A general theory for elastic phase transitions in crystals

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Summary. We derive a general theory for elastic phase transitions in solids subject to diffusion under possibly large deformations. After stating the physical model, we derive an existence result for measure-valued solutions that relies on a new approximation result for cylinder functions in infinite settings.

1 Introduction

The general idea of the present work is to derive a satisfying mathematical theory of phase transitions in single-crystals where the elastic properties of the material are described by nonlinear laws, see [23], [14]. This generalises common existing models with linear stress-strain laws, starting with pioneering works by Khattchaturyan, [15], and makes the model applicable to a somewhat broader class of materials.

Beside prescribing the elastic behaviour of the material, the other fundamental assumption is that all occuring phase transitions are reconstitutive, i.e. that there are no plastic deformations of the crystal.

For the proof of existence of solutions to our new model, the experiences with the Stefan problem, [29] and [20], were found to be very valuable. But as it turns out, due to the nonlinear aspects of elasticity, a formulation within the framework of Sobolev functions is not general enough. This leads in a natural way to the formulation of the solution as Young measures presented in Section 4.1.

Historically, there is a variety of approaches to phase transitions in solids and it is not possible to give here a comprehensive overview. Instead, we refer the interested reader to the monographs and survey articles [29], [30], [21], [5], [28] and [11].

After these classifying comments we give now a general survey of this article.
We consider the elastic theory of single crystals at constant temperature where the free energy density depends on the local concentration of one or more species of particles in such a way that for a given local concentration vector certain lattice geometries (phases) are preferred.

The local concentration of the molecules may change due to diffusion. The time scales typical of diffusion and of elastic deformation are usually significantly different and in good approximation it is admissible to assume that the deformation adjusts infinitely fast to the local situation. In the developed model there is surface energy contributing to the free energy of the crystal and the model allows for m different coexisting macroscopic phases. We will assume that the crystal does not possess interstitials and that the time-evolution of the boundary of the domain is known.

After deriving the physical model with the above properties we will discuss the existence of solutions to this model by means of an implicit time discretisation and will show that in the limit of vanishing time step the time-discrete solutions converge in the sense of Young measures on suitable Banach spaces with separable dual. To achieve this goal, we will derive a general approximation result for cylinder functions in the infinite setting. Finally we can proof an energy inequality for the limit solution.

2 Model and implicit time discretisation

In this section we present our model. In the first subsection the mathematical equations are derived whereas the second subsection presents a reasonable solution strategy. This section is only heuristic and shall make the reader familiar with the general ideas. A deep mathematical treatment is done later.

2.1 Derivation of the model

To describe the physical phenomenon presented in the introduction, we make use of non-equilibrium thermodynamics, see [12], [18], and of continuum mechanics, see [13], [6]. We neglect the atomistic structure of the crystal and disregard possible effects of the microstructure. The model is based upon the following basic considerations: The diffusion is caused by the gradients of the chemical potentials. The diffusive flux causes a local change of the free energy of the crystal. The free energy shall depend on particle density, elasticity of the crystal and phase parameter only with a term representing the surface energy of the boundary layers.

In good approximation we can assume that the system is in mechanical equilibrium. For the analytical treatment, we will assume in this work that deformation and phase parameters are global minimisers of the free energy with respect to the present particle densities.

At starting time $t = 0$ the crystal is described by a non-empty, bounded Lipschitz domain $\Omega \subset \mathbf{R}^3$. Let $\mathbf{R}_+ := [0, \infty[$. The evolution of Ω is given by a family of C^2-diffeomorphisms $\{\Psi_t : \mathbf{R}^3 \to \mathbf{R}^3 : t \in \mathbf{R}_+\}$ with

$$\Psi_0(x) = x \text{ for all } x \in \Omega, \tag{2.1}$$

$$\big(\mathbf{R}_+ \times \mathbf{R}^3 \ni (t,x) \mapsto \Psi_t(x) \in \mathbf{R}^3\big) \in \mathrm{C}^2(\mathbf{R}_+ \times \mathbf{R}^3, \mathbf{R}^3), \tag{2.2}$$

$$\big(\mathbf{R}_+ \times \mathbf{R}^3 \ni (t,x) \mapsto \Psi_t^{-1}(x) \in \mathbf{R}^3\big) \in \mathrm{C}^2(\mathbf{R}_+ \times \mathbf{R}^3, \mathbf{R}^3). \tag{2.3}$$

The domain occupied by the crystal at time $t \geq 0$ is denoted by $\Omega_t := \Psi_t(\Omega)$.

The mechanical deformation is given by a family of mappings $\{\Phi_t : \mathbf{R}_+ \times \Omega \to \Omega_t : t \in \mathbf{R}_+\}$ that satisfy for all $t \in \mathbf{R}_+$ and for all $x \in \Omega$

$$\Phi_0(x) = x, \tag{2.4}$$

$$\Phi_t \in \mathrm{W}^{1,3+\delta}(\Omega, \mathbf{R}^3) \text{ and } \Phi_t^{-1} \in \mathrm{W}^{1,3+\delta}(\Omega_t, \mathbf{R}^3) \text{ exists}, \tag{2.5}$$

$$\det \nabla \Phi_t > 0 \text{ a.e. in } \Omega. \tag{2.6}$$

Here, $\delta > 0$ can be arbitrary. The conditions (2.5) and (2.6) ensure that Φ_t are deformations. The condition $\delta > 0$ guarantees the integrability of the functional determinant and therefore that the volume is finite. Condition (2.4) reflects the fact that the initial state is undeformed.

The space- and time-dependent particle densities of the $n \in \mathbf{N}$ different species of molecules are described by $\rho_i : \mathbf{R}_+ \times \mathbf{R}^3 \to \mathbf{R}$, $i = 1, \ldots, n$. The following natural conditions are postulated for $t \in \mathbf{R}_+$ and $1 \leq i \leq n$:

$$\rho_i(t) \in \mathrm{L}^1(\Omega_t), \tag{2.7}$$

$$\rho_i(t) \geq 0 \quad \text{a.e. in } \Omega_t, \tag{2.8}$$

$$\int_{\Omega_t} \rho_i(t,x)\, dx = \int_{\Omega} \rho_{0_i}(x)\, dx > 0, \tag{2.9}$$

$$\sum_{i=1}^{n} \rho_i(t) \circ \Phi_t \det \nabla \Phi_t \leq 1 \qquad \text{a.e. in } \Omega. \tag{2.10}$$

The functions ρ_{0_i} are given initial values with

$$\rho_{0_i} \in \mathrm{L}^1(\Omega), \quad 0 < \int_{\Omega} \rho_{0_i}(x)\, dx, \quad 0 \leq \rho_{0_i} \quad \text{a.e. in } \Omega, \tag{2.11}$$

$$\sum_{i=1}^{n} \rho_i \leq 1 \text{ a.e. in } \Omega, \qquad \int_{\Omega} \sum_{i=1}^{n} \rho_{0_i}(x)\, dx < |\Omega|. \tag{2.12}$$

Equation (2.9) ensures the conservation of mass, (2.10) is due to the fact that the crystal does not possess interstitials and that the number of lattice positions in a volume element is a uniform constant. We assume $(2.12)_2$ with strict inequality as we assume a non-vanishing vacancy density.

Let $m \in \mathbf{N}$ denote the number of different possible phases. The phases are described by a family of phase vectors $\left\{\chi_t := (\chi_{j_t})_{j=1}^m : \Omega_t \to \mathbf{R} : t \in \mathbf{R}_+\right\}$, where the initial value χ_0 is given. Here, $\chi_{j_t}(x)$ determines whether the material point x at time $t \in \mathbf{R}_+$ is in phase j, $1 \le j \le m$, i.e. χ_{j_t} are characteristic functions. As any point in the crystal belongs to exactly one phase, the functions χ_{j_t} fulfil for any $1 \le j \le m$ and $t \in \mathbf{R}_+$

$$\chi_{j_t}(1-\chi_{j_t}) \;=\; 0, \tag{2.13}$$

$$\sum_{j=1}^m \chi_{j_t} \;=\; 1, \tag{2.14}$$

$$\chi_{j_t} \in \mathrm{BV}(\;\Omega_t\;). \tag{2.15}$$

With (2.14) we may write the surface energy between phase i and j at time t as

$$S_t : \mathrm{L}^1(\Omega_t) \times \mathrm{L}^1(\Omega_t) \to \bar{\mathbf{R}}_+ := \mathbf{R}_+ \cup \{+\infty\},$$

$$(p_1,p_2) \mapsto \begin{cases} \frac{1}{2}\int\limits_{\Omega_t} \left(|\nabla p_1| + |\nabla p_2| - |\nabla(p_1+p_2)|\right), \text{ if } \int\limits_{\Omega_t} |\nabla p_i| < \infty, i=1,2, \\ \infty, \text{ otherwise.} \end{cases} \tag{2.16}$$

Assuming further that the densities of the surface energy ς_{ij} on the interface between phase i and phase j are positive constants with $\varsigma_{ij} = \varsigma_{ji}$, the surface energy $F_t^s(\chi_t)$ at time $t \in \mathbf{R}_+$ can be introduced by

$$F_t^s : \mathrm{L}^1\left(\Omega_t, \mathbf{R}^m\right) \to \mathbf{R}_+, \quad p = (p_k)_{k=1}^m \mapsto \sum_{i=1}^m \sum_{j=1}^m \sigma_{ij} S_t(p_i,p_j) \tag{2.17}$$

with $\sigma_{ij} := \frac{\varsigma_{ij}}{2}$, $1 \le i,j \le m$. Additionally we postulate for $1 \le i,j,k \le m$

$$\sigma_{ij} \;=\; \sigma_{ji}, \tag{2.18}$$

$$(i \ne j \text{ and } k \notin \{i,j\}) \Rightarrow \sigma_{ij} \le \sigma_{ik} + \sigma_{kj}. \tag{2.19}$$

So, energetically it is not favourable to add a third phase between two other existing phases.

We assume that the volume density of phase j depends on the particle concentrations and the gradients of the deformations. It is given by a measurable function (see p.9 in [3]) $f_j : \mathbf{R}^n \times \mathsf{M}^3 \to \bar{\mathbf{R}}_+$, $\mathsf{M}^k := \mathrm{M}(k \times k, \mathbf{R})$, $k \in \mathbf{N}$.

Let for $t \in \mathbf{R}_+$

$$B_t := \mathrm{L}^1\left(\Omega_t, \mathbf{R}^n\right) \times \mathrm{W}^{1,3+\delta}\left(\Omega_t, \mathbf{R}^3\right) \times \mathrm{L}^1\left(\Omega_t, \mathbf{R}^m\right), \tag{2.20}$$

$$\mathrm{Def}_t := \{(r,d,p) \in B_t : \det \nabla d \ne 0 \text{ a.e. in } \Omega_t\}, \tag{2.21}$$

$$F_t^v \;:\; \mathrm{Def}_t \to \bar{R} := \mathbf{R} \cup \{-\infty, +\infty\},$$

$$(r,d,p=(p_k)_{k=1}^m) \mapsto \sum_{j=1}^m \int\limits_{\Omega_t} p_j(x) f_j\left(r(x), (\nabla d)^{-1}(x)\right)\, dx. \tag{2.22}$$

By (2.22) the volumetric free energy $F_t^v\left(\rho_t, \Phi_t^{-1}, \chi_t\right)$ of the crystal at time $t \in \mathbf{R}_+$ is introduced. For the total free energy of the system at time $t \in \mathbf{R}_+$ we write $F_t(\rho(t), \Phi_t^{-1}, \chi_t)$ with

$$F_t : \mathrm{Def}_t \to \bar{\mathbf{R}}, \ \ (r, d, p) \mapsto F_t^v(r, d, p) + F_t^s(p). \tag{2.23}$$

For the subsequent formal derivation we assume that all functions are sufficiently smooth. We extend the density vector $\rho(t)$ by 0 to a function on the whole of $\mathbf{R}^n$. We use the notation $\partial v := (\partial v_l)_{l=1}^k$, where ∂ is an arbitrary differential operator.

The evolution in time of the particle densities is described by the continuity equation

$$\partial_t \rho(t) = -\mathrm{div}\mathcal{F}_t \text{ in } \Omega_t, \tag{2.24}$$

where $\mathcal{F}_t := (\mathcal{F}_{i_t})_{i=1}^n$, and $\mathcal{F}_{i_t}$ is the particle flux of species i, $1 \le i \le n$, at time $t \in \mathbf{R}_+$. In our case, $\mathcal{F}_{i_t}$ consists of two components, the diffusive flux $\tilde{J}_{i_t}$, and the mechanical flux M_{i_t}.

We write

$$\mathcal{F}_t = -J_t + M_t, \ \ \left(J_t := (-\tilde{J}_{i_t})_{i=1}^n, M_t := (M_{i_t})_{i=1}^n\right), \quad t \in \mathbf{R}_+. \tag{2.25}$$

For the mechanical flux we easily find

$$M_{i_t} = \rho_i(t)\partial_t \Phi_t \circ \Phi_t^{-1} \text{ in } \Omega_t, \ t \in \mathbf{R}_+, 1 \le i \le n. \tag{2.26}$$

We introduce the notations $\rho(t)\partial_t\Phi_t \circ \Phi_t^{-1} := \left(\rho_i(t)\partial_t\Phi_t \circ \Phi_t^{-1}\right)_{i=1}^n$ and write (2.24) as

$$\partial_t \rho(t) = \mathrm{div}\left(J_t - \rho(t)\partial_t\Phi_t \circ \Phi_t^{-1}\right) \text{ in } \Omega_t, \ t \in \mathbf{R}_+, \tag{2.27}$$

or equivalently

$$\partial_t\left(\rho(t) \circ \Phi_t \det\nabla\Phi_t\right) = \mathrm{div}J_t \circ \Phi_t \det\nabla\Phi_t \text{ in } \Omega, \ t \in \mathbf{R}_+. \tag{2.28}$$

At fixed constant temperature the diffusive fluxes are caused by the negative gradients of the chemical potentials which are the thermodynamic forces, [17], [12]. According to Onsager's postulate, [16], [24], [25], [12], every thermodynamic flux is a linear combination of the thermodynamic forces. So we set

$$J_{i_t} = \sum_{k=1}^n L_{ik}\nabla\mu_{k_t} \text{ in } \Omega_t, \quad 1 \le i \le n, \quad t \in \mathbf{R}^+, \tag{2.29}$$

$$\text{or } J_t = L\nabla\mu_t \text{ in } \Omega_t, \quad \left(\mu_t = (\mu_{k_t})_{k=1}^n\right), \quad t \in \mathbf{R}_+ \tag{2.30}$$

with a symmetric and positive definite matrix $L := (L_{ik})_{i,k=1}^n$ and the chemical potential μ_i of species i, where the symmetry and positive definiteness of L comes from Onsager's reciprocity relation, [24], [25], [12].

According to the definition of the chemical potential one has in Ω_t for any $t \in \mathbf{R}_+$ and $i = 1, \ldots, n$

$$\mu_{i_t} = \sum_{j=1}^{m} \chi_{j_t} \partial_{r_i} f_j \left(\rho(t), \nabla\Phi_t \circ \Phi_t^{-1}\right) = \sum_{j=1}^{m} \chi_{j_t} \partial_{r_i} f_j (\rho(t), (\nabla\Phi_t^{-1})^{-1}). \quad (2.31)$$

Now we formulate the aforementioned minimality condition on the free energy. Considering the time-evolution of the deformation of a representative volume element and keeping in mind that the number of particles only changes due to diffusion, we find for two possible deformations Φ_t^1, Φ_t^2 the relation

$$\rho^1(t) \circ \Phi_t^1 \det\nabla\Phi_t^1 = \rho^2(t) \circ \Phi_t^2 \det\nabla\Phi_t^2 \text{ in } \Omega, \quad (2.32)$$

where $\rho^1(t), \rho^2(t)$ are the densities corresponding to Φ_t^1, Φ_t^2. So the minimality condition for any $t \in \mathbf{R}_+$ reads

$$F_t \left(\rho(t), \Phi_t^{-1}, \chi_t\right) = \min_{\tilde{\Phi} \in D_t, \tilde{\chi} \in P_t} F_t \left(\hat{\rho}(t) \circ \tilde{\Phi}^{-1} \det \nabla\tilde{\Phi}^{-1}, \tilde{\Phi}^{-1}, \tilde{\chi}\right), \quad (2.33)$$

with

$$D_t := \left\{\Phi \in \mathcal{W}^\delta : \tilde{\Phi}(\Omega) = \Omega_t, \exists \Phi^{-1} \in \mathcal{W}_t^\delta, \det\nabla\Phi > 0 \text{ a.e. in } \Omega\right\}, \quad (2.34)$$

$$P_t := \left\{\chi \in \mathcal{BV} : \sum_{j=1}^{m} \chi_j = 1, \chi_j(1 - \chi_j) = 0, j = 1, \ldots, m\right\}, \quad (2.35)$$

$$\hat{\rho}(t) := \rho(t) \circ \Phi_t \det\nabla\Phi_t \quad (2.36)$$

for $t \in \mathbf{R}_+$ and the setting $\mathcal{BV} := \mathrm{BV}(\Omega_t, \mathbf{R}^m)$, $\mathcal{W}^\delta := \mathrm{W}^{1,3+\delta}(\Omega, \mathbf{R}^3)$, $\mathcal{W}_t^\delta := \mathrm{W}^{1,3+\delta}(\Omega_t, \mathbf{R}^3)$.

To conclude, our model consists of the equations (2.4)–(2.6), (2.7)–(2.10), (2.13)–(2.15), (2.27) or (2.28), (2.29) or (2.30), (2.31) and (2.33).

2.2 Solution strategy - implicit time discretisation

The objective is to solve the model equations. To this end we discretise the equations implicitly in time. The ansatz is the same as in [29], [19], [20].

The following argument is only heuristic. We exploit the minimality condition on the free energy (2.33) and choose a suitable approximation of (2.28).

If we formally consider the time derivative of $F = F(\rho, \Phi, \chi)$, we find (omitting the dependence on t)

$$\mathrm{d}_t F = \partial_\rho F \partial_t \rho + \partial_\Phi F \partial_t \Phi + \partial_\chi F \partial_t \chi.$$

From (2.33) it follows $\partial_\chi F \partial_t \chi = 0$, $\partial_\rho F \partial_\Phi \rho + \partial_\Phi F = 0$. Consequently,

$$\mathrm{d}_t F = \partial_\rho F(\partial_t \rho - \partial_\Phi \rho \partial_t \Phi). \quad (2.37)$$

Now we compute $\partial_\Phi \rho \partial_t \Phi$ from (2.32) to obtain

$$\partial_\Phi \rho \partial_t \Phi = -\rho \mathrm{Tr}(\nabla \Phi^{-1} \nabla \partial_t \Phi \circ \Phi^{-1}) - \langle \nabla \rho, \partial_t \Phi \circ \Phi^{-1} \rangle \tag{2.38}$$

$$= -\mathrm{div}(\rho \partial_t \Phi \circ \Phi^{-1}) = -\mathrm{div} M, \tag{2.39}$$

where $\mathrm{Tr}(A) := \sum_{k=1}^{3} A_{kk}$ is the trace of $A \in \mathsf{M}^3$. If we plug (2.27) and (2.39) into (2.37) we find

$$d_t F = \partial_\rho F(\mathrm{div} J - \mathrm{div} M + \mathrm{div} M) = \partial_\rho F \mathrm{div} J.$$

Assuming that the surface terms do not depend on ρ, it follows, see [4] p.58,

$$d_t F(t) = \sum_{i=1}^{n} \int_{\Omega_t} \sum_{j=1}^{m} \chi_{j_t}(x) \partial_{r_i} f_j \left(\rho_t(x), \nabla \Phi_t \circ \Phi_t^{-1}(x) \right) \mathrm{div} J_{i_t}(x)\, dx$$

$$= \sum_{i=1}^{n} \int_{\Omega_t} \mu_{i_t}(x) \mathrm{div} J_{i_t}(x)\, dx, \quad t \in \mathbf{R}_+. \tag{2.40}$$

Assuming further that the normal component of $J_{i,t}$ vanishes on $\partial \Omega_t$, which follows from (2.28) and (2.9), we get with the inner product $\langle a, b \rangle := \sum_{k=1}^{3} a_k b_k$ in $\mathbf{R}^3$

$$\sum_{i=1}^{n} \mu_{i_t} \mathrm{div} J_{i_t} = \sum_{i=1}^{n} \mathrm{div}(\mu_{i_t} J_{i_t}) - \langle \nabla \mu_{i_t}, J_{i_t} \rangle,\ t \in \mathbf{R}_+.$$

With the divergence theorem and (2.30) we find

$$d_t F(t) = -\int_{\Omega_t} \sum_{i=1}^{n} \langle \nabla \mu_{i_t}(x), J_{i_t}(x) \rangle\, dx = -2\mathrm{Q}_t(J_t) = -2\mathrm{Q}_t^*(\nabla \mu_t) \tag{2.41}$$

$$= -\mathrm{Q}_t(J_t) - \mathrm{Q}_t^*(\nabla \mu_t), \tag{2.42}$$

where for $t \in \mathbf{R}_+$

$$\mathrm{Q}_t : \left(\mathrm{L}^2(\Omega_t, \mathbf{R}^3) \right)^n \to \mathbf{R},\ G \mapsto \frac{1}{2} \int_{\Omega_t} (L^{-1} G, G)\, dx, \tag{2.43}$$

$$Q_t^* : \left(\mathrm{L}^2(\Omega_t, \mathbf{R}^3) \right)^n \to \mathbf{R},\ G \mapsto \frac{1}{2} \int_{\Omega_t} (G, LG)\, dx. \tag{2.44}$$

Here we introduced the symbol

$$(\cdot, \cdot) : \left(\mathbf{R}^3 \right)^n \to \mathbf{R},\ (a, b) \mapsto \sum_{k=1}^{n} \langle a_k, b_k \rangle. \tag{2.45}$$

In (2.41) and (2.42), Q_t^* denotes the Fenchel conjugate to Q_t. We call (2.42) the $Q-Q^*$-formulation of the problem. In general, every system of equations originating from non-equilibrium thermodynamics can be written in the form

$$\mathrm{d}_t F + Q + Q^* + G + G^* \leq 0,$$

where Q and G are certain convex functionals and Q^*, G^* are their convex conjugates. Therefore, Equation (2.41) can be written in the form

$$\int\limits_{\Omega_t} \langle \nabla_r f(x), \mathrm{div} J_t(x) \rangle \, dx + \partial_J \mathrm{Q}_t(J_t)(J_t) = 0, \quad t \in \mathbf{R}_+, \tag{2.46}$$

with $\langle \nabla_r f, \mathrm{div} J_t \rangle := \sum\limits_{i=1}^{n} \sum\limits_{j=1}^{m} \chi_{j_t} \partial_{r_i} f_j \left(\rho_t, \left(\nabla \Phi_t^{-1} \right)^{-1} \right) \mathrm{div} J_{i_t}$.

Now we approximate (2.28) for given discrete step size $h > 0$ by

$$\rho(t+h) = \hat{\rho}(t) \circ \Phi_{t+h}^{-1} \det \nabla \Phi_{t+h}^{-1} + h \mathrm{div} J_{t+h}. \tag{2.47}$$

We see that for known $(\rho(t), \Phi_t, \chi_t)$, a minimiser (Φ, χ, J) of the functional

$$\begin{aligned}(\tilde{\Phi}, \tilde{\chi}, \tilde{J}) \mapsto E_{t+h}(\tilde{\Phi}, \tilde{\chi}, \tilde{J}) := F_{t+h} &\left(\hat{\rho}(t) \circ \tilde{\Phi}^{-1} \det \nabla \tilde{\Phi}^{-1} + h \mathrm{div} \tilde{J}, \tilde{\Phi}^{-1}, \tilde{\chi} \right) \\ &+ h \mathrm{Q}_{t+h}(\tilde{J})\end{aligned} \tag{2.48}$$

satisfies (2.46). Additionally, due to $\rho := \hat{\rho}(t) \circ \tilde{\Phi}^{-1} \det \nabla \tilde{\Phi}^{-1} + h \mathrm{div} J$, every minimiser fulfils the equation

$$\begin{aligned} 0 = \partial_J E_{t+h}(\Phi, \chi, J)(\delta J) &= h \int\limits_{\Omega_{t+h}} \langle \nabla_\rho f(\rho, \nabla \Phi, \chi), \mathrm{div} \delta J \rangle \, dx + h \partial_J Q(J)(\delta J) \\ = -h \int\limits_{\Omega_{t+h}} (\nabla \mu, \delta J) \, dx + h \int\limits_{\Omega_{t+h}} (L^{-1} J, \delta J) \, dx \end{aligned}$$

and it holds $J = L \nabla \mu$ and (2.33) is fulfilled.

Motivated by these considerations we arrive at the following implicit time discrete version of our original problem:

Let $\rho(t)$, Φ_t, χ_t be the solutions of the problem at time t. Then $\rho(t+h)$, Φ_{t+h} and χ_{t+h} are given by $\rho(t+h) := \hat{\rho}(t) \circ \tilde{\Phi}^{-1} \det \nabla \tilde{\Phi}^{-1} + h \mathrm{div} J$, $\Phi_t := \Phi$, $\chi_t := \chi$, where (Φ, χ, J) is a minimiser of (2.48).

3 The time-discrete system

In this paragraph we show the existence of minimisers of (2.48) in a suitable function space. To this end it is necessary to make (2.48) precise. We make further assumptions on the structure of $f_1, \dots, f_m$, which are motivated by the direct method in the calculus of variations, see [4], [7] and (2.6), (2.10).

First we want to extend Def_t on B_t (see (2.20), (2.21)) and want to ensure that the domain where F_t is finite is closed. The difficulty here is that in the definition of F_t the inverse of the gradients of the deformations occur. The following ansatz solves this problem, taking (2.6) and (2.10) into account.

For $A \in \mathsf{M}^3$ let

$$\mathrm{cof} A := \begin{pmatrix} A_{22}A_{33} - A_{23}A_{32} & A_{13}A_{32} - A_{12}A_{33} & A_{12}A_{23} - A_{22}A_{23} \\ A_{23}A_{31} - A_{21}A_{33} & A_{11}A_{33} - A_{13}A_{31} & A_{13}A_{21} - A_{11}A_{23} \\ A_{21}A_{32} - A_{22}A_{32} & A_{12}A_{31} - A_{11}A_{32} & A_{11}A_{22} - A_{12}A_{21} \end{pmatrix}.$$

With this definition we have $A\,\mathrm{cof}A = (\mathrm{cof}A)A = (\det A)E_3 := (\det A)(\delta_{kl})_{k,l=1}^3$. It is important to notice that for invertible $A \in \mathsf{M}^3$ it holds $\frac{1}{\det A}\mathrm{cof}A = A^{-1}$. Therefore we make the following conditions on $f_1, \dots, f_m$:

$$\text{There exist } g_j : \mathbf{R}^n \times \mathsf{M}^3 \times \mathsf{M}^3 \times \mathbf{R} \to \bar{\mathbf{R}}_+ \text{ such that for all } (r, A) \in \mathbf{R}^n \times \mathsf{M}^3$$
$$f_j(r, A^{-1}) = g_j(r, A, \mathrm{cof}A, \det A), \text{ if } \det A \neq 0. \tag{3.1}$$

Furthermore we demand that for all $(r, A, B, d) \in \mathbf{R}^n \times \mathsf{M}^3 \times \mathsf{M}^3 \times \mathbf{R}$

$$g_j(r, A, B, d) \in \mathbf{R}_+ \text{ iff } (r, A, B, d) \in \mathrm{Z}, \quad 1 \le j \le m, \tag{3.2}$$

with the admissible set

$$\mathrm{Z} := \left\{ (r, A, B, d) \in \mathbf{R}^n \times \mathsf{M}^3 \times \mathsf{M}^3 \times \mathbf{R} : d \ge 0, \sum_{i=1}^n r_i d \le 1 \text{ and } r \ge 0 \right\}. \tag{3.3}$$

Here, the condition $r \ge 0$ for $r \in \mathbf{R}^n$ has to be understood componentwise.

As given in (3.1), g_j denotes the argument of F_t^v in the position of f_j. Now we define for $t \in \mathbf{R}_+$ with the abbreviation $\mathbf{d} := (\nabla d, \mathrm{cof}\nabla d, \det\nabla d)$, $d \in \mathcal{W}_t^\delta$,

$$F_t^v : \mathrm{B}_t \to \bar{\mathbf{R}}, \ (r, d, p) \mapsto$$
$$\begin{cases} \sum_{j=1}^m \int_{\Omega_t} p_j(x) g_j(r(x), \mathbf{d}(x)) dx, \text{ if } \sup_{j=1}^m \int_{\Omega_t} |p_j(x)|\, g_j(r(x), \mathbf{d}(x))\, dx < \infty, \\ +\infty, \text{ otherwise}, \end{cases} \tag{3.4}$$
$$F_t : \mathrm{B}_t \to \bar{\mathbf{R}}, \quad (r, d, p) \mapsto F_t^s(p) + F_t^v(r, d, p). \tag{3.5}$$

Since Q_t is defined on $\left(\mathrm{L}^2(\Omega_t, \mathbf{R}^3)\right)^n$, it remains to define the divergence on $\mathrm{L}^2(\Omega_t, \mathbf{R}^3)$. This is done in a way adapted to the equations such that the conservation of mass (2.9) and the implication (2.40)⇒(2.41) holds.

$$\mathrm{div}_t : L^2(\Omega_t, \mathbf{R}^3) \to W^{1,-2}(\Omega_t),$$
$$\mathrm{div}_t j(\xi) := -\int_{\hat{\Omega}} \langle j, \nabla \xi \rangle\, dx, \quad \xi \in W^{1,2}(\hat{\Omega}, \mathbf{R}^n). \tag{3.6}$$

In the following we write div instead of div_t.

Remark. *As is shown in [1], for a lower semicontinuous convex function* $g : \mathbf{R}^n \to \bar{\mathbf{R}}$ *that satisfies* $C_1 g(x) + C_2 \geq \|x\|^q$ *for all* $x \in \mathbf{R}^n$ *and positive constants* C_1*,* C_2 *and* $q > 1$*, one can define* $\int_\Omega g(\mathrm{div}J)$ *in a natural way by setting*

$$\int\limits_\Omega g(\mathrm{div}J) = +\infty, \quad \textit{if } \mathrm{div}J \notin \mathrm{L}^q(\Omega, \mathbf{R}^n).$$

Now we are in the position to formulate (2.48) appropriately. Let $t \in \mathbf{R}_+$, $h > 0$, $\rho(t)$ and Φ_t be given such that (2.4)–(2.6) and (2.7)–(2.10) are satisfied. Then introduce

$$\begin{aligned} E_{t+h} &: \mathrm{B}_t \times \left(\mathrm{L}^2(\Omega_t, \mathbf{R}^3)\right)^n \mapsto \bar{\mathbf{R}}, \\ &(d, p, G) \mapsto F_{t+h}(\hat{\rho}(t) \circ d\det\nabla d + h\mathrm{div}G, d, p) + h\mathrm{Q}_{t+h}(G). \quad (3.7) \end{aligned}$$

We call the variational problem $E_{t+h} \to \min$ the *time-discrete* system. The existence of minimisers is ensured by the following theorem.

Theorem 1. *Let* $t \in \mathbf{R}_+$ *and* $h > 0$*. In addition to the earlier assumptions, let* $f_1, \ldots, f_m$ *be lower semicontinuous and convex, satisfying*

$$c_1^j f_j(r, A, B, d) + c_2^j \geq \|A\|^{3+\delta}, \quad (3.8)$$

$$c_3^j f_j(r, A, B, d) + c_4^j \geq \frac{\|B\|^{3+\delta}}{|d|^{2+\delta}}, \quad (3.9)$$

$$c_5^j f_j(r, A, B, d) + c_6^j \geq |d|^{1+\frac{\delta}{3}} \quad (3.10)$$

for all $(r, A, B, d) \in \mathbf{R}^n \times \mathsf{M}^3 \times \mathsf{M}^3 \times \mathbf{R}$ *with non-negative constants* c_k^j*,* $k = 1, \ldots, 6$*. Then* E_{t+h} *possesses a minimiser* (Φ, χ, J) *that fulfils (2.5), (2.6), (2.7)–(2.10) and (2.13)–(2.15) with* $\rho := \hat{\rho}(t) \circ \tilde{\Phi}^{-1}\det\nabla\tilde{\Phi}^{-1} + h\mathrm{div}J$*.*

The proof of this theorem can be found in [1].

Idea of proof: We use the direct method in the calculus of variations. First we show the lower semicontinuity of the functionals in a suitable topology (weak topology for J and Φ, strong topology for χ; a new proof for the lower semicontinuity of F_t^s with methods from elementary convex algebra is given in [2]). For a minimising sequence $(\Phi_k, \chi_k, J_k)_{k\in\mathbf{N}}$, Equation (3.8) yields the boundedness of $\|\Phi_k^{-1}\|_{\mathcal{W}_t^\delta}$, (3.9) gives the boundedness of $\|\Phi_k\|_{\mathcal{W}^\delta}$, (3.10) gives the boundedness of $\|\det\nabla\Phi_k^{-1}\|_{\mathrm{L}^{1+\frac{\delta}{3}}}$ which implies the boundedness of $\|\mathrm{div}J_k\|_{\mathrm{L}^{1+\frac{\delta}{3}}}$.

The norm $\|\chi_k\|_{\mathrm{BV}}$ can be estimated by F_t^s, see [2], which guarantees the compactness in L^1, whereas the L^2-norm of J_k is estimated by Q_t.

Exploiting the differentiability properties of functions in $\mathcal{W}_t^\delta$, see [10], and properties of the weak convergence in these spaces, see [6], the existence of minimisers with the stated properties can be proved.

Corollary 2. *If for* $1 \leq i \leq n$*,* $1 \leq j \leq m$ *the derivatives* $\partial_{r_i} f_j$ *exist in* $\overset{\circ}{\mathrm{Z}}$ *and if* $\lim\limits_{k\to\infty} |\partial_{r_i} f_j(r_k, A_k, B_k, d_k)| = +\infty$ *for every sequence* $(r_k, A_k, B_k, d_k)_{k\in\mathbf{N}}$

with $\lim_{k\to\infty}(r_k, A_k, B_k, d_k) = (r, A, B, d) \in \partial\mathrm{Z}$*, then for a minimiser of Theorem 1 it holds* $J = \nabla\mu$ *with* $\mu_i = \sum_{j=1}^{m} \chi_j \partial_{r_i} f_j(\rho, \mathbf{\Phi})$, $1 \leq i \leq n$.

The complete proof of this statement is given in [1].

Idea of proof: Since the formal method presented at the end of Section 2.2 cannot be applied, we approximate f_j by suitable smooth and convex functions f_j^k from below and solve the corresponding variational problem $E_{t+h}^k \to \min$ for which we have $J^k = \nabla\mu^k$, $\mu^k = \nabla_r f^k(\rho^k, \mathbf{\Phi}^k) \in \mathrm{W}^{1,2}(\Omega_t)$.

Using convexity arguments and elementary measure-theoretic results one can then show with the Poincaré inequality the existence of a subsequence with $J^{k_l} \to J$, $\nabla\mu^{k_l} \to \nabla\mu$ and $\nabla_r f^{k_l}(\rho^{k_l}, \mathbf{\Phi}^{k_l}) \to \nabla_r f(\rho, \mathbf{\Phi})$ as $l \to \infty$.

4 The continuous system

According to Theorem 1 we can construct for given $h > 0$ a sequence of time-discrete solutions. We discuss the limit $h \to 0$ and show that the discrete solutions converge in a sense that has yet to be specified to a solution of the original problem. As we have at most weak convergence, due to the non-linearity of F_t we cannot expect that the weak limit satisfies (2.33). Additionally, the equations do not provide a condition on Φ_t and χ_t in time. If we consider the problem on a fixed given time interval $[0, T]$ for $T > 0$ and regard ρ, Φ, χ, J, μ as mappings from $[0, T]$ to a certain topological space X, we notice the analogy to Young measures that yield solutions to our problem in case X is finite-dimensional (or locally compact), see [9], [22], [27].

4.1 Formulation of the problem with Young measures

As the domain Ω_t is time dependent, so is the function space X_t containing $\rho(t), \Phi_t, \chi_t, J_t, \mu_t$. The space $X := \bigcup_{t\in[0,T]} X_t$ has no 'nice' topological properties. Therefore we consider the quantities $\hat{\rho}(t) := \rho(t) \circ \Phi_t \det\nabla\Phi_t, \hat{\Phi}_t := \Psi_t^{-1} \circ \Phi_t, \hat{\chi}_t := \chi_t \circ \Psi_t, \hat{J}_t := J_t \circ \Psi_t, \hat{\mu}_t := \mu_t \circ \Psi_t$ on the reference domain Ω to formulate the equations. So we transform with Φ_t respectively Ψ_t for $t \in \mathbf{R}_+$. The corresponding time-discrete solutions exist according to Theorem 1 since Φ_t possesses the transformation property, see [10]. In the following, $\hat{\alpha}$ always denotes the transform of α. In analogy to the common weak formulation, the measure-valued formulation reads:

Let $\hat{X} := \mathrm{L}^2(\Omega, \mathbf{R}^n) \times \mathcal{W}^\delta \times \mathrm{L}^{1+\frac{3}{\delta}}(\Omega, \mathbf{R}^m) \times \left(\mathrm{L}^2(\Omega, \mathbf{R}^3)\right)^n \times \mathrm{W}^{1,2}(\Omega, \mathbf{R}^n)$ be equipped with the product topology of the weak topology in coordinates 2, 4, 5 and the strong topology in coordinates 1 and 3. We look for a mapping $\mathcal{P} : [0, T] \to \mathcal{R}(\hat{X}), t \mapsto \mathcal{P}_t$, where $\mathcal{R}(\hat{X})$ is the space of signed Radon measures over $\hat{X}$ with $\mathcal{P}_t \geq 0$ and $\mathcal{P}_t(\hat{X}) = 1$ for almost all $t \in [0, T]$ such that (with $\hat{x} := (\hat{\rho}, \hat{\phi}, \hat{\chi}, \hat{J}, \hat{\mu})$)

$$\int_0^T \vartheta'(t) \int_{\hat{X}} \int_{\Omega} \hat{\rho}(y)\hat{\xi}(y)\, dy\, d\mathcal{P}_t(\hat{x})\, dt$$
$$= \int_0^T \vartheta(t) \int_{\hat{X}} \int_{\Omega} \hat{J}(y)\nabla(\hat{\xi} \circ \hat{\boldsymbol{\Phi}}^{-1} \circ \Psi_t^{-1}) \circ \Psi_t(y) \det\nabla\Psi_t(y)\, dy\, d\mathcal{P}_t(\hat{x})\, dt, \tag{4.1}$$

$$\int_0^T \vartheta(t) \int_{\hat{X}} \int_{\Omega} \hat{\xi}(y)L^{-1}\hat{J}(y)\det\nabla\Psi_t(y)\, dy\, d\mathcal{P}_t(\hat{x})\, dt$$
$$= -\int_0^T \vartheta(t) \int_{\hat{X}} \int_{\Omega} \hat{\mu}(y)\mathrm{div}(\hat{\xi} \circ \Psi_t^{-1}) \circ \Psi_t(y)\det\nabla\Psi_t(y)\, dy\, d\mathcal{P}_t(\hat{x})\, dt, \tag{4.2}$$

$$\int_0^T \vartheta(t) \int_{\hat{X}} \int_{\Omega} \hat{\mu}(y)\hat{\xi}(y)\det\nabla\Psi_t(y)\, dy\, d\mathcal{P}_t(\hat{x})\, dt$$
$$= \int_0^T \vartheta(t) \int_{\hat{X}} \int_{\Omega} \sum_{j=1}^m \hat{\chi}_j \circ \hat{\Phi}(y)\partial_r \hat{f}_j \left(\hat{\rho}(y), \hat{\boldsymbol{\Phi}}(y)\right) \hat{\xi}(y)\, dy\, d\mathcal{P}_t(\hat{x})\, dt \tag{4.3}$$

for all $\vartheta \in \mathrm{C}_0^\infty([0,T])$, $\hat{\xi} \in \mathrm{C}_0^\infty(\bar{\Omega}, \mathbf{R}^n)$ and

$$\mathrm{supp}\,\mathcal{P}_t \subset \Big\{(\hat{\rho}, \hat{\phi}, \hat{\chi}, \hat{J}, \hat{\mu}) \in \hat{X} : \hat{\rho} \in \mathrm{supp}\,\mathcal{P}_t\big|_{\hat{X}_1}, \quad \hat{F}(\hat{\rho}, \hat{\phi}, \hat{\chi}) = \min_{(\tilde{\Phi},\tilde{\chi}) \in \hat{X}_2 \times \hat{X}_3} F(\hat{\rho}, \tilde{\Phi}, \tilde{\chi})\Big\} \tag{4.4}$$

for almost all $t \in [0,T]$. Here, $\hat{X}_l$ denotes the l-th component of $\hat{X}$, $1 \le l \le 5$. Furthermore, let the conditions analogous to (2.4)–(2.6), (2.7)–(2.10), (2.13)–(2.15) be fulfilled for almost all $t \in [0,T]$ on $\mathrm{supp}\,\mathcal{P}_t$.

4.2 Construction of the Young measures

The key to the proof of existence of measure-valued solutions to the continuous problem is given by the following theorem.

Theorem 3. *(Analogon to Young measures in the infinite setting)*
Let $I_T := [0,T] \subset \mathbf{R}$ for $T > 0$ and λ_T be the Lebesgue measure on I_T, $(\nu_i)_{i\in\mathbf{N}}$ be a sequence of positive Radon measures on I_T with $\nu_i \overset{*}{\rightarrow} \lambda_T$ for $i \to \infty$, let X_1, X_2 be Banach spaces with separable X_1^*, X_2^*, define

$$(X, \|\cdot\|_X) := (X_1 \times X_2, \|\cdot\|_{X_1} + \|\cdot\|_{X_2}), \quad (X, \tau) := (X_1 \times X_2, \|\cdot\|_{X_1} \times w_{X_2}),$$

and $(\gamma_i : [0,T] \to X)_{i\in\mathbf{N}}$ be a mapping.

If $K_1^n \subset\subset (X_1, \|\cdot\|_{X_1})$, $K_2^n \subset\subset (X_2, w_{X_2})$ *and*

$$\nu_i \left(M_i^n := \{t \in I_T : \gamma_i(t) \notin K_1^n \times K_2^n\}\right) < \frac{1}{n} \quad \text{for } i \in \mathbf{N}, \tag{4.5}$$

then there exists a subsequence $(\gamma_{i_k})_{k\in\mathbf{N}}$ *and a mapping* $\mathcal{P} : I_T \to \mathcal{R}(X)$ *with*

$$\mathcal{P}_t \geq 0, \quad \mathcal{P}_t(X) = 1 \ \text{ for almost all } t \in I_T \tag{4.6}$$

and

$$\left([0,T] \ni t \mapsto \int_X f(t,x)\, d\mathcal{P}_t(x) \in \mathbf{R}\right) \in \mathrm{L}^\infty([0,T]), \tag{4.7}$$

$$\lim_{k\to\infty} \int_0^T f(t, \gamma_{i_k}(t))\, d\nu_{i_k}(t) = \int_0^T \int_X f(t,x)\, d\mathcal{P}_t(x)\, dt \tag{4.8}$$

for all $f \in \mathrm{C}_b([0,T] \times X)$.

Corollary 4. *Additional to the assumptions of Theorem 3 let there exist a* $q \geq 0$ *such that for all* $i \in \mathbf{N}$

$$\|\gamma_i\|_X \in \mathrm{L}^1(I_T) \text{ and } \int_{M_i^n} \|\gamma_i\|_X^q\, d\nu_i(t) < \frac{1}{n}. \tag{4.9}$$

Let $f : (I_T \times X, |\cdot| \times \tau) \to \mathbf{R}$ *fulfil for a constant* $C > 0$

$$f(t,x) \leq C\,(1 + \|x\|^q) \quad \text{for all } (t,x) \in I_T \times X. \tag{4.10}$$

Let f *be bounded from below and let* f *be either lower semi-continuous or lower semicontinuous with respect to the second argument and satisfy a uniform continuity in time, i.e. for any* $n \in \mathbf{N}$ *and given* $\epsilon > 0$ *there exists a* $\delta(n,\epsilon)$ *with* $|f(x,t) - f(x,t')| < \epsilon$ *for* $|t - t'| < \delta(n,\epsilon)$, $t, t' \in I_T$ *and all* $x \in K_1^n \times K_2^n$. *If one of these two conditions is met, it follows*

$$f(t,\cdot) \in \mathrm{L}^1\left(X, \mathcal{B}_X, \mathcal{P}_t\right) \ \text{ for almost all } t \in I_T, \tag{4.11}$$

$$\left([0,T] \ni t \mapsto \int_X f(t,x)\, d\mathcal{P}_t(x)\, dt \in \mathbf{R}\right) \in \mathrm{L}^1([0,T]), \tag{4.12}$$

$$\liminf_{k\to\infty} \int_0^T f\left(t, \gamma_{i_k}(t)\right)\, d\nu_{i_k}(t) \geq \int_0^T \int_X f(t,x)\, d\mathcal{P}_t(x)\, dt. \tag{4.13}$$

A continuous function f *that is not necessarily bounded from below and satisfies (4.10) fulfils*

$$\lim_{k\to\infty} \int_0^T f\left(t, \gamma_{i_k}(t)\right)\, d\nu_{i_k}(t) = \int_0^T \int_X f(t,x)\, d\mathcal{P}_t(x)\, dt. \tag{4.14}$$

We remind that a cylinder function is defined as follows:

Definition 5. *Let X be a topological vector space. A function $f : X \to \mathbf{R}$ is called a cylinder function on X if for some $p \in \mathbf{N}$ there exists a $\alpha \in X^{*^p}$ and a $g \in \mathrm{C}_b(\mathbf{R}^p)$ such that f has the representation $f = g \circ \alpha$. The symbol Z_X denotes the set of all cylinder functions on X.*

Corollary 6. *From the assumptions of Theorem 3 it follows*

$$\mathcal{P}_t\left(X \setminus \bigcup_{n=1}^{\infty} K_1^n \times K_2^n\right) = 0 \text{ for almost all } t \in I_T. \tag{4.15}$$

The longer, technical proofs of this statement can be found in [1]. Crucial is the following Lemma that is also proved in [1].

Lemma 7. *(Approximation Lemma.) Let X be a Banach space, $f : X \to \mathbf{R}$ be strongly continuous, $g : X \to \mathbf{R}$ be weakly continuous, $K \subset X$ strongly compact and $L \subset X$ weakly compact. Then for any $\epsilon > 0$ there exist cylinder functions $\Gamma_\epsilon : X \to \mathbf{R}$ and $\Theta_\epsilon : X \to \mathbf{R}$ with*

$$\max_{x\in K} |f(x) - \Gamma_\epsilon(x)| < \epsilon \text{ and } \max_{x\in L} |g(x) - \Theta_\epsilon(x)| < \epsilon.$$

In addition it holds $\max_{x\in X} |\Gamma_\epsilon(x)| \leq \max_{x\in K} |f(x)|$ and $\max_{x\in X} |\Theta_\epsilon(x)| \leq \max_{x\in L} |g(x)|$

Remark. *The approximating cylinder functions can be chosen as elements of a fixed countable set.*

Idea of proof: The strategy to prove Theorem 3 is to first show the statements in the finite-dimensional case using slicing theorems, [26],, and then to approximate with cylinder functions. Essentially, the extension to the infinite-dimensional case is an application of Riesz' representation theorem for positive linear forms on the space of continuous functions on completely regular spaces.

The proofs of the corollaries rely on the fact that lower continuous functions can be approximated on compact sets from below by continuous functions, see [1].

4.3 Measure valued solutions

In earlier sections we have established the mathematical tools needed to formulate the final theorem. The proof of the next theorem is contained in [1].

Theorem 8. *The continuous system (2.4)–(2.6), (2.7)–(2.10), (2.13)–(2.15), (2.27) or (2.28), (2.29) or (2.30), (2.31) and (2.33) possesses a solution in the sense of Section 4.1 if the requirements of Theorem 1 and Corollary 2 are met. There exists $\hat{\rho} \in \mathrm{L}^2([0,T] \times \Omega, \mathbf{R}^n)$ with $\mathcal{P}_t = \delta_{\hat{\rho}(t)} \times \tilde{\mathcal{P}}_t$ for almost all $t \in [0,T]$ and the following energy inequality holds:*

$$\mathsf{E}(\tau_2) - \mathsf{E}(\tau_1) \leq - \int_{\tau_1}^{\tau_2} \mathsf{Q}(t) + \mathsf{Q}^*(t)\, dt \text{ for almost all } \tau_1, \tau_2 \in [0,T], \tag{4.16}$$

where

$$\mathsf{E} : [0,T] \to \mathbf{R},\ t \mapsto \int_{\hat{X}} \hat{F}(\hat{\rho}, \hat{\Phi}, \hat{\chi}, t)\, d\mathcal{P}_t(\hat{x}), \tag{4.17}$$

$$\mathsf{Q} : [0,T] \to \mathbf{R},\ t \mapsto \int_{\hat{X}} \hat{Q}(\hat{J}, t)\, d\mathcal{P}_t(\hat{x}), \tag{4.18}$$

$$\mathsf{Q}^* : [0,T] \to \mathbf{R},\ t \mapsto \int_{\hat{X}} \hat{Q}^*(\nabla\hat{\mu}, t)\, d\mathcal{P}_t(\hat{x}). \tag{4.19}$$

Idea of proof: (All subsequences are labelled as the original sequence; we use the abbreviation $\hat{x} := (\hat{\rho}, \hat{\Phi}, \hat{\chi}, \hat{J}, \hat{\mu})$.)

For $i \in \mathbf{N}$ let $h(i) := \frac{T}{2^i}$. Then, according to Theorem 1 and Corollary 2, we can construct recursively a finite sequence $\left(\hat{x}_{lh(i)}\right)_{l=0}^{2^i}$ which solves the time-discrete problem. Now we define $\hat{x}_i$ for $i \in \mathbf{N}$ as the step function corresponding to the sequence which is continuous from left. One can show that $\left(\gamma_i := (\hat{\rho}_i, \hat{\Phi}_i, \hat{\chi}_i, \hat{J}_i, \hat{\mu}_i)\right)_{i\in\mathbf{N}}$ satisfies the assumptions of Theorem 3. In the next step one proves with the help of Kolmogoroff's compactness criterium, see [31], the existence of a subsequence with the property

For a given smooth Dirac sequence $(\phi_j)_{j\in\mathbf{N}}$ there exists for every $j \in \mathbf{N}$ a $\hat{\rho}^j \in \mathrm{L}^2([0,T] \times \Omega, \mathbf{R}^n)$ such that

$$\lim_{k\to\infty} \int_0^T \int_\Omega \left| \hat{\rho}_i^j(t,x) - \hat{\rho}^j(t,x) \right|^2 dx\, dt = 0.$$

Furthermore we need:

Lemma 9. *Let X be a T3a-space, $\nu \in \mathcal{PM}(X)$ with $\nu(X) = 1$ and $g \in \mathrm{C}(X,X)$. If for every $f \in \mathrm{C_b}(X)$*

$$\int_X f^2(g(x))\, d\nu(x) - \left(\int_X f(g(x))\, d\nu(x) \right)^2 = 0, \tag{4.20}$$

then there exists $x_0 \in X$ with $g(x) = x_0$ for all $x \in \operatorname{supp} \nu$.

Applying Theorem 3 and the above Lemma on the subsequence $(\gamma_i)_{i\in\mathbf{N}}$, we find the existence of $\hat{\rho}$ with $\mathcal{P}_t = \delta_{\hat{\rho}(t)} \times \tilde{\mathcal{P}}_t$ for almost all $t \in [0,T]$.

With the exception of (4.2) and (4.4), the remaining equations follow essentially from Theorem 3 and the Corollaries 4 and 6.

For the proof of the minimality condition (4.4), we show with (4.1) that

$$\mathsf{E}(t) = \min_{(\Phi,\chi)\in\hat{X}_2\times\hat{X}_3} \hat{F}(t,\hat{\rho}(t),\Phi,\chi) \quad \text{for } t\in[0,T].$$

The validity of (4.2) relies on the subgradient-inequality

$$\int_{\hat{X}}\int_{\Omega} \mu(\tilde{\rho}-\rho)\,dy\,d\mathcal{P}_t(\hat{x}) \le \int_{\hat{X}}\int_{\Omega} f(\tilde{\rho})-f(\rho)\,dy\,d\mathcal{P}_t(\hat{x}),$$

where (4.4) is used.

The proof of the energy inequality is based on the following considerations.

Define for $i\in\mathbf{N}$, $1\le k\le 2^i$ and $t:=kh(i)$

$$J_{t_i}^{\inf} := \operatorname*{argmin}_{J\in \mathrm{L}^2(\Omega_t,\mathbf{R}^3)^n} \left[F_t\left(\rho_i(t)+h(i)\mathrm{div}J,\Phi_{t_i},\chi_{t_i}\right)+h(i)Q_t(J)\right],$$
$$\rho_i^{\inf}(t) := \rho_i(t)+h\,\mathrm{div}J_{t_i}^{\inf}$$

and the corresponding continuation for $t\neq kh(i)$. Then it holds

$$h(i)\mu_{j_i}^{\inf}\mathrm{div}J_i^{\inf} = \mu_{j_i}^{\inf}\left(\rho_i^{\inf}-\rho_i\right) \ge f_j\left(\rho_i^{\inf},\mathbf{\Phi}_i\right)-f_j\left(\rho_i,\mathbf{\Phi}_i\right)$$

and (Young's inequality)

$$\begin{aligned} Q_t\left(J_{t_i}^{\inf}\right)+Q_t^*\left(\nabla\mu_{t_i}^{\inf},t\right) &= \int_{\Omega_t}\left\langle J_{t_i}^{\inf},\nabla\mu_{t_i}^{\inf}\right\rangle dx \\ &= -\sum_{j=1}^{m}\int_{\Omega_t}\chi_{j_{t_i}}\mu_{j_{t_i}}^{\inf}\mathrm{div}J_{t_i}^{\inf}\,dx \end{aligned}$$

for $i\in\mathbf{N}$, $1\le j\le m$, $t\in[0,T]$ and $x\in\Omega_t$. This yields

$$\begin{aligned} &F_t\left(\rho_i^{\inf}(t),\Phi_{t_i},\chi_{t_i}\right)-F\left(\rho_i(t),\Phi_{t_i},\chi_{t_i}\right)\\ &\qquad \le -h(i)\left[Q_t\left(J_{t_i}^{\inf}\right)+Q_t^*\left(\nabla\mu_{t_i}^{\inf}\right)\right] \end{aligned}$$

which can be rewritten as

$$\begin{aligned} &F_t\left(\rho_i^{\inf}(t),\Phi_{t_i},\chi_{t_i}\right)+h(i)Q_t\left(J_{t_i}^{\inf}\right)\\ &\qquad \le F_t\left(\rho_i(t),\Phi_{t_i},\chi_{t_i}\right)-h(i)Q_t^*\left(\nabla\mu_{t_i}^{\inf}\right). \end{aligned}$$

Therefore, due to

$$\begin{aligned} &F_{t+h(i)}\left(\rho_i(t+h(i)),\Phi_{(t+h(i))_i},\chi_{(t+h(i))_i}\right)+h(i)Q_{t+h(i)}\left(J_{(t+h(i))_i}\right)\\ &\qquad \le F_t\left(\rho_i^{\inf}(t),\Phi_{t_i},\chi_{t_i}\right)+h(i)Q_t\left(J_{t_i}^{\inf}\right), \end{aligned}$$

we obtain the estimate

$$F_{t+h(i)}\left(\rho_i(t+h(i)), \Phi_{(t+h(i))_i}, \chi_{(t+h(i))_i}\right) - F_t\left(\rho_i^{\inf}(t), \Phi_{t_i}, \chi_{t_i}\right) \\ \leq -h(i)\left[Q_{t+h(i)}\left(J_{(t+h(i))_i}\right) + Q_t^*\left(\nabla\mu_{t_i}^{\inf}\right)\right]. \quad (4.21)$$

Next, the inequality (4.21) is rewritten in terms of $\hat{F}$, $\hat{Q}$, $\hat{Q}_{\inf}$. Then we consider the two sequences

$$\left(\gamma_i^1 := (\hat{\rho}_i, \hat{\Phi}_i, \hat{\chi}_i, \hat{J}_i, \hat{\mu}_i, \hat{\mu}_{\inf_i})\right)_{i\in\mathbf{N}} \text{ and } \left(\gamma_i^2 := (\hat{\rho}_{\inf_i}, \hat{\Phi}_i, \hat{\chi}_i, \hat{J}_i, \hat{\mu}_i, \hat{\mu}_{\inf_i})\right)_{i\in\mathbf{N}}$$

and show that they generate the same measure $\breve{\mathcal{P}}_t = \delta_{\hat{\rho}(t)} \times \bar{\mathcal{P}}_t$ for almost all $t \in [0, T]$. From (4.21) it follows (4.16) with the corresponding $\mathsf{Q}_{\inf}^*$. Estimating the subgradient inequality we can finally show $\mathsf{Q}_{\inf}^* = \mathsf{Q}^*$.

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