Leiden Elasticity Lectures I

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Overview

The field of elasticity is concerned with the mechanical response of "solid" bodies. It is an old subject that has its roots in work by Euler, Lagrange, and others in the 18th century. This work is based on the idea that extended matter is a mathematical continuum of mass points with preferred relative positions that stretch or compress in response to stress. This is the approach that will be followed in most of these lectures. It should be noted, however, that there is another, more restrictive but nonetheless very useful, approach to elasticity, namely one in which elastic distortions are viewed as Goldstone modes associated with the formation of periodic crystalline states. In the description, elasticity arises from spatial variation of phases of mass density waves.

Course Outline
(subject to change as lectures progress)

I. Preliminaries
   A. Mapping from reference to target space
   B. Deformation and Strain
   C. Cauchy-Green tensors and nonlinear strain
   D. Eulerian Strain
II. Elastic energy
   A. Elastic moduli
   B. Isotropic and uniaxial solids
   C. Voight notation
III. Force and stress
   A. First and second Pila-Kirchhoff stress tensor
   B. The Cauchy stress tensor
IV. Polar Decomposition Theorem and target-reference conversion.
V. Nonaffine Response

Classical Lagrangian Description

Engineering notation: $\mathbf{x}$->$\mathbf{X}$
$\mathbf{R}$->$\mathbf{x}$

$$\mathbf{R}(\mathbf{x}) = \mathbf{x} + \mathbf{u}(\mathbf{x})$$

Reference material in D dimensions described by a continuum of mass points x. Neighbors of points do not change under distortion

Material distorted to new positions $\mathbf{R}(\mathbf{x})$ in $d \geq D$ dimensions.

$$\Lambda_{i\alpha} = \frac{\partial R_i}{\partial x_\alpha} = \delta_{i\alpha} + \eta_{i\alpha}$$

Cauchy deformation tensor $\eta_{i\alpha} = \partial_\alpha u_i$

Linear and Nonlinear Elasticity

Linear: Small deformations – Λ near 1

Nonlinear: Large deformations – Λ >>1

Why nonlinear?

- Systems can undergo large deformations – rubbers, polymer networks , …
- Non-linear theory needed to understand properties of statically strained materials
- Non-linearities can renormalize nature of elasticity
- Elegant an complex theory of interest in its own right

Why now:

- New interest in biological materials under large strain
- Liquid crystal elastomers – exotic nonlinear behavior
- Old subject but difficult to penetrate – worth a fresh look

Deformations and Strain

Complete information about shape of body in $\mathbf{R}(\mathrm{x}) = \mathbf{x} + \mathbf{u}(\mathbf{x})$;

$\mathbf{u} = \mathrm{const.}$ – translation no energy.

No energy cost unless $\mathbf{u}(\mathbf{x})$ varies in space.

For slow variations, use the Cauchy deformation tensor

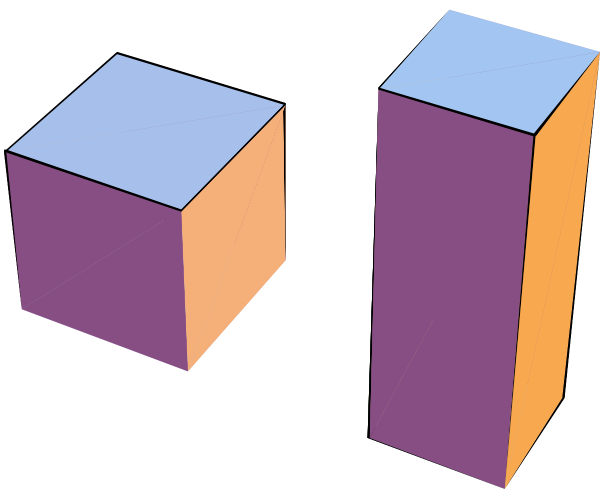
$$\Lambda_{i\alpha} = \delta_{i\alpha} + \partial_\alpha u_i = \delta_{i\alpha} + \eta_{i\alpha}$$

$$d^3R = \det \underset{\sim}{\Lambda}\, d^3x$$

$\det \underset{\sim}{\Lambda} = 1$: No volume change

$$\underset{\sim}{\Lambda} = \begin{pmatrix} \Lambda^{-1/2} & 0 & 0 \\ 0 & \Lambda^{-1/2} & 0 \\ 0 & 0 & \Lambda \end{pmatrix} \quad \text{3D}$$

$$\underset{\sim}{\Lambda} = \begin{pmatrix} \Lambda & 0 \\ 0 & \Lambda^{-1} \end{pmatrix} \quad \text{2D}$$

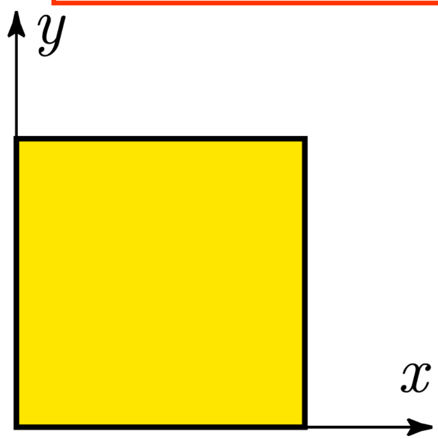


Volume preserving stretch along z-axis: This is pure shear

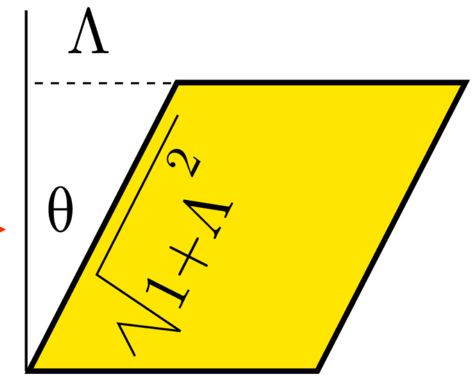
Simple shear strain

Constant Volume, but note stretching of sides originally along x or y.

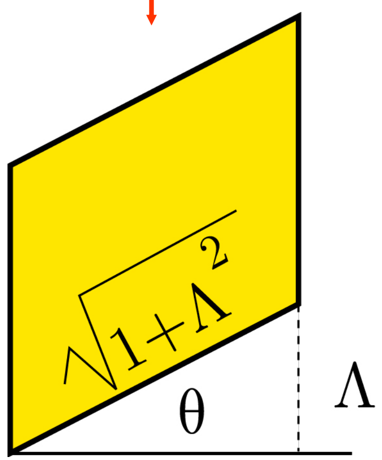
Note: Λ is not symmetric



$$\underset{\sim}{\Lambda} = \begin{pmatrix} 1 & \Lambda \\ 0 & 1 \end{pmatrix}$$

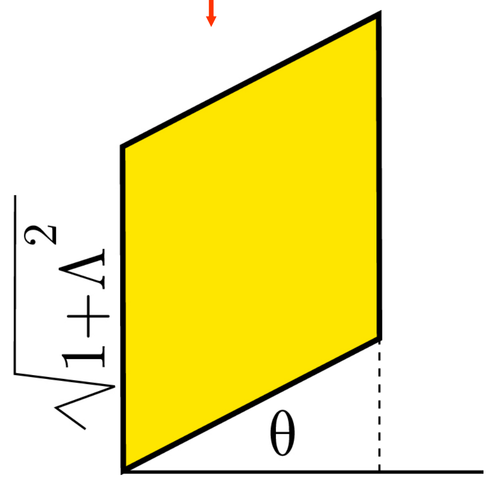


Rotate



$$\underset{\sim}{\Lambda} = \begin{pmatrix} 1 & 0 \\ \Lambda & 1 \end{pmatrix}$$

Not equivalent to



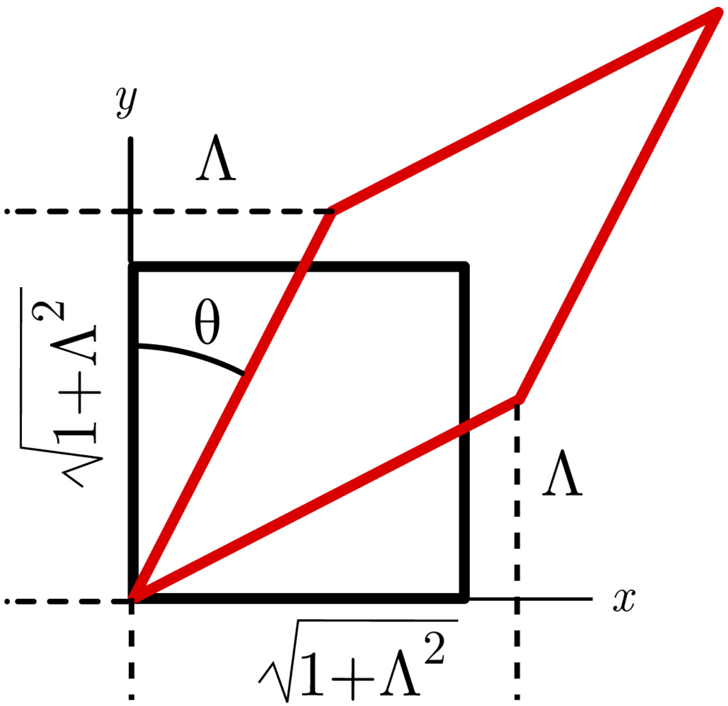
More Complex Shear

Shear: symmetric deformation tensor with unit determinant – equivalent to stretch along 45 deg.

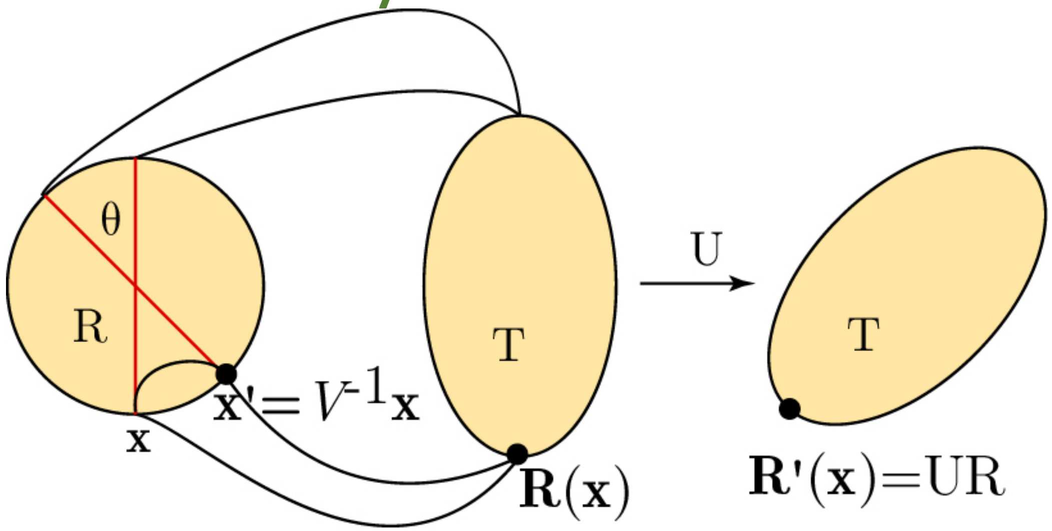
$$\underset{\sim}{\Lambda} = \begin{pmatrix} \sqrt{1+\Lambda^2} & \Lambda \\ \Lambda & \sqrt{1+\Lambda^2} \end{pmatrix}$$

$$\det \underset{\sim}{\Lambda} = 1$$

Again volume preserving:
All nonlinear shears
preserve volume.



Cauchy-Green Tensors



R=Reference space

T=Target space

$$dR^2 - dx^2 = 2u_{\alpha\beta}dx_\alpha dx_\beta$$

$$dR^2 = g_{\alpha\beta}dx_\alpha dx_\beta$$

$$g_{\alpha\beta} = \partial_\alpha R_i \partial_\beta R_i = \Lambda^T_{\alpha i}\Lambda_{i\beta}$$

$$\Lambda_{i\alpha} = \frac{\partial R_i}{\partial x_\alpha} = \delta_{i\alpha} + \eta_{i\alpha}$$

Metric tensor: Right Cauchy-Green tensor ($C_{\alpha\beta}$): Invariant under any U

$$h_{ij} = \partial_\alpha R_i \partial_\alpha R_j = \Lambda_{i\alpha}\Lambda^T_{\alpha j}$$

Standard Engineering notation in blue: Λ_{ia} → $F_{i\alpha}$

Left Cauchy-Green tensor (B_{ij}) (or Finger tensor): Invariant under any V

Nonlinear Strain

Symmetric!

$$\underset{\sim}{u} = \tfrac{1}{2}(\underset{\sim}{\Lambda}^T \underset{\sim}{\Lambda} - \underset{\sim}{\delta}) = \tfrac{1}{2}(\underset{\sim}{g} - \underset{\sim}{\delta}) \approx \tfrac{1}{2}(\underset{\sim}{\eta} + \underset{\sim}{\eta}^T)$$

$$u_{\alpha\beta} = \tfrac{1}{2}\left(\partial_\alpha u_\beta + \partial_\beta u_\alpha + \partial_\alpha u_k \partial_\beta u_k\right)$$

$$\underset{\sim}{u}^{st} = \underset{\sim}{u} - \tfrac{1}{D}\underset{\sim}{\delta}\,\mathrm{Tr}\,\underset{\sim}{u}$$

Assumes flat reference metric with $dx^2 = dR^2$

$u_{\alpha\beta}$ is invariant under rotations in the target space but transforms as a tensor under rotations in the reference space. It contains no information about orientation of object. This is the strain physicists use.

$$\underset{\sim}{v} = \tfrac{1}{2}(\underset{\sim}{\Lambda}\underset{\sim}{\Lambda}^T - \underset{\sim}{\delta}) \approx \tfrac{1}{2}(\underset{\sim}{\eta} + \underset{\sim}{\eta}^T)$$

$$v_{ij} = \tfrac{1}{2}\left(\partial_i u_j + \partial_j u_i + \partial_\alpha u_i \partial_\alpha u_j\right)$$

v_{ij} is invariant under symmetry operations in the reference space, but it transforms as a tensor in the target space.

Eulerian Strain

Treat $\boldsymbol{x}$ as a function of $\mathbf{R}$ rather than $\mathbf{R}$ as a function of $\mathbf{x}$

$$\mathbf{u}(\mathbf{x}) \to \mathbf{u}(\mathbf{x}(\mathbf{R})) \qquad \frac{\partial R_i}{\partial x_\alpha}\frac{\partial x_\alpha}{\partial R_j} = \delta_{ij} \Rightarrow \Lambda^{-1}_{\alpha j} = \frac{\partial x_\alpha}{\partial R_j}$$

$$dx^2 = h^E_{ij} dR_i dR_j$$

$$dx^2 - dR^2 = -2u^E_{ij} dR_i dR_j$$

$$h^E_{ij} = \frac{\partial x_\alpha}{\partial R_i}\frac{\partial x_\alpha}{\partial R_j} = (\Lambda^T)^{-1}_{i\alpha}\Lambda^{-1}_{\alpha j} = h^{-1}_{ij}$$

$$u^E_{ij} = \tfrac{1}{2}(\delta_{ij} - h^E_{ij}) = \frac{1}{2}\left(\frac{\partial u_i}{\partial R_j} + \frac{\partial u_j}{\partial R_i} - \frac{\partial u_k}{\partial R_j}\frac{\partial u_k}{\partial R_i}\right)$$

Elastic energy

The elastic energy should be invariant under rigid rotations in the target space (unless there are externals fields): it is if it is a function of $u_{\alpha\beta}$.

$$\mathcal{F} = \tfrac{1}{2}\int d^D x\, f(u_{\alpha\beta})$$

$$= \tfrac{1}{2}\int d^D x[K_{\alpha\beta\gamma\delta} u_{\alpha\beta} u_{\gamma\delta} + \tilde{\boldsymbol{\sigma}}_{\alpha\beta} u_{\alpha\beta}]$$

This energy is automatically invariant under rotations in target space. It must also be invariant under the point-group operations of the reference space. These place constraints on the form of the elastic constants.

Note there can be a linear "stress"-like term. This can be removed (except for transverse random components) by redefinition of the reference space

Elastic modulus tensor/isotropic solid

$K_{\alpha\beta\chi\delta}$ is the elastic constant or elastic modulus tensor. It has inherent symmetry and symmetries of the reference space.

$$K_{\alpha\beta\gamma\delta} = K_{\gamma\delta\alpha\beta} = K_{\beta\alpha\gamma\delta} = K_{\alpha\beta\delta\gamma}$$

Isotropic system $\quad K_{\alpha\beta\gamma\delta} = \lambda\delta_{\alpha\beta}\delta_{\gamma\delta} + \mu(\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\delta})$

$$f = f(\underset{\sim}{\Lambda}) = f(\underset{\sim}{U}\underset{\sim}{\Lambda}\underset{\sim}{V}^{-1})$$

$$f = f(\underset{\sim}{u}) = f(\underset{\sim}{V}\underset{\sim}{u}\underset{\sim}{V}^{-1})$$

$$= \tfrac{1}{2}\lambda u_{\alpha\alpha}^2 + \mu u_{\alpha\beta}u_{\alpha\beta} - C\,\mathrm{Tr}(\underset{\sim}{u}^{st})^3 + D\,\mathrm{Tr}(\underset{\sim}{u}^{st})^4$$

$$= \tfrac{1}{2}B(\mathrm{Tr}\underset{\sim}{u})^2 + \mu\,\mathrm{Tr}(\underset{\sim}{u}^{st})^2$$

U and V symmetry operations: invariance

$$\mathbf{R}(\mathbf{x}) \rightarrow \underline{U}\mathbf{R}(\underline{V^{-1}}\mathbf{x})$$

μ = shear modulus; B =λ+2μ/D= bulk modulus

Isotropic: free energy density f has two harmonic elastic constants

Uniaxial Solid

Uniaxial ($\mathbf{n}$ = unit vector along uniaxial direction)

$$K_{\alpha\beta\gamma\delta} = C_1 n_\alpha n_\beta n_\gamma n_\delta + C_2 (n_\alpha n_\beta \delta^T_{\gamma\delta} + n_{\gamma\delta} n_\beta \delta^T_{\alpha\beta}) + C_3 \delta^T_{\alpha\beta}\delta^T_{\gamma\delta} + 2C_4 (\delta^T_{\alpha\gamma}\delta^T_{\beta\delta} + \delta^T_{\alpha\delta}\delta^T_{\beta\gamma}) + + C_5 (n_\alpha n_\gamma \delta^T_{\beta\delta} + n_\alpha n_\delta \delta^T_{\beta\gamma} + n_\beta n_\delta \delta^T_{\alpha\gamma} + n_\beta n_\gamma \delta^T_{\alpha\delta})$$

Uniaxial: five harmonic elastic constants

$$f = \tfrac{1}{2} C_1 u_{zz}^2 + C_2 u_{zz} u_{\nu\nu} + \tfrac{1}{2} C_3 u_{\nu\nu}^2 + 2C_4 u_{\nu\tau}^2 + 2C_5 u_{\nu z}^2;$$

$$\mathbf{x}_\alpha = (\mathbf{x}_\nu, x_z)$$

Invariant under

$$\mathbf{R}(\mathbf{x}) \;\rightarrow\; \underset{\sim}{\mathrm{U}}\mathbf{R}(\underset{\sim}{\mathrm{V}}_{\mathrm{uni}}^{-1}\mathbf{x})$$

Summation convention on repeated ν and τ understood.

Voigt Notation

Because the strain matrix is symmetric, it has only D(D+1)/2 independent components:

$$2D : \underset{\sim}{u} = (u_{xx}, u_{yy}, u_{xy});$$

$$3D : \underset{\sim}{u} = (u_{xx}, u_{yy}, u_{zz}, u_{xy}, u_{xz}, u_{yz})$$

The elastic energy can then be written in matrix form

$$f = \frac{1}{2} \underset{\sim}{u}^T \underset{\sim}{K} \underset{\sim}{u}$$

$$\underset{\sim}{K} = \begin{pmatrix} K_{xxxx} & K_{xxyy} & 2K_{xxxy} \\ K_{xxyy} & K_{yyyy} & 2K_{yyxy} \\ 2K_{xxyy} & 2K_{yyxy} & 4K_{xyxy} \end{pmatrix}$$

$\underset{\sim}{K}$ must be positive definite for mechanical stability: 3 positive eigenvalues in 2D and 6 in 3D.

Force and stress I: Lagrangian Picture

$$f_i^L = \partial_\alpha \sigma^I_{i\alpha} \qquad F_i = \int d^d x f_i^L = \text{force}$$

f_i^L : internal "Lagrangian" force density in reference space– vector in target space.

The stress tensor $\sigma^I{}_{i\alpha}$ is mixed. This is the engineering or 1st Piola-Kirchhoff stress tensor = force per area of reference space. It is not necessarily symmetric!

$$\begin{aligned}\delta \mathcal{F}^{\text{int}} &= -\int_\infty d^D x f_i^L \delta u_i \\ &= -\int_\infty d^D x \delta u_i \partial_\alpha \sigma^I_{i\alpha} \\ &= -\int_{\partial \mathcal{D}_\infty} dS_\alpha \sigma^I_{i\alpha} \delta u_i + \int_{\mathcal{D}} d^D x \sigma^I_{i\alpha} \partial_\alpha \delta u_i \\ &= \int_{\mathcal{D}} d^D x \sigma^I_{i\alpha} \partial_\alpha \delta u_i = \delta \mathcal{F}\end{aligned}$$

The first integral is over all space because f_i^L is zero outside matter, the surface integral is zero because the stress outside matter. $\mathcal{D}$ is the volume of the sample

Force and Stress II

$$-\frac{\delta \mathcal{F}}{\delta u_i(\mathbf{x})} = -\int d^D x' \frac{\partial f}{\partial u_{\alpha\beta}(\mathbf{x}')} \frac{\delta u_{\alpha\beta}(\mathbf{x}')}{\delta u_i(\mathbf{x})} = f_i^L = \partial_\alpha \sigma_{i\alpha}^I$$

$$\frac{\delta u_{\alpha\beta}(\mathbf{x}')}{\delta u_i(\mathbf{x})} = \tfrac{1}{2}(\Lambda_{i\alpha}\partial'_\beta + \Lambda_{i\beta}\partial'_\alpha)\delta(\mathbf{x}-\mathbf{x}')$$

$$-\frac{\delta \mathcal{F}}{\delta u_i(\mathbf{x})} = -\int d^D x' \frac{\partial f}{\partial u_{\alpha\beta}(\mathbf{x}')} \Lambda_{i\alpha}\partial'_\beta \delta(\mathbf{x}-\mathbf{x}') = f_i^L = \partial_\alpha \sigma_{i\alpha}^I$$

$$\sigma_{i\alpha}^I = \frac{\partial f}{\partial \Lambda_{i\alpha}} = \Lambda_{i\beta}\frac{\partial f}{\partial u_{\beta\alpha}} \equiv \Lambda_{i\beta}\sigma_{\beta\alpha}^{II}$$

Note: In a linearized theory, $\sigma^I{}_{i\alpha} = \sigma_{i\alpha}{}^{II}$

$\sigma_{\alpha\beta}{}^{II}$ is the second Piola-Kirchhoff stress tensor - symmetric

$$\delta\mathcal{F} = \int d^D x\, \sigma_{i\alpha}^I \partial_\alpha \delta u_i = \int d^D x\, \sigma_{\alpha\beta}^{II}\Lambda_{i\beta}\delta\Lambda_{i\alpha} = \int d^D x\, \sigma_{\alpha\beta}^{II}\delta u_{\alpha\beta}$$

Cauchy stress

The Cauchy stress is the familiar force per unit area in the target space. It is a symmetric tensor in the target space.

$$\int d^D x\, \sigma^I_{i\alpha}\, \partial_\alpha \delta u_i = \int d^D R\, \sigma^C_{ij} \nabla_j \delta u_i$$

$$\nabla_i \equiv \frac{\partial}{\partial R_i}$$

$$= \int d^D R\, \sigma^C_{ij} (\nabla_j \delta u_i + \nabla_i \delta u_j)$$

$$d^d R = \det \underset{\sim}{\Lambda}\, d^d x$$

$$\partial_\alpha = \frac{\partial}{\partial x_\alpha} = \frac{\partial R_i}{\partial x_\alpha} \frac{\partial}{\partial R_i} = \Lambda_{i\alpha} \nabla_i$$

$$\sigma^C_{ij} = \frac{1}{\det \underset{\sim}{\Lambda}} \sigma^I_{i\alpha} \Lambda^T_{\alpha j} = \frac{1}{\det \underset{\sim}{\Lambda}} \Lambda_{i\alpha} \sigma^{II}_{\alpha\beta} \Lambda^T_{\alpha j}$$

$$\underset{\sim}{\sigma}^C = \frac{1}{\det \underset{\sim}{\Lambda}} \underset{\sim}{\Lambda}\, \underset{\sim}{\sigma}^{II} \underset{\sim}{\Lambda}^T$$

Symmetric as required

Exercise: Show

$$\partial_j \sigma^C_{ij} \equiv f^C_i = f^L_i \,/\, \det \Lambda$$

Coupling to other fields

We are often interested in the coupling of target-space vectors like an electric field or the nematic director to elastic strain. How is this done? The strain tensor $u_{\alpha\beta}$ is a scalar in the target space, and it can only couple to target-space scalars, not vectors.

Answer lies in the polar decomposition theorem

$$\underset{\sim}{\Lambda} = \underset{\sim}{\Lambda}(\underset{\sim}{\Lambda}^T\underset{\sim}{\Lambda})^{-1/2}(\underset{\sim}{\Lambda}^T\underset{\sim}{\Lambda})^{1/2} \equiv \underset{\sim}{O}\underset{\sim}{g}^{1/2}$$

$$\underset{\sim}{\Lambda} = (\underset{\sim}{\Lambda}\underset{\sim}{\Lambda}^T)^{1/2}(\underset{\sim}{\Lambda}\underset{\sim}{\Lambda}^T)^{-1/2}\underset{\sim}{\Lambda} = \underset{\sim}{h}^{1/2}\underset{\sim}{O}$$

$$\underset{\sim}{g} = (\underset{\sim}{\delta} + 2\underset{\sim}{u}); \quad \underset{\sim}{O} = \underset{\sim}{\Lambda}\underset{\sim}{g}^{-1/2}$$

$$\underset{\sim}{O}\underset{\sim}{O}^T = \underset{\sim}{\Lambda}\underset{\frown}{\underset{\sim}{g}}^{-1/2}(\underset{\sim}{\Lambda}\underset{\sim}{g}^{-1/2})^T = \underset{\sim}{\Lambda}\underset{\sim}{g}^{-1/2}\underset{\sim}{g}^{-1/2}\underset{\sim}{\Lambda}^T = \underset{\sim}{\Lambda}(\underset{\sim}{\Lambda}^T\underset{\sim}{\Lambda})^{-1}\underset{\sim}{\Lambda}^T = \underset{\sim}{\delta}$$

$\underset{\sim}{g}$ is symmetric and depends on $\underset{\sim}{u}$ only.

$\underset{\sim}{O}$ is an orthogonal, unimodular rotation matrix

Exercise: Show $\underset{\sim}{\Lambda}(\underset{\sim}{\Lambda}^T\underset{\sim}{\Lambda})^{-1/2} = (\underset{\sim}{\Lambda}\underset{\sim}{\Lambda}^T)^{-1/2}\underset{\sim}{\Lambda}$

Target-reference conversion

The rotation matrix $\underset{\sim}{O}$ converts target-space

vectors E_i to reference-space vectors $\tilde{E}_a$ and vice-versa

$$E_i = O_{i\alpha}\tilde{E}_\alpha; \quad \tilde{E}_\alpha = O^T_{\alpha i} E_i$$

If $\underset{\sim}{\Lambda}$ is symmetric, $\mathrm{O}_{i\alpha} = \delta_{i\alpha}$.

$$\underset{\sim}{O} = \underset{\sim}{\Lambda}\,\underset{\sim}{g}^{-1/2} = (\underset{\sim}{\delta} + \underset{\sim}{\eta})[(\underset{\sim}{\delta} + \underset{\sim}{\eta}^T)(\underset{\sim}{\delta} + \underset{\sim}{\eta})]^{-1/2}$$

$$\approx \underset{\sim}{\delta} + \underset{\sim}{\eta} - \tfrac{1}{2}\underset{\sim}{\eta}^T - \tfrac{1}{2}\underset{\sim}{\eta} = \underset{\sim}{\delta} + \tfrac{1}{2}(\underset{\sim}{\eta} - \underset{\sim}{\eta}^T)$$

$$O_{i\alpha} \approx \delta_{i\alpha} + \tfrac{1}{2}(\partial_\alpha u_i - \partial_i u_\alpha) \approx \delta_{i\alpha} - \varepsilon_{i\alpha k}\Omega_k$$

To linear order in $\boldsymbol{u}$, $O_{i\alpha}$ has a term proportional to the antisymmetric part of the strain matrix.

Sample couplings

Coupling of electric field to strain

$$u_{\alpha\beta}\tilde{E}_{\alpha}\tilde{E}_{\beta} = E_{i}O_{i\alpha}u_{\alpha\beta}O^{T}_{\beta j}E_{j} \equiv v_{ij}E_{i}E_{j}$$

$$\underset{\sim}{O}\underset{\sim}{u}\underset{\sim}{O}^{T} = \tfrac{1}{2}\underset{\sim}{\Lambda}(\underset{\sim}{\Lambda}^{T}\underset{\sim}{\Lambda})^{-1/2}(\underset{\sim}{\Lambda}^{T}\underset{\sim}{\Lambda} - \underset{\sim}{\delta})(\underset{\sim}{\Lambda}^{T}\underset{\sim}{\Lambda})^{-1/2}\underset{\sim}{\Lambda}^{T}$$

$$= \tfrac{1}{2}(\underset{\sim}{\Lambda}\underset{\sim}{\Lambda}^{T} - \underset{\sim}{\delta}) = \underset{\sim}{v}$$

Free energy no longer depends on the strain $u_{\alpha\beta}$ only. The electric field defines a direction in the target space as it should

$$f^{T} = f(\underset{\sim}{u}) - gE_{i}E_{j}v_{ij}$$

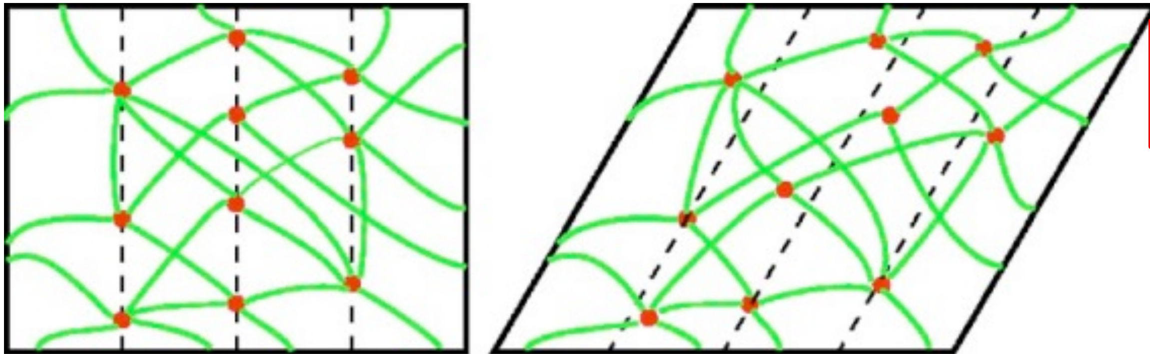
$$\Lambda_{i\alpha} = \frac{\partial R_{i}}{\partial x_{\alpha}} = \frac{\partial R_{i}}{\partial x'_{\beta}}\frac{\partial x'_{\beta}}{\partial x_{\alpha}} = \Lambda'_{i\beta}\Lambda_{0\beta\alpha}$$

Energy depends on both symmetric and anti-symmetric parts of η’

$$\Lambda'_{i\alpha} = \delta_{i\alpha} + \eta'_{i\alpha}$$

Nonaffine response

B. A. DiDonna and TCL, PRE **72** (6), 066619 (2005).



$$K_{ijkl}(\mathbf{x}) = K_{ijkl}$$
$$+ \delta K_{ijkl}(\mathbf{x})$$

$$\mathcal{H} = \int d^d x \left(\frac{1}{2} K_{ijkl}(\mathbf{x}) u_{ij}(\mathbf{x}) u_{kl}(\mathbf{x}) + \tilde{\sigma}_{ij}(\mathbf{x}) u_{ij}(\mathbf{x}) \right)$$

K_{ijkl} and σ_{ij} are random variables. Chose $\mathbf{u}$ so that the system is in equilibrium at $\mathbf{u}=0$. Thus the local force must be zero.

$$f_i(\mathbf{x}) = \partial_j \tilde{\sigma}_{ij}(\mathbf{x}) = \partial_j \tilde{\sigma}_{ji} = 0$$

$$\mathcal{H} = \frac{1}{2} \int d^d x [K_{ijkl}(\mathbf{x}) u_{ij}(\mathbf{x}) u_{kl}(\mathbf{x}) + \tilde{\sigma}_{ij}(\mathbf{x}) \partial_i u_k(\mathbf{x}) \partial_j u_k(\mathbf{x})]$$

Linear term in $\mathbf{u}$ does not survive.

Deviations from Affine Response

$$R_i(\mathbf{x}_B) = \Lambda_{ij} x_{Bj}$$

$\mathbf{x}_B$: boundary sites

$$R_i(\mathbf{x}) = \Lambda_{ij} x_j + u'_i(\mathbf{x})$$

$$u_i(\mathbf{x}) = \gamma_{ij} x_j + u'_i(\mathbf{x})$$

u': Nonaffine response

$$u_{ij}(\mathbf{x}) \approx \gamma^S_{ij} x_j + (\partial_i u'_j + \partial_j u'_i + \gamma_{ip}\partial_j u'_p + \gamma_{jp}\partial_i u'_p)/2$$

$$\delta\mathcal{H} = \frac{1}{2}\int \{K_{ijkl}\partial_j u'_i \partial_l u'_k + [\delta K_{ijkl}(\mathbf{x}) + \delta_{ik}\tilde{\sigma}_{jl}(\mathbf{x})]\partial_j u'_i \partial_l u'_k$$

$$+ 2\,\delta K_{ijkl}(\mathbf{x})\,\gamma_{kl}\partial_j u'_i\}$$

Response to Strain with Random K

$$u_i'(\mathbf{x}) = \int d^d x' \chi_{ip}(\mathbf{x}-\mathbf{x}')\partial_j' \delta K_{pjkl}(\mathbf{x}')\gamma_{kl}$$

$$\chi_{ik}^{-1}(\mathbf{x},\mathbf{x}') = -\partial_j K_{ijkl}^T(\mathbf{x})\partial_l \delta(\mathbf{x}-\mathbf{x}')$$

$$K_{ijkl}^T(\mathbf{x}) = K_{ijkl} + \delta K_{ijkl}(\mathbf{x}) + \delta_{ik}\tilde{\sigma}_{jl}$$

$$\chi_{ij}^0(\mathbf{q}) = \frac{1}{(\lambda+2\mu)q^2}\hat{q}_i\hat{q}_j + \frac{1}{\mu q^2}(\delta_{ij} - \hat{q}_i\hat{q}_j)$$

$$G_{ij}(\mathbf{x},\mathbf{x}') = \langle u_i'(\mathbf{x})u_j'(\mathbf{x}')\rangle$$

Nonaffine correlator: average over random modulus and internal stress

$$\propto \chi(q)q\left\langle \delta K \delta K \right\rangle q\chi(q) \propto \left\langle \delta K \delta K \right\rangle / (K^2 q^2)$$

Nonaffine Correlations

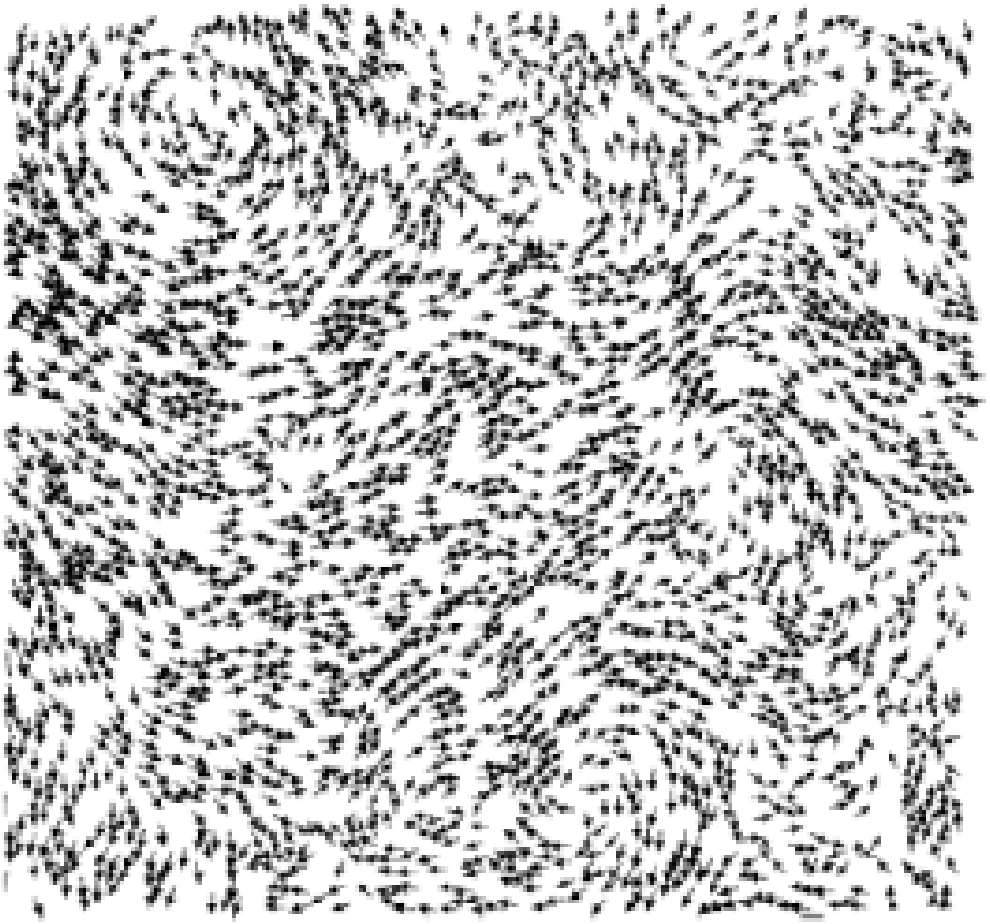
$$G(\mathbf{q}) \equiv G_{ii}(\mathbf{q}) \sim \frac{\gamma^2}{q^2}\Delta^S(\mathbf{q}) \sim \frac{\gamma^2}{q^2}\frac{\Delta^K(\mathbf{q})}{K^2}$$

$$G(\mathbf{q}) = \frac{\gamma_{xy}^2}{\mu^2 q^2}(\Delta_A + \Delta_B \hat{q}_\perp^2 - \Delta_C \hat{q}_x^2 \hat{q}_y^2)$$

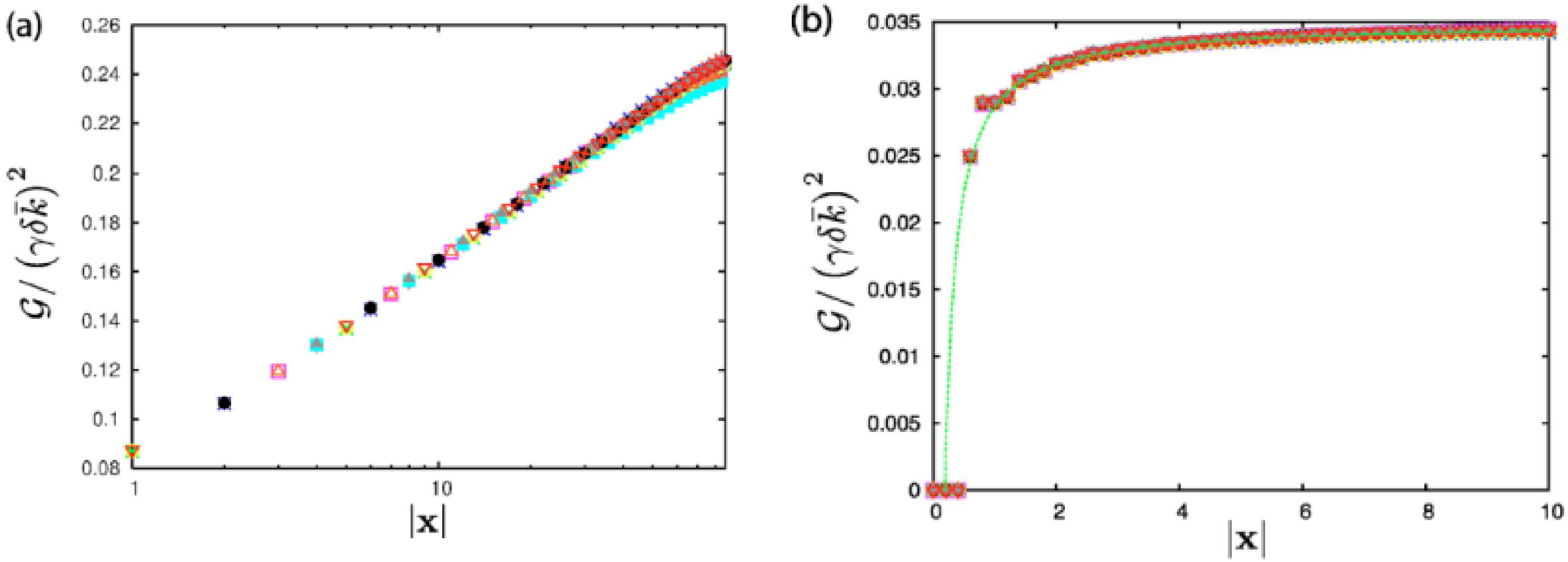
$$\begin{aligned} \mathcal{G}(\mathbf{x}) &= \langle (\mathbf{u}'(\mathbf{x}) - \mathbf{u}'(0))^2 \rangle \\ &\sim A \ln(|\mathbf{x}|/B) \qquad d = 2 \\ &\sim C - D|\mathbf{x}|^{-1} \qquad d = 3 \end{aligned}$$

$$\mathcal{G}_\theta(\mathbf{x}) = \epsilon_{ij}\epsilon_{kl}\frac{x_i x_j}{|\mathbf{x}|^4}\mathcal{G}_{kl}(\mathbf{x}) \sim \frac{1}{|\mathbf{x}|^2}\mathcal{G}(\mathbf{x})$$

Map of Nonaffine Displacement Directions



Numerical Calculations of G



"Relaxed" Elastic Moduli

$$Z = \int \mathfrak{D}u(x)\exp\left[-\frac{1}{T}\int d^D x\Big(K\,\partial u\,\partial u + \delta K(\mathbf{x})K\,\partial u\,\partial u\Big)\right]$$

$$K^{\text{ren}} = K - T\int d^D x\Big\langle\big(\delta K(\mathbf{x})\,/\,T\big)^2\Big\rangle T\,\partial\partial'\chi(\mathbf{x},\mathbf{x}')\big|_{\mathbf{x}=\mathbf{x}'}$$
$$= K - \int_{\mathbf{q}}\big\langle\delta K(\mathbf{q})\delta K(-\mathbf{q})\big\rangle q^2\chi(\mathbf{q})$$

Elastic moduli are reduced by nonaffine relaxation

Example: Incompressible Rubber

$$P(R)=\sqrt{\frac{3}{2\pi Nb^2}}\,\exp\left[-\frac{3R^2}{2Nb^2}\right]$$

Probability distribution of a random walk of N steps of length b.

$$V(R)=-T\ln P(R)=\frac{3}{2}T\,\frac{R^2}{Nb^2}$$

Purely entropic force

$$f=n_b\left\langle V(\underset{\sim}{\Lambda}\mathbf{R})\right\rangle_R=\frac{3}{2}\frac{T}{Nb^2}\left\langle \mathbf{R}_0\underset{\sim}{\Lambda}^T\underset{\sim}{\Lambda}\mathbf{R}_0\right\rangle_{R_0}$$

$$\left\langle R_{0i}R_{0j}\right\rangle=\frac{1}{3}\delta_{ij}Nb^2$$

Average is over the end-to-end separation in a random walk: random direction, Gaussian magnitude

$$\mathrm{f}=\tfrac{1}{2}n_bT\ \mathrm{Tr}\underset{\sim}{\Lambda}^T\underset{\sim}{\Lambda}=\tfrac{1}{2}n_bT\ \mathrm{Tr}(\underset{\sim}{\delta}+2\underset{\sim}{u})$$

Rubber : Incompressible Stretch

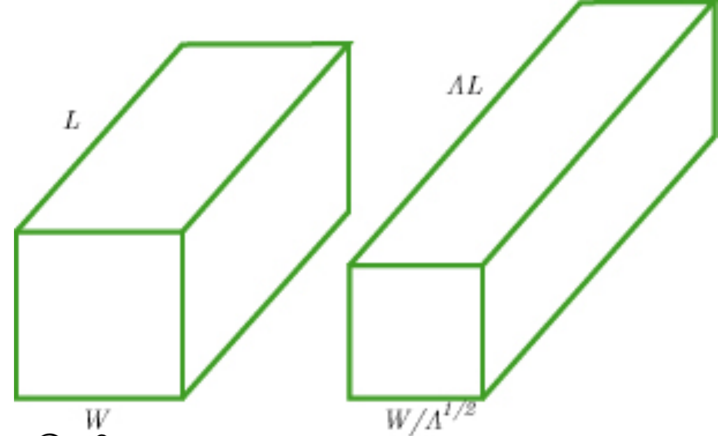
$$\Box f = \frac{1}{2} T n_b \mathrm{Tr} \underset{\sim}{\Lambda}^T \underset{\sim}{\Lambda} = \frac{1}{2} T n_b \mathrm{Tr}(1 + 2\underset{\sim}{u})$$

Unstable: nonentropic forces between atoms needed to stabilize; Simply impose incompressibility constraint.

$$\mathbf{\Lambda} = \begin{pmatrix} \Lambda^{-1/2} & 0 & 0 \\ 0 & \Lambda^{-1/2} & 0 \\ 0 & 0 & \Lambda \end{pmatrix}$$

$$\Box f == \frac{1}{2} n_b T \left(\Lambda^2 + \frac{2}{\Lambda} \right)$$

Rubber: stress -strain



$$F_z = \frac{\partial}{\partial L}\left(V\Box f\right) = \frac{\partial(A_R L_R \Box f)}{\partial \Lambda L_R} = A_R\frac{\partial f}{\partial \Lambda}$$

A_R= area in reference space

Engineering stress

$$\sigma^I = \frac{F_z}{A_R} = \frac{\partial \Box f}{\partial \Lambda} = nT\left(\Lambda - \frac{1}{\Lambda^2}\right)$$

Physical Stress

$A = A_R/\Lambda$ = Area in target space

$$\sigma^C = \frac{F_z}{A} = \Lambda\frac{\partial f}{\partial \Lambda} = nT\left(\Lambda^2 - \frac{1}{\Lambda}\right)$$

Y=Young's modulus: $\Lambda = 1+\gamma$

$$Y = \frac{\sigma^C}{\gamma} = \frac{nT}{\gamma}\left((1+\gamma)^2 - \frac{1}{1+\gamma}\right) \sim 3nT$$

Rubber elasticity: Neo-Hookean Model

$$\Box f = \tfrac{1}{2} T n_b \mathrm{Tr}\,\underset{\sim}{g} + \tfrac{1}{2} B (J-1)^2$$

$$= \tfrac{D}{2} T n_b + T n_b \mathrm{Tr}\,\underset{\sim}{u} + \tfrac{1}{2} B (\mathrm{Tr}\,\underset{\sim}{u})^2$$

$$J = \det \underset{\sim}{\Lambda} = (\det \underset{\sim}{g})^{1/2}$$

Add nonlinear compression energy to rubber entropic part: linear term: compression of crosslinked system

Neo-Hookean model: No linear term: most common of many semi-empirical theories for nonlinear elasticity in the engineering literature. Note isotropy in the reference space means g can be replace by h anywhere.

$$\Box f = \frac{1}{2}\mu\left(\frac{\mathrm{Tr}\,\underset{\sim}{g}}{J^{2/3}} - 3\right) + \lambda (J-1)^2$$

$$\rightarrow \mu \mathrm{Tr}\,\underset{\sim}{u}^2 + \tfrac{1}{2}\lambda\left(\mathrm{Tr}\,\underset{\sim}{u}\right)^2$$