

Geometric Theory of Defects

M. O. Katanaev

Steklov Mathematical Institute, Moscow

Katanaev, Volovich Ann. Phys. 216(1992)1; ibid. 271(1999)203

Katanaev Theor.Math.Phys.135(2003)733; ibid. 138(2004)163

Physics – Uspekhi 48(2005)675.

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

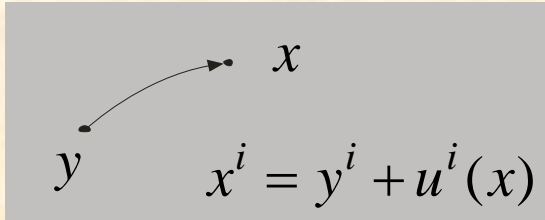
$\partial_i \sigma^{ij} + f^j = 0$ - Newton's law

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

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

λ, μ - Lamé coefficients

Differential geometry of elastic deformations



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

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

$$\delta_{ij} \quad g_{ij}$$

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

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

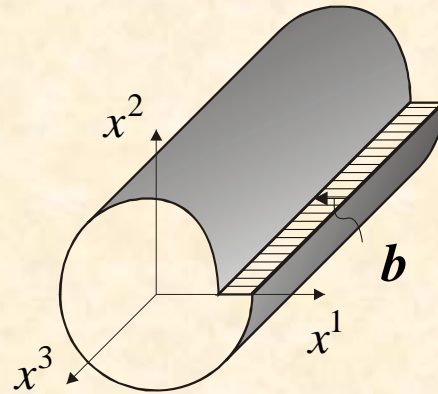
$$\tilde{R}_{ijk}{}^l = \partial_i \tilde{\Gamma}_{jk}{}^l - \tilde{\Gamma}_{ik}{}^m \tilde{\Gamma}_{jm}{}^l - (i \leftrightarrow j) = 0 \text{ - curvature tensor}$$

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

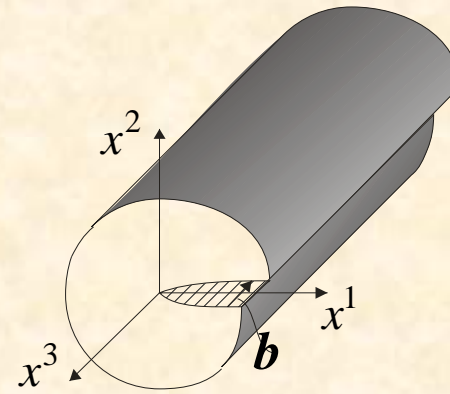
$$T_{ij}{}^k = \tilde{\Gamma}_{ij}{}^k - \tilde{\Gamma}_{ji}{}^k = 0 \text{ - torsion tensor}$$

Dislocations

Linear defects:



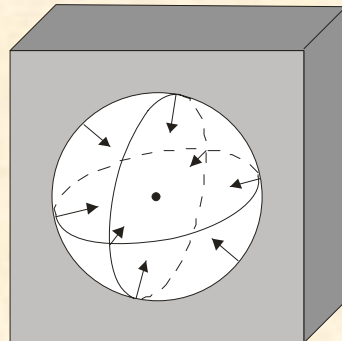
Edge dislocation



Screw dislocation

b - Burgers vector

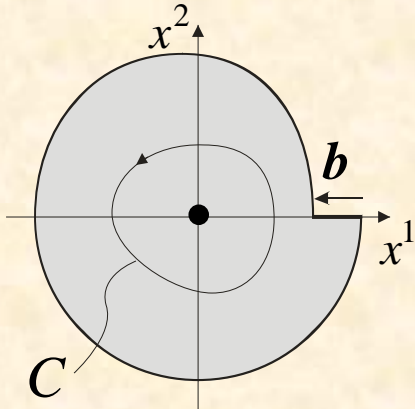
Point defects:



Vacancy

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

Edge dislocation



$$\oint_C dx^\mu \partial_\mu u^i = -\oint_C dx^\mu \partial_\mu y^i = -b^i \quad (*)$$

$x^\mu, \mu = 1, 2, 3$ - 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)

$$(*) \Rightarrow b^i = \oint_C dx^\mu e_\mu^i = \iint_S dx^\mu \wedge dx^\nu (\partial_\mu e_\nu^i - \partial_\nu e_\mu^i) \quad \text{- Burgers vector in elasticity}$$

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

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

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

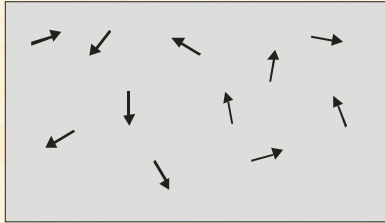
SO(3)-connection

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

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

Disclinations

Ferromagnets



$n^i(x)$ - unit vector field

n_0^i - fixed unit vector

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

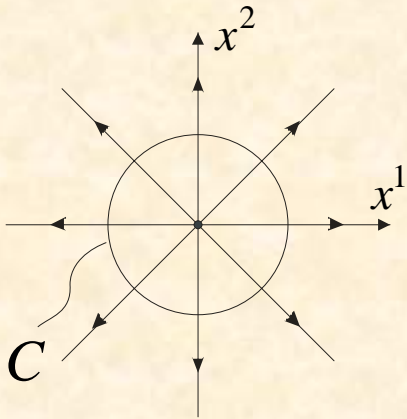
$S_i^j \in \mathbb{SO}(3)$ - orthogonal matrix

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

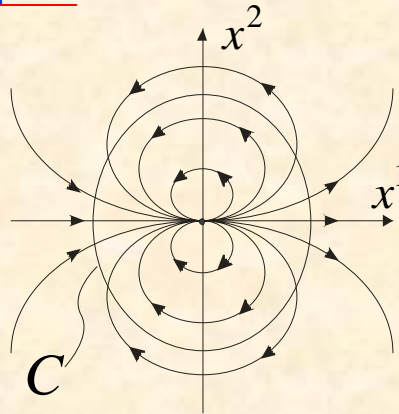
$$\omega_i = \frac{1}{2} \varepsilon_{ijk} \omega^{jk} \text{ - rotational angle}$$

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

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

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

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

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)

$$\Omega^{ij} = \oint dx^{\mu} \omega_{\mu}^{ij} = \iint dx^{\mu} \wedge dx^{\nu} (\partial_{\mu} \omega_{\nu}^{ij} - \partial_{\nu} \omega_{\mu}^{ij}) \quad \text{- the Frank vector}$$

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

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

- definition of the Frank vector
in the geometric theory

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

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

$$S = \int d^3x eL, \quad e = \det e_\mu^i \quad L = \kappa R - \frac{1}{4} T_{ijk} (\beta_1 T^{ijk} + \beta_2 T^{kij} + \beta_3 T^j \delta^{ik}) \\ + \frac{1}{4} R_{ijkl} (\gamma_1 R^{ijkl} + \gamma_2 R^{klij} + \gamma_3 R^{ik} \delta^{jl}) + \Lambda$$

$$T_{ij}^k = e^\mu_i e^\nu_j T_{\mu\nu}^k, \dots \text{ - transformation of indices}$$

$$T_j = T_{ij}^i \text{ - trace of torsion} \quad \kappa, \beta_1, \beta_2, \beta_3 \text{ - coupling constants}$$

$$R_{ik} = R_{ijk}^j \text{ - Ricci tensor} \quad \gamma_1, \gamma_2, \gamma_3, \Lambda$$

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

Postulate: equations of equilibrium admit solutions

$$\left\{ \begin{array}{l} R = 0, \quad T \neq 0 \text{ - only dislocations} \\ R \neq 0, \quad T = 0 \text{ - only disclinations} \\ R = 0, \quad T = 0 \text{ - elastic deformations} \end{array} \right.$$

The result:

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

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

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

Elastic gauge

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

$$\sigma = \frac{\lambda}{2(\lambda + \mu)} \quad - \text{Poisson ratio}$$

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

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

Lorentz gauge

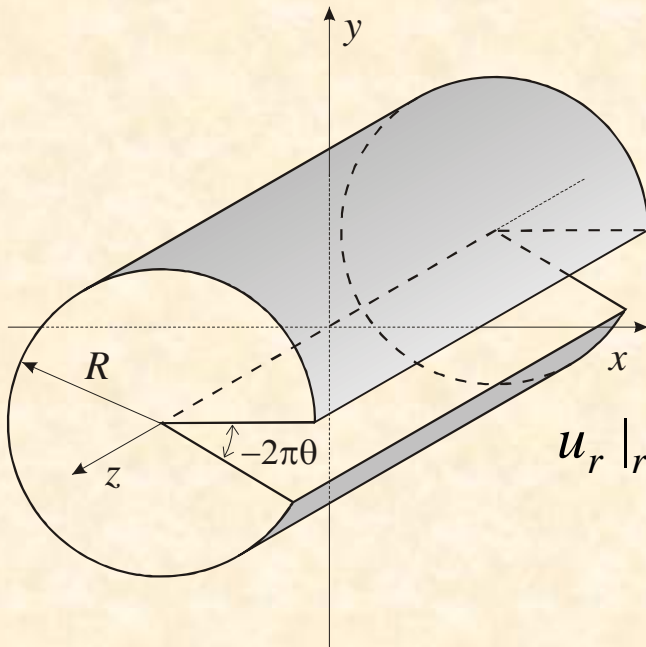
$$\partial^\mu \omega_\mu{}^{ij} = 0 \quad - \text{the Lorenz gauge (fixes SO(3)-invariance)}$$

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

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

Wedge dislocation in elasticity theory



r, φ, z - cylindrical coordinates

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

Boundary conditions:

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

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

θ - deficit angle

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

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

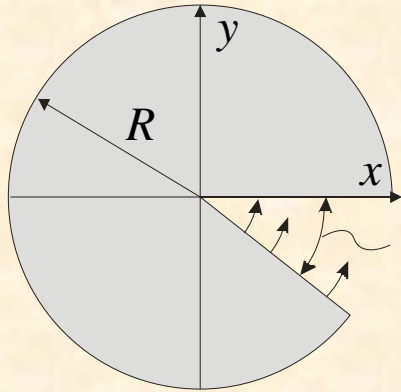
$$u = \frac{D}{2} r \ln r + c_1 r + \frac{c_2}{r}, \quad c_{1,2} = \text{const} \text{ - a general solution}$$

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

induced metric

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

Wedge dislocation in the geometric theory



θ - deficit angle

$$\alpha = 1 + \theta$$

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

Where is the Poisson ratio σ ???

The elastic gauge:

$$(1 - 2\sigma)\partial^\mu e_{\mu i} + \partial_i e_\mu{}^\mu = 0$$

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

$$dl^2 = \left(\frac{r}{R}\right)^{2(n-1)} \left(dr^2 + \frac{\alpha^2 r^2}{n^2} d\varphi^2 \right) \text{ - exact solution of the Einstein equations in the elastic gauge}$$

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

Comparison of the elasticity theory with the geometric model

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

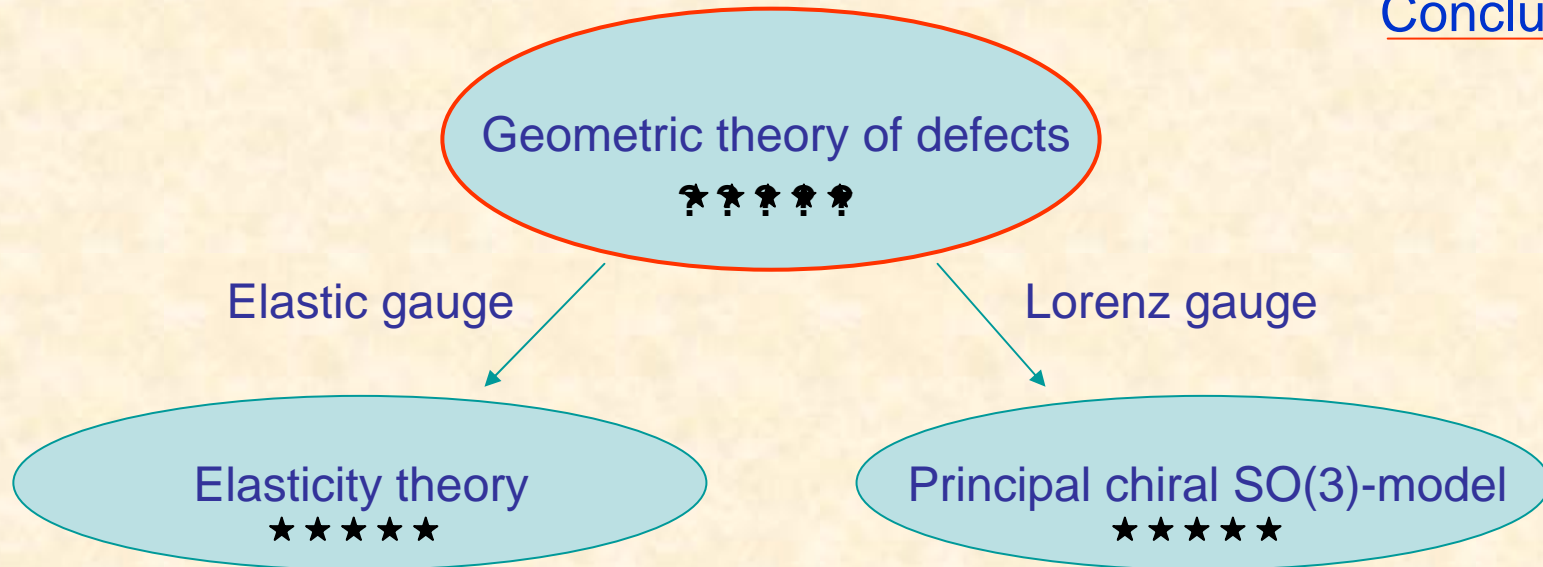
$$\leftarrow \theta \ll 1, \quad n \approx 1 + \theta \frac{1-2\sigma}{2(1-\sigma)}$$

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

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



- 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.