

Moving martensitic phase boundaries: from micro to macro

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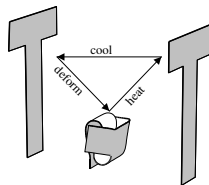


Work with Karsten Matthies, Hartmut Schwetlick, Daniel Sutton (Bath) and Michael Herrmann (Saarbrücken)

Background: Martensitic phase transitions

Weak phase transitions

One class of martensitic materials exhibits the *shape-memory effect*:



Microscopic picture

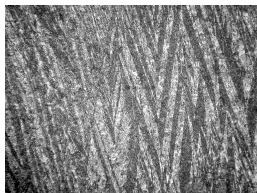


Figure: Needles and wedges in NiTi (weak transition)

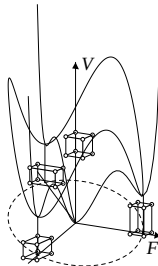


Figure: Potential energy Φ nonconvex (variants coexist)

Mathematical challenge: PDE models for martensites

Motivation (1D case only)

Landau theory: phase transitions modelled by a *nonconvex* potential Φ .

$\implies$ The *stress* $\sigma = \Phi'$ is non-monotone.

$\implies$ The equations of elasticity are of elliptic-hyperbolic type,

$$u_{tt} = (\sigma(u_x))_x. \quad (1)$$

Eq. (1) is ill-posed (generically infinitely many solutions).

Mathematical work since the '80s: viscous / capillary / hysteresis models (e.g., Andrews, Ball, Bonetti, Chen, Colli, Frémond, Gilardi, Hoffmann, Niezgódka, Pego, Rybka, Sprekels, Stefanelli, Visintin, Watson, ...).

Applied mechanics viewpoint

(1) is ill-posed since no law defines the *velocity of the interface*(s).

$\implies$ *Postulate* a *kinetic relation*, which relates the configurational force f and the velocity c : $f = f(c)$.

Can we derive a kinetic relation from “first principles” = atomistic model?

A brief on kinetic relations

Continuum setting of elasticity

Where the solution is smooth:

$$r_t = v_x \quad (r = u_x \text{ strain, } v = u_t \text{ velocity}) \quad (2)$$

$$\rho v_t = \hat{\sigma}(r)_x = \hat{\sigma}'(r)r_x \quad (\sigma = \Phi' = \text{stress}); \quad (3)$$

Rankine-Hugoniot conditions for nonsmooth solutions ($\dot{s} = c = \text{velocity}$ of the discontinuity, $x = \dot{s}t$, $\llbracket f \rrbracket = \lim_{h \rightarrow 0} f(x+h) - f(x-h) = \text{jump}$):

$$\llbracket r \rrbracket \dot{s} = - \llbracket v \rrbracket \quad (4)$$

$$\rho \llbracket v \rrbracket \dot{s} = - \llbracket \hat{\sigma} \rrbracket \quad (5)$$

Mechanical energy $E(t) = \int_{x_1}^{x_2} \left[\frac{\rho}{2} v(x, t)^2 + \Phi(r(x, t)) \right] dx$. Then

$$\underbrace{\sigma(x_2, t)Av(x_2, t) - \sigma(x_1, t)Av(x_1, t)}_{\text{rate of work of external forces}} - \underbrace{\dot{E}(t)}_{\text{rate of storage of mech. en.}} = f(t)A\dot{s}(t),$$

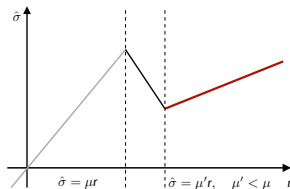
with *driving traction* $f(t) = \int_{r^-}^{r^+} \hat{\sigma}(r) dr - \frac{1}{2}[\hat{\sigma}(r^-) + \hat{\sigma}(r^+)](r^+ - r^-)$.

(Short: $f = \llbracket \Phi(r) \rrbracket - \{\Phi'(r)\} \llbracket r \rrbracket$). Thermodynamics: $f\dot{s} \geq 0$.

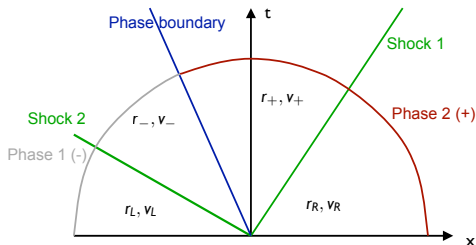
A brief on kinetic relations: sharp interface model

Abeyaratne, Knowles ARMA 1991

- ▶ trilinear stress-strain relation
- ▶ Riemann problem (data r_l, v_l, r_R, v_R).



- ▶ 7 unknowns:
 r_-, v_-, r_+, v_+ ,
 three velocities
 (shocks + phase
 boundary)
- ▶ 6 equations (3 · 2
 jump conditions)



Rankine-Hugoniot $\Rightarrow \rho \dot{s}^2 = \llbracket \hat{\sigma} \rrbracket / \llbracket r \rrbracket$; determines shock velocities, but *not* phase boundary velocity. Abeyaratne, Knowles, *Arch. Rational Mech. Anal.*, **114** (1991), 119–154): assume phenomenological *kinetic relation*: traction $f = \llbracket \Phi(r) \rrbracket - \{ \Phi'(r) \} \llbracket r \rrbracket \stackrel{!}{=} \hat{f}(\dot{s})$. Main question of this talk: *is such a kinetic relation derivable from microscopic model?*

An atomistic (nonlocal) model

The problem setting

Model (similar Fermi-Pasta-Ulam 1953)



Discrete model of elasticity: chain of particles coupled by elastic springs. The longitudinal motion of atom k is $u_k(t)$; the equations of motion are

$$\ddot{u}_k(t) = \Phi'(u_{k+1}(t) - u_k(t)) - \Phi'(u_k(t) - u_{k-1}(t)), \quad k \in \mathbb{Z}.$$

Nearest neighbour interaction: *elastic potential* $\Phi(u_{k+1}(t) - u_k(t))$.

Naïve continuum limit:

$$u_{tt} = (\sigma(u_x))_x = (\Phi'(u_x))_x$$

So

- ▶ Second order (inertial) dynamics
- ▶ Double-well potential Φ ,
- ▶ Potential depends on strain (= gradient),
- ▶ Lattice problem is nonlocal.

The problem setting

Model (similar Fermi-Pasta-Ulam 1953)



Equations of motion again:

$$\ddot{u}_k(t) = \Phi'(u_{k+1}(t) - u_k(t)) - \Phi'(u_k(t) - u_{k-1}(t)), \quad k \in \mathbb{Z}.$$

Travelling wave ansatz

We seek *travelling waves* $u_j(t) = u(j - ct)$ for $j \in \mathbb{Z}$ and $t \in \mathbb{R}$:

$$c^2 \ddot{u}(x) = \Phi'(u(x+1) - u(x)) - \Phi'(u(x) - u(x-1)). \quad (6)$$

For the *discrete strain* $r(x) := u(x+1/2) - u(x-1/2)$: discrete (nonlinear, nonlocal) wave equation

$$c^2 r''(x) = \Delta_1 \Phi'(r(x)) \quad (7)$$

with $\Delta_1 g(x) := g(x+1) - 2g(x) + g(x-1)$.

Supersonic speeds: existence of soliton solutions for FPU

Existence of soliton solutions, *convex* Φ and *supersonic* c

- ▶ *Constrained minimisation*: Friesecke, Wattis, *Comm. Math. Phys.*, **161** (1994), 391–418:
 $\frac{1}{2} \int_{\mathbb{R}} \dot{u}(t)^2 dt \stackrel{!}{=} \min$ with prescribed $K = \int_{\mathbb{R}} \Phi(u(t+1) - u(t)) dt$.
 $\Rightarrow c$ given by Lagrange multiplier associated with constraint.
Main assumption: $\left(\frac{\Phi(r)}{r^2}\right)' > 0$.
- ▶ *Centre manifold analysis*: Iooss, *Nonlinearity*, **13** (2000), 849–866.
- ▶ *Mountain pass methods*: Smets, Willem, *J. Funct. Anal.*, **149** (1997), 266–275; Arioli, Gazzola, *Nonlinear Anal.*, **26** (1996), 1103–1114.
Mountain pass argument, using convexity of energy. Monotone waves are found as saddle points of the action functional.
- ▶ *Nonlinear eigenvalue problem*: Filip, Venakides, *Comm. Pure Appl. Math.*, **52** (1999), 693–735

Heteroclinic supersonic solution, minimal action: Rademacher & Herrmann (2009); Herrmann (2010)

Special case: piecewise quadratic potential

Subsonic waves: existence of waves?

Mechanics literature

- ▶ Balk, Cherkaev, Slepian, *J. Mech. Phys. Solids*, **49** (2001), 131–148
- ▶ Slepian, Cherkaev, Cherkaev, *J. Mech. Phys. Solids*, **53** (2005), 407–436
- ▶ Truskinovsky, Vainchtein, *SIAM J. Appl. Math.*, **66** (2005), 533–553

Use piecewise bi-quadratic energy, equal depth wells and elastic modulus.

Reason: $\Phi(r) = \frac{1}{2} \min\{(r+1)^2, (r-1)^2\}$

$\Rightarrow$ equation for discrete strain,

$$c^2 r''(x) = \Delta_1 \Phi'(r(x))$$

becomes semilinear (H = Heaviside function),

$$c^2 r''(x) = \Delta_1 r(x) - 2\Delta_1 H(r(x)).$$

Further, *if* $r(x)$ and x have the same sign, the equation becomes inhomogeneous,

$$c^2 r''(x) = \Delta_1 r(x) - 2\Delta_1 H((x)).$$

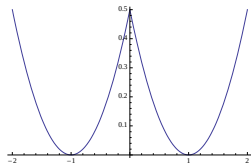


Figure: Special Φ

(Non-)existence results

Bounded travelling waves with one phase boundary

Results (Schwetlick & Z., *SIAM Math Anal.*, **41** (2009), 1231–1271; Schwetlick, Sutton, *Z. J Nonlin. Sci.*, '12))

- ▶ *Existence* of travelling waves for almost sonic waves,
- ▶ *Nonexistence* of travelling waves for some slow velocities.

Föster, Scheil, *Z. Metallkd.*, **32** (1940), 165–201: martensite trafs:

- ▶ fast (*umklapp*): velocity close to the speed of sound;
- ▶ slow (*schiebung*): observable under an optical microscope

Relevant part of the (technical) proofs

Assume there is only one interface at 0, then for distance ≥ 1 from interface spatially discrete wave equation. Split solution $r := r_{\text{pr}} - r_{\text{cor}}$ with explicit function r_{pr} so that *corrector* r_{cor} is solution of

$$(c^2 \partial^2 - \Delta_1)[r_{\text{cor}}](x) = \Phi(x) \in L^2(\mathbb{R}) \quad (8)$$

Fourier estimates to show that single interface assumption is (not) met.

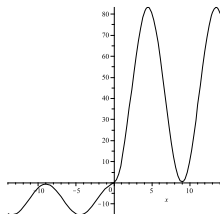
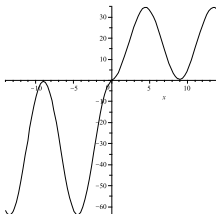
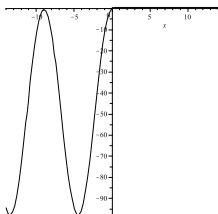
Macroscopic non-uniqueness

Solution family and selection criteria

Useful bit of argument: $L := c^2 \partial^2 - \Delta_1$;

- ▶ $Lr = -2\Delta_1 H(x)$ gives formally in Fourier space $F[r](\kappa) = F[-2H](\kappa)/D(\kappa)$;
- ▶ this is not invertible since $D(\kappa) = c^2 \kappa^2 - 4 \sin^2(\kappa/2)$ has real roots.
- ▶ But if $r = r_{\text{cor}} + r_{\text{pr}}$ then $F[r_{\text{cor}}](\kappa) = F[-2H](\kappa)/D(\kappa) - F[r_{\text{pr}}]$ which is invertible for “correct” r_{pr} (removable singularity).

Note that L has nontrivial kernel $\implies$ *three-parameter family of solutions* (Schwetlick & Z., *Arch. Rat. Mech. Anal.*, **206** (2012), 707–724).



Macroscopic non-uniqueness

Solution family and selection criteria

In mechanics / physics literature: only one solution. Selection principle based on Sommerfeld's selection criteria for Helmholtz equation with source at the origin,

The energy radiated from the sources has to scatter to infinity,
energy must not be radiating from infinity into the prescribed singularities of the field. (SOM1)

However, this criterion is applied in *travelling wave coordinates*, which are *not* related to an inertial frame by a Galilei transformation. An energy flux is missed (Herrmann, Schwetlick, Z., *Contin. Mech. Thermodyn.*, **1** (2012), 21–36).

Two consequences:

1. All solutions of the solution family have a thermodynamic meaning.
2. Another selection principle by Sommerfeld's can be extended,

Sources have to be *sources*, not sinks of the energy. (SOM2)

Potentials with spinodal region

Potentials with spinodal region

Perturbation setting

Now consider potentials with spinodal region (“elliptic-hyperbolic”):

$$\Phi_\delta(r) = \frac{1}{2}r^2 - \Psi_\delta(r), \quad \Psi_\delta(0) = 0,$$

where Ψ'_δ is a perturbation of $\Psi'_0 = \text{sgn}$ in a small neighbourhood of 0 (recall $\Phi_0 := \Phi = \frac{1}{2} \min\{(r+1)^2, (r-1)^2\}$, so $\Phi'_0 = r - \text{sgn}(r)$).

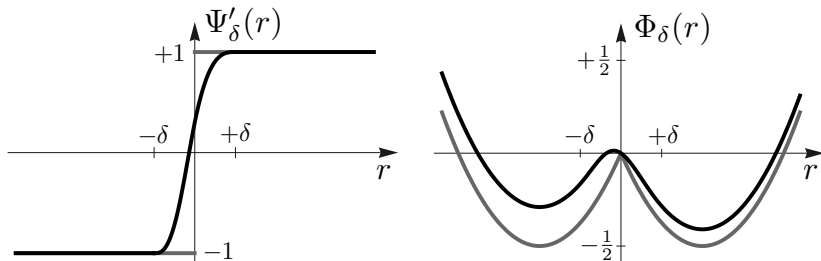


Figure: Sketch of Ψ'_δ and Φ_δ for $\delta = 0$ (grey) and $\delta > 0$ (black)

$\Psi'_\delta = \Psi'_0$ outside $(-\delta, \delta)$; $|\Psi'_\delta(r)| \leq C_\Psi$ and $|\Psi''_\delta(r)| \leq \frac{C_\Psi}{\delta}$ for all $r \in \mathbb{R}$.

Potentials with spinodal region

Existence result

Herrmann, Matthies, Schwetlick & Z., *SIAM J. Math Anal.*, to appear

Set $I_\delta := \frac{1}{2} \int_{\mathbb{R}} [\Psi'_\delta(r) - \Psi'_0(r)] \, dr$.

Let r_0 be a solution for degenerate potential (fast subsonic waves, family!)

Theorem

For all $c_1 \in (c_0, 1)$ there exists $\delta_0 > 0$ such that for any $0 < \delta < \delta_0$, any speed $c_0 < c < c_1$, and any given wave r_0 there exists a travelling wave solution r with

$$r = r_0 - I_\delta + s, \tag{9}$$

where the corrector $s \in W^{2,\infty}(\mathbb{R})$

1. *vanishes at $x = 0$,*
2. *is small in the sense of*

$$\|S\|_\infty = O(\delta^2), \quad \|S'\|_\infty = O(\delta), \quad \|S''\|_\infty = O(1).$$

3. *is non-oscillatory as $x \rightarrow +\infty$ (and oscillates in a well-understood way in the limit $x \rightarrow -\infty$).*

Moreover, for small δ there exists only one r with these properties.

Potentials with spinodal region

Sketch of the strain r

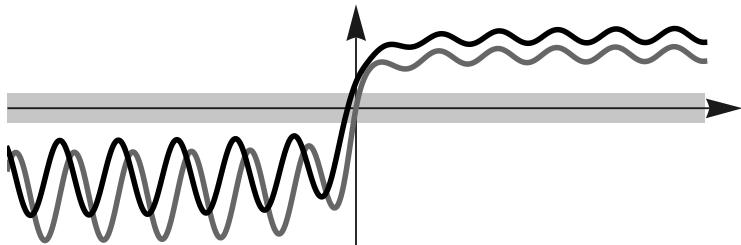


Figure: Sketch of the waves for $\delta = 0$ (grey) and $\delta > 0$ (black); the shaded region indicates the spinodal interval $(-\delta, +\delta)$.

Sketch of proof

Reformulation as integral equation

Let

$$(\mathcal{A}F)(x) := \int_{x-1/2}^{x+1/2} F(s) \, ds.$$

The travelling wave equation is

$$c^2 r'' = \Delta_1 r - \Delta_1 \Psi'_\delta(r); \quad (10)$$

two integrations yield the equation

$$\mathcal{M}r = \mathcal{A}^2 \Psi'_\delta(r) + \mu, \quad (11)$$

with $\mathcal{M} = \mathcal{A}^2 - c^2 \text{Id}$.

Lemma

A function $W \in W^{2,\infty}(\mathbb{R})$ solves the travelling wave equation (10) if and only if there exists a constant $\mu \in \mathbb{R}$ such that (r, μ) solves (11).

Approach to show the existence

Difficulties

- ▶ Problem can be interpreted as bifurcation phenomenon in presence of essential spectrum;
- ▶ no suitable Fredholm properties of the operator, usual Lyapunov-Schmidt reduction cannot be used because of presence of essential spectrum.

Key ideas

- ▶ “Regularise” linear part in Fourier space in form of a split, by identifying suitable oscillating functions;
- ▶ thus linear part becomes invertible on space of *localised* functions.
- ▶ Deal with nonlinearity by careful estimates to obtain sharp bounds.

Sketch of proof I

Perturbation setting (after normalisation to $l_\delta = 0$)

1. To solve $\mathcal{M}r = \mathcal{A}^2 \Psi'_\delta(r) + \mu$, make the anchor-corrector ansatz

$$r = r_0 + s, \quad \mu = \mu_0 + \eta,$$

and seek correctors (s, η) such that

$$\mathcal{M}s = \mathcal{A}^2 \mathcal{G}(s) + \eta, \quad (12)$$

with $\mathcal{G}(s)(x) = \Psi'_\delta(r_0(x) + s(x)) - \Psi'_0(r_0(x))$.

2. Study fine properties of $\mathcal{G}$.

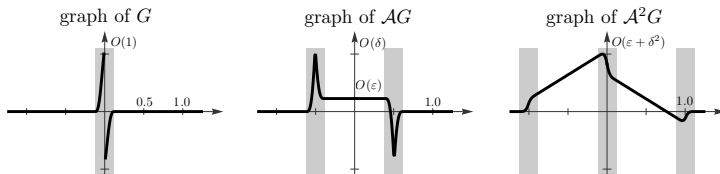


Figure: Properties of $G = \mathcal{G}(s)$ for δ -admissible s . The shaded regions indicate intervals with length of order $O(\delta)$.

Sketch of proof II

Perturbation setting

3. Fixed point argument. Let $X := \{s \in W^{2,\infty}(\mathbb{R}) \mid s(0) = 0\}$, and

$$X_\delta := \left\{ s \in X \mid \|S\|_\infty \leq C_0\delta^2, \quad \|S'\|_\infty \leq C_1\delta, \quad \|S''\|_\infty \leq C_2 \right\}.$$

Proposition

Self-mapping: For all sufficiently small δ there exists an operator $\mathcal{T}: X_\delta \rightarrow X_\delta$ such that for any $s \in X_\delta$

$$\mathcal{MT}(s) = \mathcal{A}^2\mathcal{G}(s) + \eta(s)$$

for some $\eta(S) \in \mathbb{R}$ with $|\eta(S)| \leq C_0\delta^2$.

Fixed point: For sufficiently small δ , the operator $\mathcal{T}$ has a unique fixed point in X_δ , so we have solved $\mathcal{M}s = \mathcal{A}^2\mathcal{G}(s) + \eta$ as desired.

Thermodynamic description

Thermodynamic framework to extend Sommerfeld's criteria

Microscopic conservation laws

Notation: $r_j := u_{j+1} - u_j$ discrete strain. Rewrite governing equations (velocity $v_j := \dot{u}_j$) as first order equations

$$\dot{r}_j = v_{j+1} - v_j, \quad \dot{v}_j = \Phi'(r_j) - \Phi'(r_{j-1}). \quad (13)$$

Hyperbolic scaling: define *macroscopic time* τ and the *macroscopic particle index* ξ (distances and velocities unscaled) by $\tau = ht$, $\xi = hj$.

Macroscopic conservation laws for mass, momentum & energy

Formal $h \rightarrow 0$ (Herrmann, Schwetlick, Z. '10) yields (cusp potential)

$$\partial_\tau R - \partial_\xi V = 0, \quad \partial_\tau V + \partial_\xi P = 0, \quad \partial_\tau E + \partial_\xi F = 0, \quad (14)$$

with *macroscopic strain* $R = \langle r \rangle$, *macroscopic velocity* $V = \langle v \rangle$, *pressure* $P = -\langle \Phi'(r) \rangle$, *energy density* $E = \langle \frac{1}{2} v^2 + \Phi(r) \rangle$, and *energy flux* $F = -\langle v \Phi'(r) \rangle$. Separate Galilean invariant part from E and F : with *internal energy density* U and *heat flux* Q ,

$$E = \frac{1}{2} V^2 + U, \quad F = VP + Q.$$

“Heat” in the chain

Oscillatory energy

Split the energy density E since weak limit (local mean values) and nonlinearities do not commute for oscillations. We write

$$E = E_{\text{non}} + E_{\text{osc}}, \quad E_{\text{non}} = \frac{1}{2} V^2 + \Phi(R),$$

$$\text{thus } E_{\text{osc}} = \frac{1}{2} \langle (v - \langle v \rangle)^2 \rangle + \langle \Phi(r) - \Phi(\langle r \rangle) \rangle.$$

Corresponding energy balances

Partial energies are balanced by

$$\partial_\tau E_{\text{osc}} + \partial_\xi Q = \Xi, \quad \partial_\tau E_{\text{non}} + \partial_\xi (PV) = -\Xi; \quad (15)$$

the *production* $\Xi = -(P + \Phi'(R))\partial_\xi V = \left(\langle \Phi'(r) \rangle - \Phi'(\langle r \rangle) \right) \partial_\xi \langle v \rangle$

describes transfer of non-oscillatory energy into oscillatory energy. Phase transition waves are driven by a constant transfer between the oscillatory and the non-oscillatory energy (Q , PV below exchange with exterior):

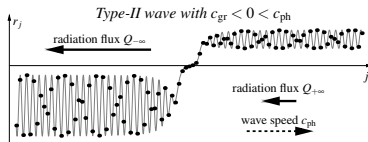
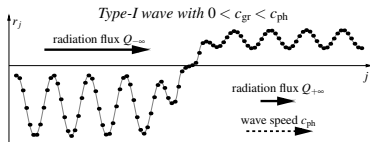
$$\frac{d}{d\tau} \int_a^b E_{\text{osc}} d\xi + Q|_{\xi=a}^{\xi=b} = \int_a^b \Xi d\xi = -\frac{d}{d\tau} \int_a^b E_{\text{non}} d\xi - (PV)|_{\xi=a}^{\xi=b}.$$

Insight I: Selection criteria, piecewise harmonic lattices

Reformulation of (SOM2)

The interface has to be a source rather than a sink of oscillatory energy. The production Ξ therefore has to be non-negative. So with **group speed** c_{gr} and **phase speed** c_{ph} , $\Xi = (c_{gr} - c_{ph}) \llbracket E_{osc} \rrbracket \geq 0$. This inequality is *equivalent* to the usual *entropy condition* for phase transition waves,

$$c_{ph} f \geq 0, \quad \text{with} \quad f := \llbracket \Phi(R) \rrbracket - \{\Phi'(R)\} \llbracket R \rrbracket \text{ kinetic relation.} \quad (16)$$



Validity of (SOM1) for moving inhomogeneity, used in physics

Provably violated for *every* (bounded single-interface) wave travelling with almost sonic speed satisfying the entropy inequality. We suggest to reject this criterion.

Back to the start: what is the kinetic relation?

Kinetic relation as a function of heat flux

Schwetlick & Z., *Arch. Rat. Mech. Anal.*, **206** (2012), 707–724; key suggestion by Kaushik Dayal).

We take a continuum mechanics expression for the kinetic relation,

$$f = \llbracket \Phi(\langle r \rangle) \rrbracket - \{ \Phi'(\langle r \rangle) \} \llbracket \langle r \rangle \rrbracket, \quad (17)$$

($\llbracket \cdot \rrbracket$ = jump, $\langle \cdot \rangle$ = average). One finds for $\Phi = \Phi_0 =$ cusp potential (α, κ_0 constants > 0)

$$f = -2 \frac{\kappa_0^2}{\alpha} \llbracket \langle \Phi(r) \rangle - \Phi(\langle r \rangle) \rrbracket. \quad (18)$$

A simple calculation shows: For spinodal potential Φ_δ , kinetic relation changes to order $O(\delta^2)$.

Back to the start: what is the kinetic relation?

Kinetic relation as a function of heat flux

Interpretation of kinetic relation for $\Phi = \Phi_0$,

$$f = -2 \frac{\kappa_0^2}{\alpha} \llbracket \langle \Phi(r) \rangle - \Phi(\langle r \rangle) \rrbracket. \quad (19)$$

- ▶ Microscopic oscillations “lost” in continuum limit lead to macroscopic dissipation $R = f \cdot c > 0$
- ▶ Thermodynamic limit suggests that there is a meaningful *thermomechanical macroscopic framework* for *mechanical microscopic model*: f depends (on speed c and) on the energy E_{osc} stored in oscillations, which can be related to a heat flux.

The end — thank you!