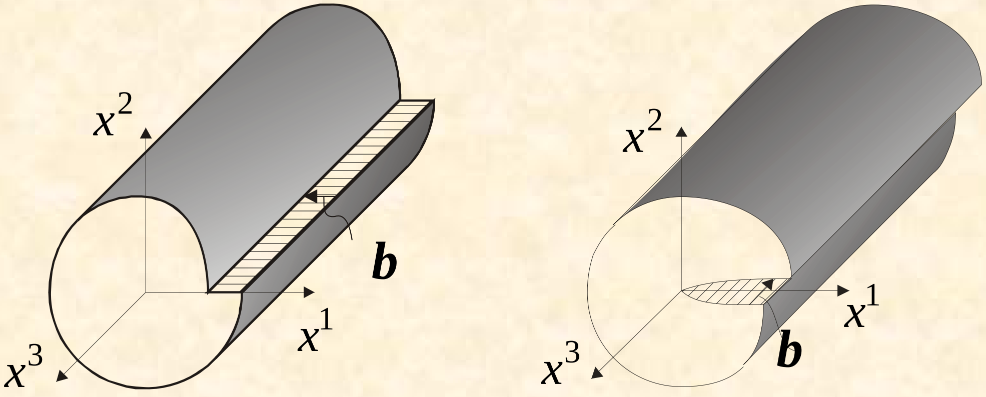
$$\tilde{R}_{ijk}{}^{l} = \partial_i \tilde{\Gamma}_{jk}{}^{l} - \tilde{\Gamma}_{ik}{}^{m}\tilde{\Gamma}_{jm}{}^{l} - (i \leftrightarrow j) = 0$$ - curvature tensor

$$\ddot{x}^i = -\tilde{\Gamma}_{jk}{}^{i}\dot{x}^j\dot{x}^k$$ - extremals (geodesics)

$$T_{ij}{}^{k} = \tilde{\Gamma}_{ij}{}^{k} - \tilde{\Gamma}_{ji}{}^{k} = 0$$ - torsion tensor

Dislocations

Linear defects:

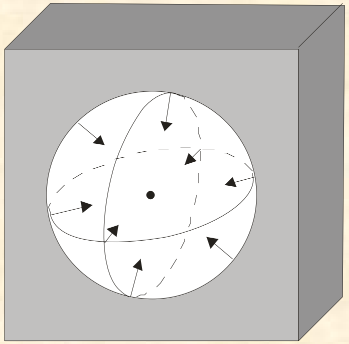


Edge dislocation

Screw dislocation

b - Burgers vector

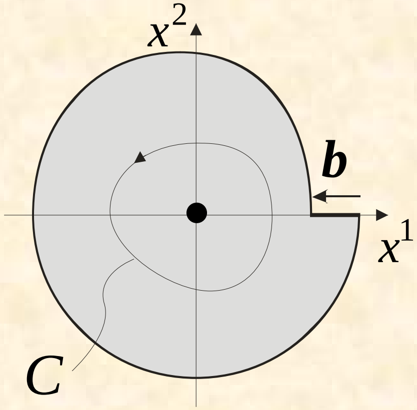
Point defects:



Vacancy

$$u^i(x) \begin{cases} \text{is continuous} & = \text{elastic deformations} \\ \text{is not continuous} & = \text{dislocations} \end{cases}$$

Edge dislocation



$$\oint\limits_C dx^\mu \partial_\mu u^i = -\oint\limits_C dx^\mu \partial_\mu y^i = -b^i \qquad (*)$$

$x^\mu,\ \mu = 1,2,3$ - arbitrary curvilinear coordinates

$y^i(x)$ - is not continuous !

$$e_\mu{}^i(x) = \begin{cases} \partial_\mu y^i & \text{- outside the cut} \\ \lim \partial_\mu y^i & \text{- on the cut} \end{cases}$$

- triad field (continuous on the cut)

$$(*) \Rightarrow\ b^i = \oint\limits_C dx^\mu e_\mu{}^i = \iint\limits_S dx^\mu \wedge dx^\nu (\partial_\mu e_\nu{}^i - \partial_\nu e_\mu{}^i)$$ - Burgers vector in elasticity

$$T_{\mu\nu}{}^i = \partial_\mu e_\nu{}^i - \omega_\mu{}^{ij} e_{\nu j} - (\mu \leftrightarrow \nu)$$ - torsion

$$R_{\mu\nu}{}^{ij} = \partial_\mu \omega_\nu{}^{ij} - \omega_\mu{}^{ik} \omega_{\nu k}{}^j - (\mu \leftrightarrow \nu)$$ - curvature

$$\omega_\mu{}^{ij} = -\omega_\mu{}^{ji}$$

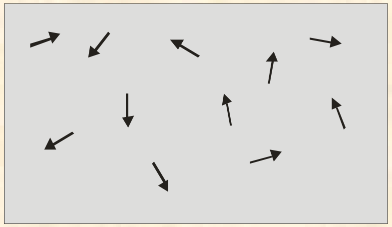
SO(3)-connection

$$\boxed{b^i = \iint dx^\mu \wedge dx^\nu T_{\mu\nu}{}^i}$$ - definition of the Burgers vector in the geometric theory

Back to elasticity: if $R_{\mu\nu}{}^{ij} = 0$ then $\omega_\mu{}^{ij} \to 0$

Disclinations

Ferromagnets



$n^i(x)$ - unit vector field $\qquad n_0^i$ - fixed unit vector

$$n^i = n_0^j S_j{}^i(\omega)$$

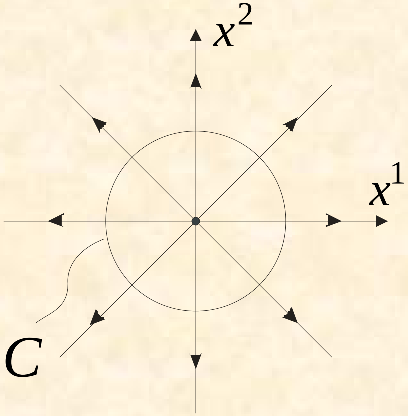
$S_i{}^j \in \mathbb{SO}(3)$ - orthogonal matrix

$\omega^{ij} = -\omega^{ji} \in \mathfrak{so}(3)$ - Lie algebra element (spin structure)

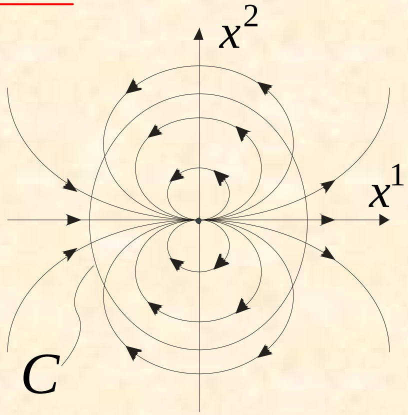
$\omega_i = \frac{1}{2}\varepsilon_{ijk}\omega^{jk}$ - rotational angle

ε_{ijk} - totally antisymmetric tensor $(\varepsilon_{123} = 1)$

Examples



$\Theta = 2\pi$



$\Theta = 4\pi$

$$\Omega^{ij} = \oint_C dx^\mu \partial_\mu \omega^{ij}$$

$\Theta_i = \varepsilon_{ijk}\Omega^{jk}$ - Frank vector
(total angle of rotation)

$$\Theta = \sqrt{\Theta^i \Theta_i}$$

Model for a spin structure:

$\omega^i(x) \in \mathfrak{so}(3)$ - basic variable

$$S_i{}^j = \delta_i^j \cos\omega + \frac{\omega^k \varepsilon_{ki}{}^j}{\omega} \sin\omega + \frac{\omega_i \omega^j}{\omega^2}(1-\cos\omega) \in \mathbb{SO}(3), \qquad \omega = \sqrt{\omega^i \omega_i}$$

$l_{\mu i}{}^j = (\partial_\mu S^{-1})_i{}^k S_k{}^j$ - trivial SO(3)-connection (pure gauge)

$\boxed{\partial^\mu l_\mu{}^{ij} = 0}$ - principal chiral SO(3)-model

Frank vector

$\omega^{ij}(x)$ - is not continuous !

$$\omega_\mu{}^{ij}(x) = \begin{cases} \partial_\mu \omega^{ij} & \text{- outside the cut} \\ \lim \partial_\mu \omega^{ij} & \text{- on the cut} \end{cases}$$

- SO(3)-connection (continuous on the cut)

$$\Omega^{ij} = \oint dx^\mu \omega_\mu{}^{ij} = \iint dx^\mu \wedge dx^\nu (\partial_\mu \omega_\nu{}^{ij} - \partial_\nu \omega_\mu{}^{ij})$$

- the Frank vector

$$R_{\mu\nu}{}^{ij} = \partial_\mu \omega_\nu{}^{ij} - \omega_\mu{}^{ik} \omega_{\nu k}{}^{j} - (\mu \leftrightarrow \nu)$$

- curvature

$$\boxed{\Omega^{ij} = \iint dx^\mu \wedge dx^\nu R_{\mu\nu}{}^{ij}}$$

- definition of the Frank vector in the geometric theory

Back to the spin structure: if $n \in \mathbb{R}^2$ then $\mathbb{SO}(3) \to \mathbb{SO}(2)$

Summary of the geometric approach

(physical interpretation)

Media with dislocations and disclinations $=$

$= \mathbb{R}^3$ with a given Riemann-Cartan geometry

Independent variables $\begin{cases} e_\mu{}^i & \text{- triad field} \\ \omega_\mu{}^{ij} & \text{- SO(3)-connection} \end{cases}$

$$T_{\mu\nu}{}^i = \partial_\mu e_\nu{}^i - \omega_\mu{}^{ij} e_{\nu j} - (\mu \leftrightarrow \nu)$$

- torsion (surface density of the Burgers vector)

$$R_{\mu\nu}{}^{ij} = \partial_\mu \omega_\nu{}^{ij} - \omega_\mu{}^{ik} \omega_{\nu k}{}^j - (\mu \leftrightarrow \nu)$$

- curvature (surface density of the Frank vector)

Elastic deformations: $R_{\mu\nu}{}^{ij} = 0, \quad T_{\mu\nu}{}^i = 0$

Dislocations: $R_{\mu\nu}{}^{ij} = 0, \quad T_{\mu\nu}{}^i \neq 0$

Disclinations: $R_{\mu\nu}{}^{ij} \neq 0, \quad T_{\mu\nu}{}^i = 0$

Dislocations and disclinations: $R_{\mu\nu}{}^{ij} \neq 0, \quad T_{\mu\nu}{}^i \neq 0$

The free energy

$$S=\int d^3x\,eL,\quad e=\det e_\mu{}^i \qquad L=\kappa R-\tfrac{1}{4}T_{ijk}(\beta_1 T^{ijk}+\beta_2 T^{kij}+\beta_3 T^j\delta^{ik})$$

$$+\tfrac{1}{4}R_{ijkl}(\gamma_1 R^{ijkl}+\gamma_2 R^{klij}+\gamma_3 R^{ik}\delta^{jl})+\Lambda$$

$T_{ij}{}^k=e^\mu{}_i e^\nu{}_j T_{\mu\nu}{}^k,\ \ldots$ - transformation of indices

$T_j=T_{ij}{}^i$ - trace of torsion

$R_{ik}=R_{ijk}{}^j$ - Ricci tensor

$R=R_i{}^i$ - scalar curvature

$\kappa,\beta_1,\beta_2,\beta_3$

$\gamma_1,\gamma_2,\gamma_3,\Lambda$ - coupling constants

Postulate: equations of equilibrium admit solutions

$$\begin{cases} R=0, & T\neq 0 \\ R\neq 0, & T=0 \\ R=0, & T=0 \end{cases}$$

- only dislocations
- only disclinations
- elastic deformations

The result:

$$\boxed{L=\kappa\tilde{R}-\gamma R_{[ij]}R^{[ij]}}$$

$\tilde{R}(e)$ - the Hilbert-Einstein action

$R_{[ij]}(e,\omega)$ - antisymmetric part of the Ricci tensor

Elastic gauge

$(1-2\sigma)\Delta u_i + \partial_i \partial_j u^j = 0$ - the elasticity equation

$\sigma = \dfrac{\lambda}{2(\lambda+\mu)}$ - Poisson ratio

$e_{\mu i} \approx \delta_{\mu i} - \partial_\mu u^i$ - the linear approximation

$\boxed{(1-2\sigma)\partial^\mu e_{\mu i} + \partial_i e_\mu{}^\mu = 0}$ - the elastic gauge (fixes diffeomorphisms)

Lorentz gauge

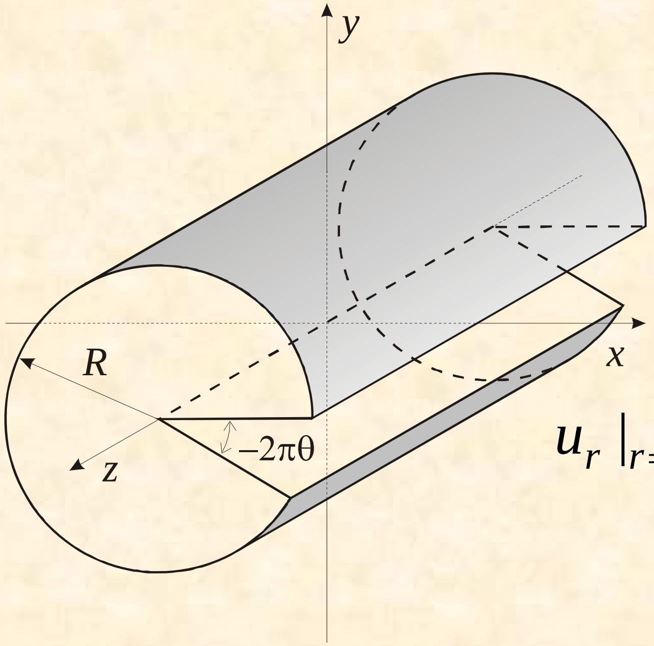
$\boxed{\partial^\mu \omega_\mu{}^{ij} = 0}$ - the Lorenz gauge (fixes SO(3)-invariance)

If there are no disclinations $R_{\mu\nu}{}^{ij} = 0$, then $\omega_{\mu i}{}^j = l_{\mu i}{}^j = (\partial_\mu S^{-1})_i{}^k S_k{}^j$

pure gauge

$\partial^\mu l_\mu{}^{ij} = 0$ - principal chiral SO(3)-model

Wedge dislocation in elasticity theory



r, φ, z - cylindrical coordinates

$u_i = \{u(r), v(r)\varphi, 0\}$ - displacement vector

Boundary conditions:

$$u_r\,|_{r=0} = 0, \quad u_\varphi\,|_{\varphi=0} = 0, \quad u_\varphi\,|_{\varphi=2\pi} = -2\pi\theta r, \quad \partial_r u_r\,|_{r=R} = 0$$

$$\longrightarrow v(r) = -\theta r$$

θ - deficit angle

$$\partial_r(r\partial_r u) - \frac{u}{r} = D$$ - elasticity equations

$$D = -\frac{1-2\sigma}{1-\sigma}\theta,$$ σ - Poisson ratio

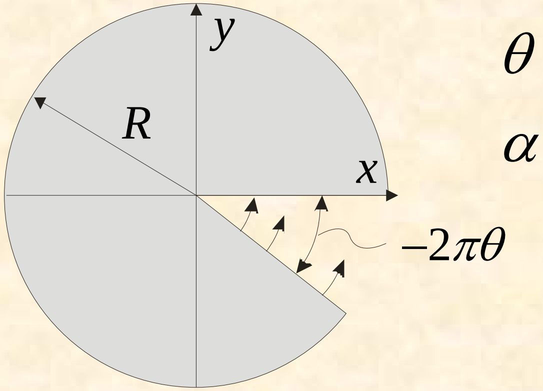
$$u = \frac{D}{2} r \ln r + c_1 r + \frac{c_2}{r}, \quad c_{1,2} = \text{const}$$ - a general solution

$$dl^2 = \left(1 + \theta\frac{1-2\sigma}{1-\sigma}\ln\frac{r}{R}\right)dr^2 + r^2\left(1 + \theta\frac{1-2\sigma}{1-\sigma}\ln\frac{r}{R} + \theta\frac{1}{1-\sigma}\right)d\varphi^2$$

induced metric

$$\theta \ll 1, \quad r \sim R$$

Wedge dislocation in the geometric theory



θ - deficit angle

$$\alpha = 1 + \theta$$

$$dl^2 = \frac{1}{\alpha^2} df^2 + f^2 d\varphi^2$$ - metric for a conical singularity (exact solution of 3D Einstein eqs.)

Where is the Poisson ratio σ ???

The elastic gauge: $$\boxed{(1-2\sigma)\partial^\mu e_{\mu i} + \partial_i e_\mu{}^\mu = 0}$$

For $e_\mu{}^i = \partial_\mu u^i$ it reduces to elasticity equations: $(1-2\sigma)\Delta u_i + \partial_i \partial_j u^j = 0$

$$dl^2 = \left(\frac{r}{R}\right)^{2(n-1)} \left(dr^2 + \frac{\alpha^2 r^2}{n^2} d\varphi^2\right)$$

- exact solution of the Einstein equations in the elastic gauge

$$n = \frac{-\theta\sigma + \sqrt{\theta^2\sigma^2 + 4(1+\theta)(1-\sigma)^2}}{2(1-\sigma)}$$

Comparison of the elasticity theory with the geometric model

$$dl^2 = \left(\frac{r}{R}\right)^{2(n-1)}\left(dr^2 + \frac{\alpha^2 r^2}{n^2}\, d\varphi^2\right)$$

- the geometric model

$$\theta \ll 1, \qquad n \approx 1 + \theta\,\frac{1-2\sigma}{2(1-\sigma)}$$

$$dl^2 = \left(1+\theta\frac{1-2\sigma}{1-\sigma}\ln\frac{r}{R}\right)dr^2 + r^2\left(1+\theta\frac{1-2\sigma}{1-\sigma}\ln\frac{r}{R}+\theta\frac{1}{1-\sigma}\right)d\varphi^2$$

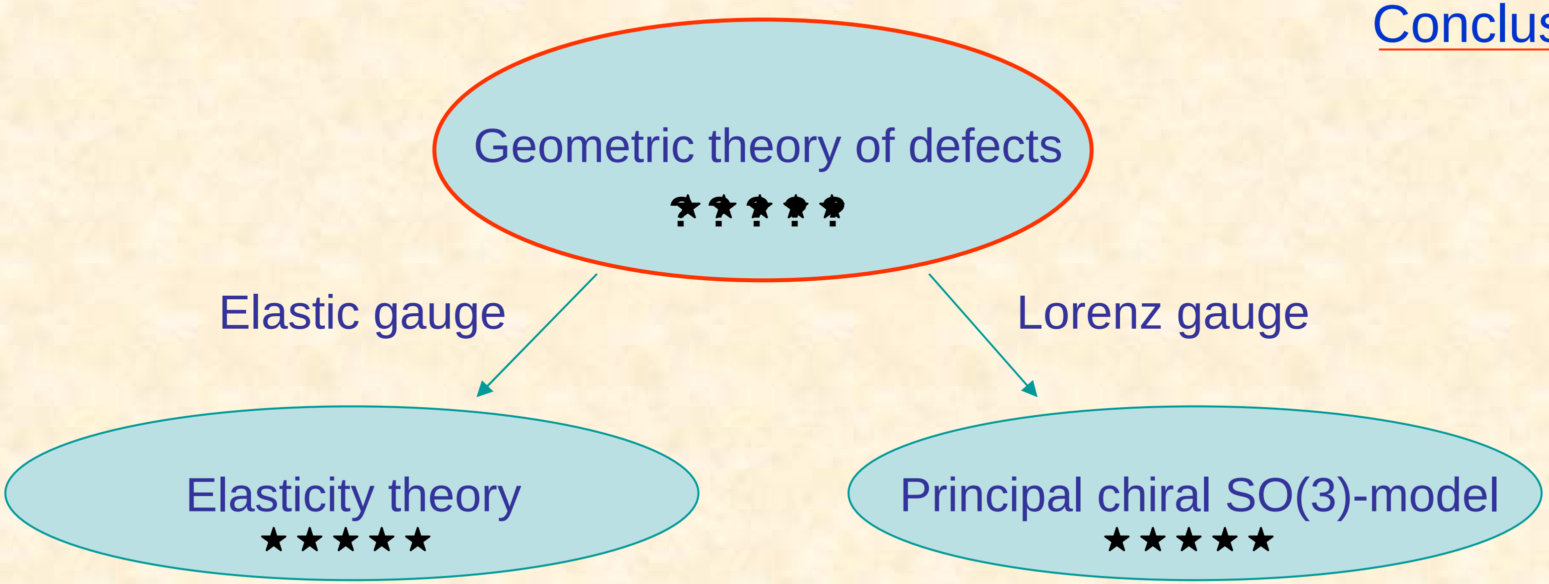
- the elasticity theory

The result of the elasticity theory is valid only for small deficit angles $\theta \ll 1$ and near the boundary $r \sim R$

The result of the geometric model is valid for all θ and everywhere

Induced metric components define the deformation tensor and can be measured experimentally

Conclusion



Geometric theory of defects

★? ★? ★? ★? ★?

Elastic gauge

Lorenz gauge

Elasticity theory

★★★★★

Principal chiral SO(3)-model

★★★★★

1) The geometric theory of defects in solids appears to be a fundamental theory of defects.

2) It describes single defects as well as continuous distribution of defects.

3) It provides a unified treatment of defects in media (dislocations) and in spin structures (disclinations).

4) In the absence of defects it reduces to the elasticity theory for the displacement vector field and to the principal chiral SO(3)-model for spin structures.