Mesoscopic and macroscopic description of material damage and magnetization

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Overview

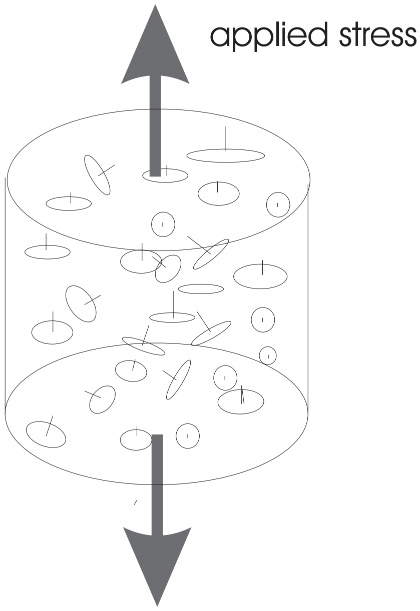
1. Complex materials and mesoscopic theory

2. Application to material damage

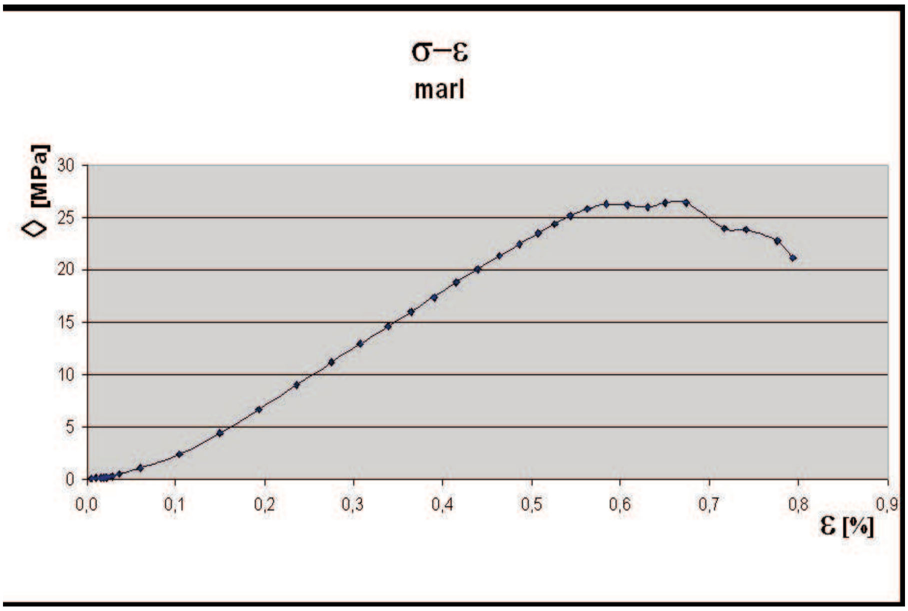
3. Application to ferrofluids

Definition of internal variables from the mesoscopic background and equations of motion for them
Different possibilites to define internal variables from mesoscopic theory
$\rightarrow$ Questions:
relevant variables?
Equation of motion?

Material damage in brittle materials



Deviation from ideal-elastic behavior, reduction of material strength



Hysteresis in cyclic loading experiments

Ferrofluids

- Viscose liquid,
  Non-Newtonian flow behavior

- Anisotropic properties, f.i. anisotropic viscosity

- properties can be influenced by an applied magnetic field

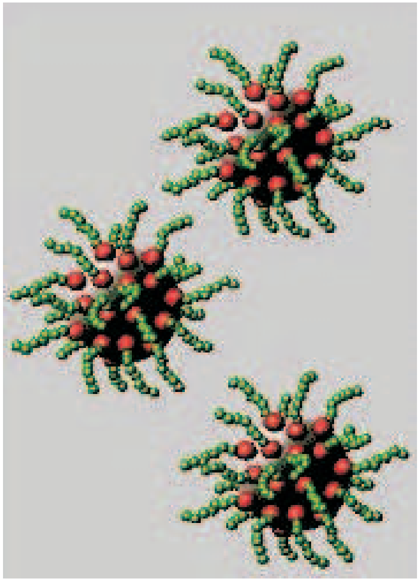
Common feature of these materials?

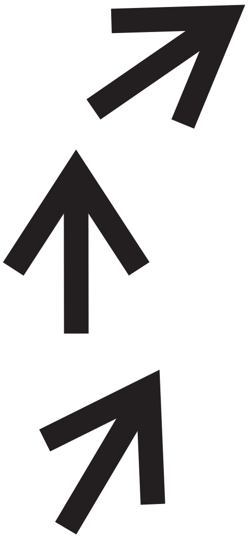
Complex internal structure which can change under external influence
$\rightarrow$ complex material behavior

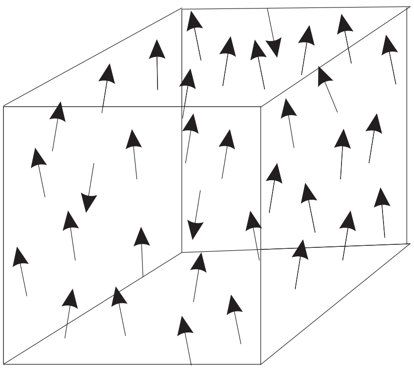
Internal structure of ferrofluids

Suspension of magnetic nano-particles

Orientational order of magnetic moments of particles → magnetization







microscopic
dipoles in a
volume element

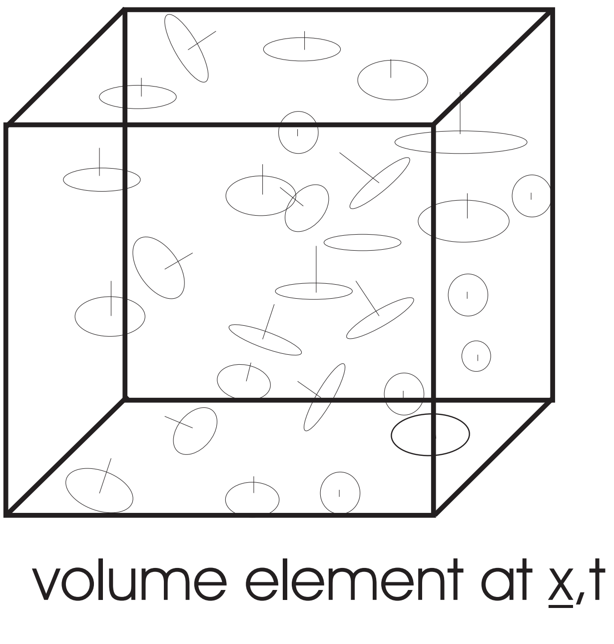
- reorientation in flow field + formation of chains $\rightarrow$ Non-Newtonian flow behavior

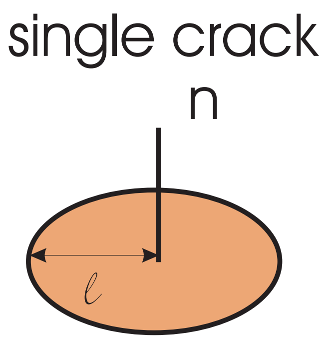
- interaction of particles with external magnetic field $\rightarrow$ influence on viscosity

Internal structure of damaged brittle material

Microcracks in a volume element

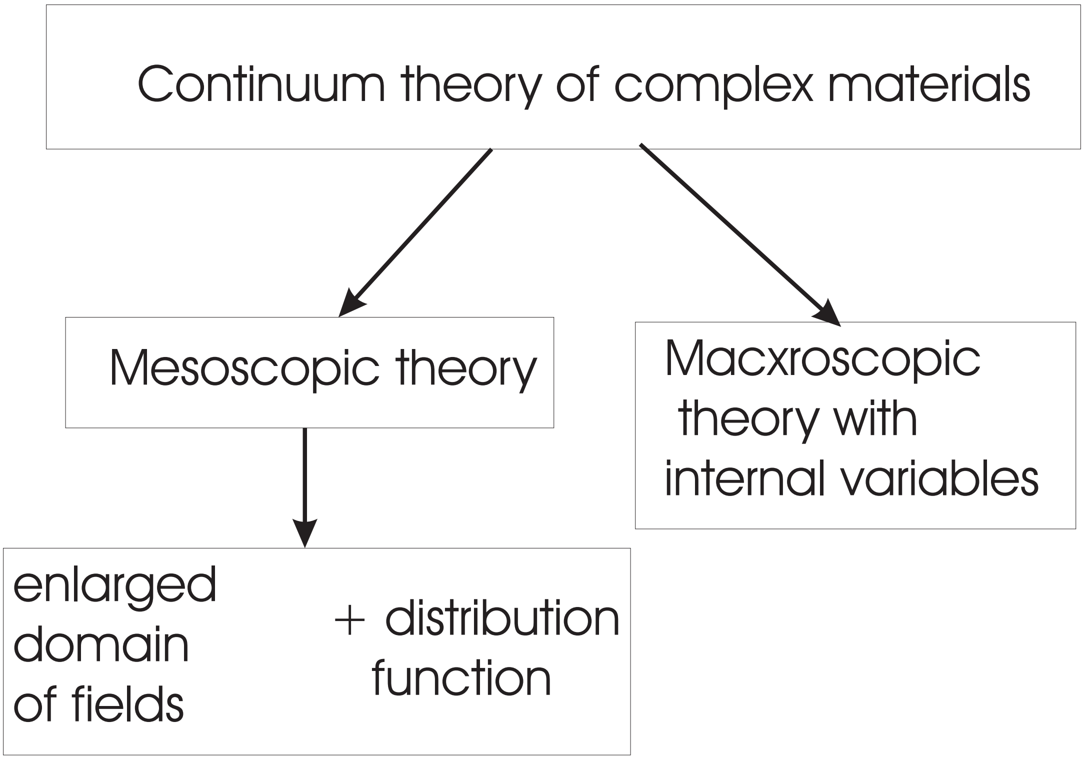
Model: Penny shaped cracks
completely described by the orientation of the surface and the diameter





cracks of different size and orientation

Mesoscopic concept



$\mathcal{M}$: set of additional mesoscopic variables

$(\cdot) := (\boldsymbol{x}, t, m) \in \mathbb{R}^3_x \times \mathbb{R}_t \times \mathcal{M}$ mesoscopic space

$\varrho(\cdot)$, $\boldsymbol{v}(\cdot)$, $e(\cdot)$, ...: mesoscopic fields

Mesoscopic balance equations

$$\underbrace{\frac{\partial}{\partial t} X(\cdot)}_{\text{change in time}}$$

$$+ \underbrace{\nabla_x \cdot (\boldsymbol{v}(\cdot)\boldsymbol{X}(\cdot) - \boldsymbol{S}(\cdot))}_{\text{flux over boundary in position space}}$$

$$+ \underbrace{\nabla_m \cdot [\boldsymbol{u}(\cdot)\boldsymbol{X}(\cdot) - \boldsymbol{R}(\cdot)]}_{\text{flux over boundary in } \mathcal{M}}$$

$$= \underbrace{\boldsymbol{\Sigma}(\cdot)}_{\text{production and supply}}$$

$\boldsymbol{u}$: mesoscopic change velocity

$$(\boldsymbol{x}, t, m) \rightarrow_{\Delta t \rightarrow 0} (\boldsymbol{x} + \boldsymbol{v}\Delta t, t + \Delta t, m + \boldsymbol{u}\Delta t)$$

Mesoscopic variable in the examples

Material	internal structure	$\mathcal{M}$
Liquid crystals of rotation symmetric particles	orientation of particle = microscopic director	S^2
Ferrofluids	orientation of magnetic moments	S^2
Material damage	orientation of and diameter of cracks	$S^2 \times [0, \infty]$

Distribution function

Definition:

$$f(\cdot) = \frac{\varrho(\cdot)}{\int_{\mathcal{M}} \varrho(\cdot) dm}$$

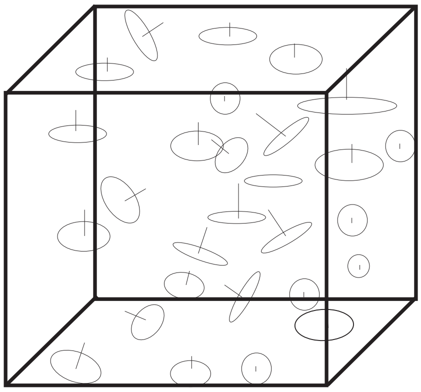
Fraction of particles with the value m of the mesoscopic variable

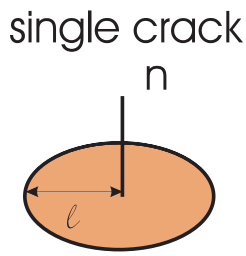
Macroscopic quantities = averages, f.e.

$$A(\boldsymbol{x}, t) = \int_{\mathcal{M}} A(\cdot) \underbrace{f(\cdot)}_{\text{Probability density}} dm$$

Application to material damage

Assumption: relevant process is the growth of microcracks





1. Penny shaped crack: flat, rotation symmetric surface

2. Much smaller than the linear dimension of the continuum element $\rightarrow$ a whole distribution of crack sizes and orientations in the volume element.

3. The cracks are fixed to the material, their motion is coupled to the motion of the volume element and cracks cannot rotate independently of the material.

4. The number of cracks is fixed, no production of cracks.

5. The cracks cannot decrease area, but can only enlarge, meaning that cracks cannot heal. A special growth law for a single crack under external load will be assumed.

variables in the mesoscopic theory: $(l, \boldsymbol{n}, \boldsymbol{x}, t)$

f.i. $N(l, \boldsymbol{n}, \boldsymbol{x}, t)$: number density of cracks of length l and orientation $\boldsymbol{n}$.
$\rightarrow$ mesoscopic crack number balance

$$\frac{\partial}{\partial t} N(\cdot) \; + \; \nabla_x \cdot \{N(\cdot)\boldsymbol{v}(\boldsymbol{x}, t)\}$$
$$+\nabla_n \cdot \{N(\cdot)\boldsymbol{u}(\boldsymbol{x}, t)\} + \frac{1}{l^2}\frac{\partial}{\partial l}\left(l^2 \dot{l} N(\cdot)\right) \; = \; 0$$

Definition of the distribution function

$$f(l, \boldsymbol{n}, \boldsymbol{x}, t) = \frac{N(l, \boldsymbol{n}, \boldsymbol{x}, t)}{N(\boldsymbol{x}, t)}$$

Mesoscopic balance of crack number

⇒ Differential equation for the distribution function

Cracks rotate with the volume element
⇒ orientation distribution rotates with the element
⇒ dynamics of size distribution is the most interesting:

$$f(l, \boldsymbol{x}, t) = \int_{S^2} f(l, \boldsymbol{n}, \boldsymbol{x}, t) d^2 n$$

$$\boxed{\frac{df(l, \boldsymbol{x}, t)}{dt} + \frac{1}{l^2} \frac{\partial}{\partial l} \left(l^2 \dot{l} f(l, \boldsymbol{x}, t) \right) = 0}$$

Crack growth velocity $\dot{l}$ as a function of crack size l and tension is needed.

Model: Rice-Griffith-dynamics for a single crack

1. Cracks can grow under tension, but not heal

2. Only tension applied normal to the crack surface leads to growth:
   relevant component for 1 crack:
   $\boldsymbol{n} \cdot \boldsymbol{t} \cdot \boldsymbol{n}$
   average over all orientations:
   $\sigma_{eff} = \boldsymbol{t} : \int_{S^2} \boldsymbol{n}\boldsymbol{n} f(l, \boldsymbol{n}, \boldsymbol{x}, t) d^2 n$
   Influence of orientational order

3. Only cracks exceeding the critical size are growing:

$$l_c = \frac{K}{\sigma^2_{eff}}$$

with constitutive constant K: Griffith-condition

4. Growth velocity

$$\dot{l} = -\alpha' + \beta' l \sigma^2_{eff} \quad \text{für} \quad l > l_c$$

in analogy to the growth law by
Rice for macroscopic cracks

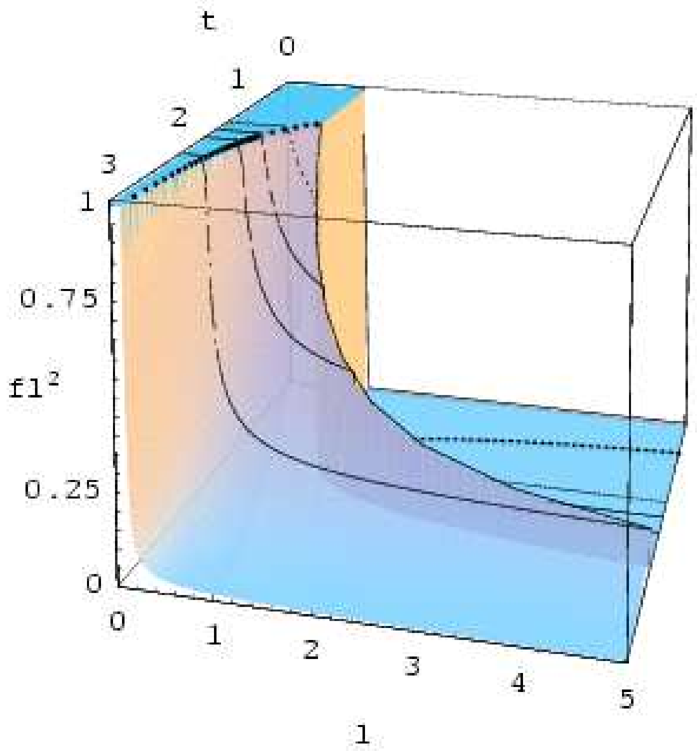
⇒ Closed differential equation for the length distribution $f(l, \boldsymbol{x}, t)$

Solutions for the length distribution

tension growing linearly with time: $\sigma_{eff} = v_\sigma t$

Stepwise initial condition

$$f(l,0) = \begin{cases} \frac{l^{-2}}{l_f} & \text{if} \quad l < l_f \\ 0 & \text{else.} \end{cases}$$



Time evolution for the length distribution

Definition of a scalar damage parameter D

Macroscopic quantity containing information on the crack growth: Average crack length

$$D(t) = < l > = \int_0^\infty l f(l,t) l^2 \mathrm{d}l = \int_0^\infty l^3 f(l,t) \mathrm{d}l$$

- Can be calculated from the solution for the distribution function
- or as a solution of a macroscopic differential equation for D:

$$\dot{D}(t) = -\alpha' + \beta' \sigma_{eff}^2 D(t)$$
$$+ \int_0^{\frac{\alpha'}{\beta' \sigma_{eff}^2}} l^2 \left(\alpha' - \beta' \sigma_{eff}^2 l \right) f(l, t = 0) dl$$

Remarks:

- Dynamics of the damage parameter depends explicitly on the initial length distribution .

- Only the initial distribution is needed, it need not to be calculated $f(l, \boldsymbol{x}, t)$ at later times.

- Stress-strain relation can be obtained with the model

Definition of a tensorial damage parameter $\boldsymbol{D}$

Accounts for the orientational order

$$\boldsymbol{D}(t) = < l\boldsymbol{n}\boldsymbol{n} > = \int_0^\infty \int_{S^2} l\boldsymbol{n}\boldsymbol{n} f(l,t) l^2 \mathrm{d}l d^2 n$$

Dynamics: growth of $D = < l >$
+ rigid rotation of orientations

Definition of other scalar damage parameters

$$\tilde{D}(t) = < l^2 > = \int_0^\infty l^2 f(l,t) l^2 \mathrm{d}l$$

...

$$\hat{D}(t) = < l^k > = \int_0^\infty l^k f(l,t) l^2 \mathrm{d}l$$

Questions:

1. Equations of motion? Derived from differential equation for the distribution function
2. Relevance in constitutive theory?
3. Infinite number of moments, eliminate higher order ones later? $\rightarrow$ higher order differential equations

Summary of the damage model

- Crack sizes and orientations are the additional variables in the mesoscopic theory

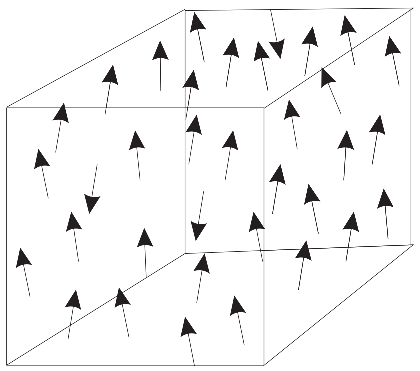
- Growth model for the single crack $\rightarrow$ differential equations for the length distribution and the damage parameter

- Definition of the damage parameter in terms of the size or size + orientation distribution.

- Growth of the damage parameter $\rightarrow$ non-linear stress-strain relation and hysteresis under cyclic load.

- Different possibilities to define damage parameters, or even include several ones.

Application to ferrofluids



microscopic
dipoles in a
volume element

Single particle with a magnetic moment
Orientational order of magnetic moments
$\Rightarrow$ macroscopic magnetization

Mesoscopic variable: $(\boldsymbol{x}, t, \boldsymbol{n})$,

$$\underbrace{\boldsymbol{n} \in S^2}_{\text{Orientation of particle moments}}$$

Orientation distribution function (ODF) = fraction of particles of orientation $\boldsymbol{n}$

$$f(\boldsymbol{n}, \boldsymbol{x}, t) = \frac{\varrho(\boldsymbol{n}, \boldsymbol{x}, t)}{\varrho(\boldsymbol{x}, t)}$$

- Analogy to mesoscopic theory of liquid crystals

- Difference: no head-tail-symmetry $\Rightarrow$ uneven moments of the distribution function

Magnetization

Magnetic moment of a particle: $\alpha \boldsymbol{n}$
average over all orientations $\Rightarrow$ Magnetization

$$\boldsymbol{M}(\boldsymbol{x}, t) = \alpha \int_{S^2} \boldsymbol{n} f(\boldsymbol{n}, \boldsymbol{x}, t) d^2 n$$

$\rightarrow$ 1st moment $\boldsymbol{a}^{(1)}$ of the ODF

Equation of motion for the distribution function

ODF:

$$f(\boldsymbol{n}, \boldsymbol{x}, t) = \frac{\varrho(\boldsymbol{n}, \boldsymbol{x}, t)}{\varrho(\boldsymbol{x}, t)}$$

differential equation for $\varrho(\boldsymbol{n}, \boldsymbol{x}, t)$: mesoscopic balance of mass
differential equation for $\varrho(\boldsymbol{x}, t)$: continuity equation

$\Downarrow$

differential equation for the ODF:

$$\frac{\partial f(\boldsymbol{x}, \boldsymbol{n}, t)}{\partial t} + \nabla \cdot (\boldsymbol{v}(\boldsymbol{x}, \boldsymbol{n}, t) f(\boldsymbol{x}, \boldsymbol{n}, t)) + \nabla_n \cdot (\boldsymbol{u}(\boldsymbol{x}, \boldsymbol{n}, t) f(\boldsymbol{x}, \boldsymbol{n}, t)) = 0$$

Orientation change velocity $\boldsymbol{u}$ of particles is needed

Solution of balance of spin $\Rightarrow \boldsymbol{u}$

(Angular velocity $\boldsymbol{\omega} = \boldsymbol{n} \times \boldsymbol{u}$ and $\boldsymbol{s} = \Theta \boldsymbol{\omega}$)

Example: Determination of angular velocity

Exploitation of the balance of spin
Assumption: the spin is stationary, $\frac{d\boldsymbol{s}}{dt} = 0$. $\Rightarrow$ Equation, determining the orientation change velocity $\boldsymbol{u}$ as a constitutive function

Constitutive assumption
set of variables = state space:

$$Z = \{ \underbrace{\varrho, T}_{\text{equilibrium variables}}, \underbrace{\boldsymbol{B}, \overline{\nabla \boldsymbol{v}}}_{\text{magnetic field and flow field}}, \underbrace{\boldsymbol{a}}_{\text{influence of the mean field of oriented particles}}, \underbrace{\boldsymbol{n}}_{\text{mesoscopic variable}} \}$$

Inserting into the differential equation for the ODF
$\Rightarrow$ equation for the ODF.
$\Rightarrow$ first moment of the equation + closure relation for the second moment

Differential equation of the magnetization

Here without $\nabla \boldsymbol{v}$:

$$\frac{d\boldsymbol{M}}{dt} = \beta_1 \alpha \varrho \boldsymbol{B} + \beta_2 \alpha \varrho \dot{\boldsymbol{B}} + \beta_4 \boldsymbol{M} - \beta_1 \frac{1}{\alpha \varrho} \boldsymbol{M}\boldsymbol{M} \cdot \boldsymbol{B} - \beta_2 \frac{1}{\alpha \varrho} \boldsymbol{M}\boldsymbol{M} \cdot \dot{\boldsymbol{B}} - \beta_4 \frac{1}{\alpha^2 \varrho^2} \boldsymbol{M}\boldsymbol{M} \cdot \boldsymbol{M}$$

with constitutive coefficients β_i.

Generalized Debye-equation

Linear limit:

$$\frac{d\boldsymbol{M}}{dt} = \beta_1 \alpha \varrho \boldsymbol{B} + \beta_2 \alpha \varrho \dot{\boldsymbol{B}} + \beta_4 \boldsymbol{M}$$

A second order differential equation for the magnetization

Consider first and second moment of the ODF:

$$\boldsymbol{M} \propto \boldsymbol{a}^{(1)} = \int_{S^2} \boldsymbol{n} f(\boldsymbol{n}, \boldsymbol{x}, t) d^2 n$$
$$\boldsymbol{a}^{(2)} = \int_{S^2} \boldsymbol{n}\boldsymbol{n} f(\boldsymbol{n}, \boldsymbol{x}, t) d^2 n$$

$$\dot{\boldsymbol{a}}^{(1)} = F\left(\boldsymbol{a}^{(1)}, \boldsymbol{B}, \dot{\boldsymbol{B}}, \boldsymbol{a}^{(2)}\right) \tag{1}$$

$$\dot{\boldsymbol{a}}^{(2)} = G\left(\boldsymbol{a}^{(1)}, \boldsymbol{B}, \dot{\boldsymbol{B}}, \boldsymbol{a}^{(2)}, \underbrace{\boldsymbol{a}^{(3)}}_{\text{closure relation}}\right)$$

$\frac{d}{dt}$ (1), assume symmetry $\boldsymbol{a}^{(1)} = S\boldsymbol{d}$, $\boldsymbol{a}^{(2)} = S^{(2)}\boldsymbol{d}\boldsymbol{d}$
eliminate $\boldsymbol{a}^{(2)} \Rightarrow$

$$\ddot{\boldsymbol{a}}^{(1)} = H\left(\boldsymbol{a}^{(1)}, \dot{\boldsymbol{a}}^{(1)}, \boldsymbol{B}, \dot{\boldsymbol{B}}, \ddot{\boldsymbol{B}}\right)$$

Differential equation of second order in time

Summary ferrofluids

- Set of variables and balance equations analogous to liquid crystals

- No head-tail-symmetry

- Magnetic interaction relevant

- Exploitation of balance equations $\Rightarrow$ differential equation for the magnetization: generalized Debye-equation

- Higher order moments relevant?
  Hierarchy of internal variables?

- Differential equation for the ODF of first order, but eliminating higher order moments can lead to second order differential equation for the magnetization

- Future work: include gradients in the state space (weakly nonlocal) $\Rightarrow$ partial differential equation for the magnetization

- Constitutive theory, f.i. anisotropic viscosity can be treated analogously to liquid crystals

Thank you very much for your attention!