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A generalized field method for multiphase transformations using interface fields

I. Steinbach*, F. Pezzolla

ACCESS e.V., Intzestrarre 5, D-52056 Aachen, Germany

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Abstract

The recently developed multiphase field method, describing the interaction between an arbitrary number of individual phase fields with individual characteristics, is reformulated by the use of interface fields. This reformulation allows for the decomposition of the nonlinear multiphase field interactions into pairwise interaction of interface fields. This removes some difficulties in the treatment of triple points or higher order interactions that occurred in the original model. The interface fields being defined in a $\binom{\tilde{N}}{2}$ dimensional space, where \tilde{N} is the order of the multiple point, can be interpreted being the generalized coordinates for this variational problem. The considered example of a multiphase change problem indicates clearly that a relaxation ansatz for the evolution of the field variables towards the minimum of the free energy is warranted only for generalized coordinates, while a relaxation ansatz using functionally dependent variables and the Lagrange formalism in general mixes time and energy scales. ©1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

The multiphase field theory [1] was originally developed for the description of first order phase transformations in a system containing $N > 2$ different phases $\phi_\alpha, \phi_\beta, \dots, \phi_N$ and their gradients $\nabla\phi_\alpha, \nabla\phi_\beta, \dots, \nabla\phi_N$. The equations of motion of the ϕ_α towards the minimum of the free energy F are derived using a relaxation ansatz

$$\tau \dot{\phi}_\alpha = \left(\nabla \frac{\partial}{\partial \nabla \phi_\alpha} - \frac{\partial}{\partial \phi_\alpha} \right) f(\{\phi_\alpha\}), \quad (1)$$

where $f(\{\phi_\alpha\})$ denotes the Gibbs free energy density of the N phase system as defined in [1], τ is a relaxation constant.

* Corresponding author.

E-mail address: i.steinbach@access.rwth-aachen.de (I. Steinbach)

Since in a multiphase problem the $\{\phi_\alpha\}$ are connected by the constraint

$$\sum_{\alpha=1}^N \phi_\alpha = 1 \quad (2)$$

or

$$\sum_{\alpha=1}^N \dot{\phi}_\alpha = 0, \quad (3)$$

the ϕ_α are not independent field variables.

In the original model [1] the nonlinearities arising from this fact were attributed to triple point energies and energies of multiple interactions of higher order. According to the physical assumption that these energies have negligible influence on the total energy of the system, the corresponding nonlinearities were neglected.

Garcke et al. [2] have shown that this approximation violates conservation of interfacial stresses at multiple points (Young's law). As an explanation for this violation one may consider that the phase boundaries in equilibrium are straight lines (2D) or planes (3D) and the angles between the boundaries are independent of the length scale. On the scale of the phase boundary thickness, the multiple phase point then fills the whole volume under consideration. Thus the multiple phase energies will influence the local physics significantly, though they are negligible in the system altogether.

By use of a Lagrange multiplier λ and treating the N phases $\alpha = 1, \dots, N$ independent, the equations of motion of the ϕ_α are found:

$$\tau \dot{\phi}_\alpha = \left(\nabla \frac{\partial}{\partial \nabla \phi_\alpha} - \frac{\partial}{\partial \phi_\alpha} \right) \left(f(\{\phi_\alpha\}) + \lambda \left(\sum_1^N \phi_\alpha - 1 \right) \right) = \left(\nabla \frac{\partial}{\partial \nabla \phi_\alpha} - \frac{\partial}{\partial \phi_\alpha} \right) f(\{\phi_\alpha\}) + \lambda. \quad (4)$$

The Lagrange multiplier λ accounts for the constraint (2) or (3).

It was shown by Garcke et al. [2] that the ansatz (4) conserves the interfacial stress balance in the sharp interface limit with isotropic interfaces and by Nestler and Wheeler [3] that it holds also for arbitrary interface anisotropy.

There arise however two severe problems. The first is the definition of the relaxation constant τ in (4). As it is well known, the relaxation rate of an interface into equilibrium strongly depends on the type of interface, e.g. solid–liquid or solid–solid. The right-hand side of (4), however – besides the pairwise contributions related to one type of interface, that were used in the original model – contains higher order contributions, related to triple points. These contributions can hardly be attributed with an individual timescale. Therefore a decomposition of these terms related to specific boundaries $\alpha \leftrightarrow \beta$ is necessary.

The second problem is the coupling of the phase field equations (4) to outer fields like temperature. The phase change $\alpha \rightarrow \beta$ results in a local energy change δE related to the latent heat of that specific phase change $L_{\alpha\beta}$, while there is no evidence that a multiple phase change can be related to a triple energy $\tilde{L}_{\alpha\beta\gamma}$. Again therefore decomposing (4) into pairwise contributions is necessary.

In fact, these problems are two facets of the same difficulty: how to fix the time and energy scale of a multiple phase change in a multiphase system. In this paper, a formal transformation of the phase field variables ϕ_α onto a set of $\binom{N}{2}$ interfacial field variables $\psi_{\alpha\beta}$ is described, that allows for the decomposition of (4) in the desired way. Moreover, this transformation leads to a definition of the multiphase change problem in a $\binom{N}{2}$ dimensional space being more general than the original definition on the $N - 1$ manifold of the N phase system, connected by the constraint (2).

2. The phase field variables ϕ_α of a multiphase system and the free energy functional F

In the classical phase field theory [4,5], the phase field variable $\phi(x, t)$ is defined as a continuous function in space and time on an Euclidean point space Ω . ϕ may be identified with the solid density that varies continuously from 1 (solid) to 0 (liquid) over the interface region with a thickness δ . The liquid density is then given by $1 - \phi(x, t)$, and $\phi(1 - \phi)$ may be interpreted as the interface density. Values of $\phi(x, t) < 0$ and $\phi(x, t) > 1$ are formally allowed but considered to be non-physical.

The multiphase system may be described by a set of N phase field variables ϕ_α , $\alpha = 1, \dots, N$, where each phase field is associated with the local density of a different phase and they are connected by the constraint (2).

We then define the open spaces $\tilde{\Omega}_\alpha \in \Omega$ where $0 < \phi_\alpha < 1$ on $\tilde{\Omega}_\alpha$ and the step function σ_α :

$$\sigma_\alpha = \begin{cases} 1 & \text{on } \tilde{\Omega}_\alpha, \\ 0 & \text{elsewhere,} \end{cases} \quad (5)$$

where $\overline{\Omega}_\alpha$ is the open space $\tilde{\Omega}_\alpha$ plus its boundary. The closed spaces $\overline{\Omega}_\alpha$ may be separated or overlapping and they change according to the evolution of the ϕ_α . We then define the number of locally present phases $\tilde{N}(x, t)$ by

$$\tilde{N}(x, t) = \sum_{\alpha=1}^N \sigma_\alpha(x, t), \quad (6)$$

and the constraint (2) reduces to

$$\sum_{\alpha=1}^{\tilde{N}} \phi_\alpha(x, t) = 1. \quad (7)$$

The number of locally present phases \tilde{N} is 2 on dual interfaces, 3 on triple points and so on.

The total free energy F is given by the volume integral over the kinetic and potential free energy densities.

$$F(\{\phi_\alpha\}) = \int_{\Omega} (f^{\text{kin}} + f^{\text{pot}}) dV = \int_{\Omega} f dV. \quad (8)$$

We here use the explicit forms for thermodynamic equilibrium

$$f^{\text{kin}} = \sum_{\gamma=1}^N \sum_{\delta=\gamma+1}^N -\frac{\varepsilon_{\gamma\delta}}{2} \nabla \phi_\gamma \nabla \phi_\delta, \quad (9)$$

$$f^{\text{pot}} = \sum_{\gamma=1}^N \sum_{\delta=\gamma+1}^N \gamma_{\gamma\delta} |\phi_\gamma| |\phi_\delta|. \quad (10)$$

The kinetic energy is a linearization of the expression $\varepsilon_{\gamma\delta}(\phi_\gamma \nabla \phi_\delta - \phi_\delta \nabla \phi_\gamma)$ used in the original model¹, and the piecewise bilinear potential replaces the double well potential $\gamma \phi_\alpha^2 \phi_\beta^2$ (see Figs. 1(a) and (b)). The explicit form of f^{kin} and f^{pot} is of minor importance for the method presented here. It is, however, considered to be essential for a multiphase method that the transition regions between the phases are finite, i.e. the $\phi_\alpha(x, t)$ have to converge to 1 or to 0 on a finite region $\overline{\Omega}_\alpha < \Omega$. Otherwise, all phases would overlap and the multiple point of order N would extend over the whole domain Ω (see Fig. 2).

¹ This expression was suggested by G.J. Schmitz, who significantly contributed to the development of the presented model.

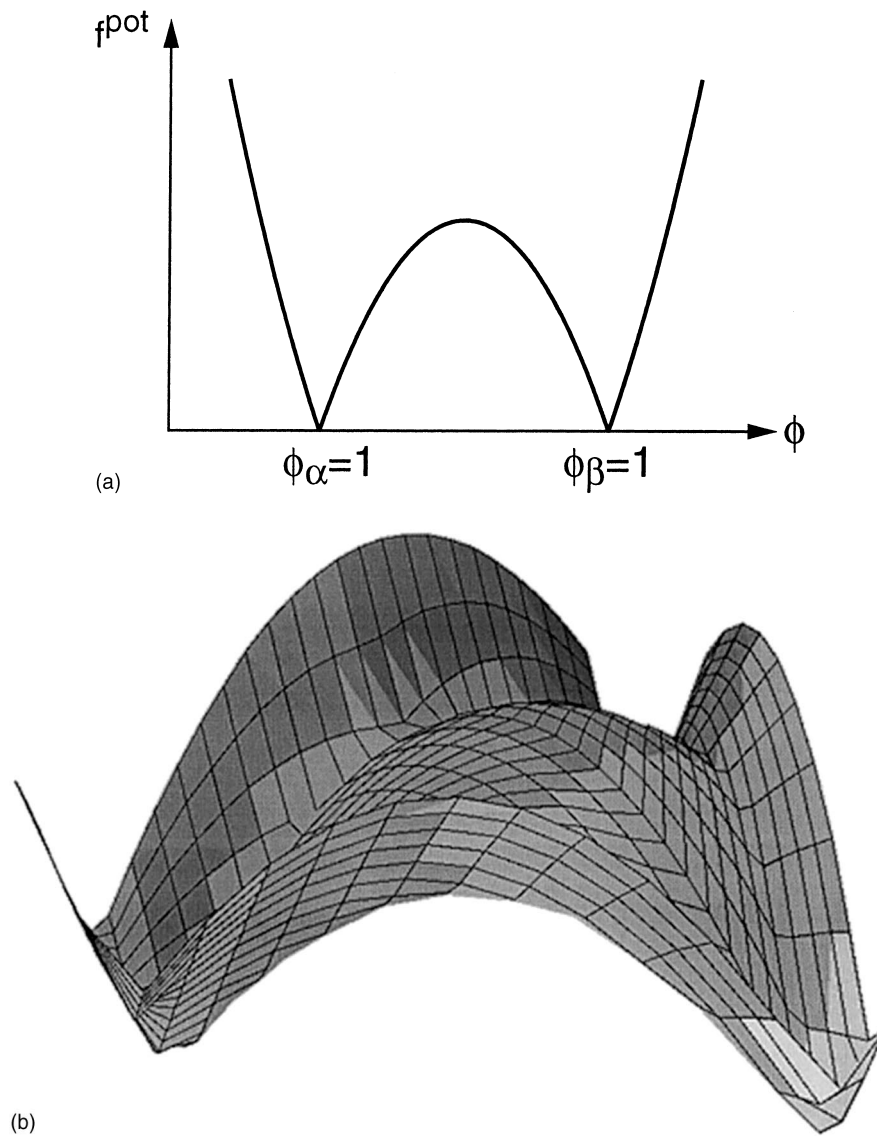


Fig. 1. (a) Piecewise “bi-linear” potential in the α - β plane, (b) Piecewise “tri-linear” potential.

The existence of finite transition regions $\bar{\Omega}_\alpha < \Omega$ is ensured by the potential (10) because of the finite derivative at the minima of f^{pot}

$$\left. \frac{\partial f^{\text{pot}}}{\partial \phi_\alpha} \right|_{\substack{\phi_\alpha=0 \\ \phi_\alpha=1}} \neq 0. \quad (11)$$

In general, we assume $\tilde{N} < N$, while $\tilde{N} = N$ is included in the method as a limiting case.

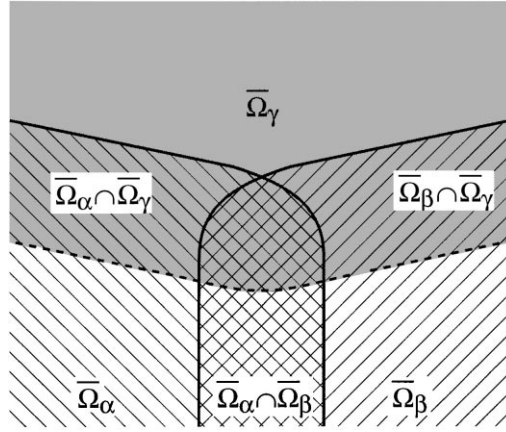


Fig. 2. The regions $\bar{\Omega}_\alpha$ and $\bar{\Omega}_\beta$, where the phase fields ϕ_α or ϕ_β are non-zero, overlap in the definition region $\bar{\Omega}_\alpha \cap \bar{\Omega}_\beta$ of the interface fields $\psi_{\alpha\beta}$. The interface fields $\psi_{\alpha\beta}$, $\psi_{\alpha\gamma}$ and $\psi_{\beta\gamma}$ overlap in the triple point $\bar{\Omega}_\alpha \cap \bar{\Omega}_\beta \cap \bar{\Omega}_\gamma$.

3. The interface fields $\psi_{\alpha\beta}$ and their equations of motion

As can be seen from the constraint (2) resp. (7) the $\{\phi_\alpha\}$ do not form an independent set of functional variables of the multiphase system. They are defined on a $\tilde{N} - 1$ dimensional manifold.

For \tilde{N} phases $\binom{\tilde{N}}{2}$ interfaces between two phases α and β can be formed. We define a set of $\binom{\tilde{N}}{2}$ antisymmetric interface fields $\{\psi_{\alpha\beta}\}$, $\alpha < \beta$ and its complement $\{\tilde{\psi}_{\beta\alpha}\}$, $\alpha < \beta$, $\tilde{\psi}_{\beta\alpha} = -\psi_{\alpha\beta}$. In the following we skip the tilde on the complement. For $\tilde{N} = 2$ a unique interface field $\psi_{\alpha\beta}$ can be defined on the basis of ϕ_α and ϕ_β :

$$\psi_{\alpha\beta} = \phi_\alpha - \phi_\beta. \tag{12}$$

Application of (12) for $\tilde{N} > 2$ projects the phase field distribution $\{\phi_\alpha\}$ into a $N - 1$ dimensional subspace of the $\psi_{\alpha\beta}$ that again is connected by the constraint (2) as (12) is a linear transformation.

The reverse transformation is

$$\phi_\alpha = \frac{1}{\tilde{N}} \left(\sum_{\beta=1}^{\tilde{N}} \psi_{\alpha\beta} + 1 \right). \tag{13}$$

On the subspace defined by (12), the equations of motion of the $\psi_{\alpha\beta}$ are found via a detour over the Lagrange density of the ϕ_α .

The Lagrange density l , that enforces the constraint (7), is defined

$$l = f + \lambda \left(\sum_{\alpha=1}^{\tilde{N}} \phi_\alpha - 1 \right). \tag{14}$$

The minimum of the free energy functional F with respect to the variation of the phase field ϕ_α may then be found from the integrated Lagrange functional $\mathcal{L} = \int_{\Omega} l dV$,

$$0 = -\frac{\delta \mathcal{L}}{\delta \phi_\alpha} = \left(\nabla \frac{\partial}{\partial \nabla \phi_\alpha} - \frac{\partial}{\partial \phi_\alpha} \right) l, \tag{15}$$

and treating the phase fields ϕ_α to be independent,

$$\frac{\delta\phi_\alpha}{\delta\phi_\beta} = \delta_{\alpha\beta} \quad (16)$$

with the Kronecker symbol $\delta_{\alpha\beta}$. We then make the relaxation ansatz

$$\overset{\circ}{\phi}_\alpha = -\frac{\delta\mathcal{L}}{\delta\phi_\alpha} = -\frac{\delta F}{\delta\phi_\alpha} - \lambda, \quad (17)$$

where $\overset{\circ}{\phi}_\alpha$ denotes the motion of the ϕ_α towards the minimum of F without specifying a timescale τ .

It is then obvious that

$$\overset{\circ}{\psi}_{\alpha\beta} = \overset{\circ}{\phi}_\alpha - \overset{\circ}{\phi}_\beta = -\frac{\delta F}{\delta\phi_\alpha} + \frac{\delta F}{\delta\phi_\beta} (+\lambda - \lambda) \quad (18)$$

is independent of the Lagrange multiplier λ .

The independence of (18) from the Lagrange multiplier indicates that the $\psi_{\alpha\beta}$ can be considered as generalized coordinates. In fact, it can be calculated explicitly that any realization of the $\{\psi_{\alpha\beta}\}$, $\psi_{\alpha\beta} \in \mathbb{R}$ leads to a set of ϕ_α that is compatible with the constraint (2), though only $\psi_{\alpha\beta} \in [0, 2]$ can be considered physically:

$$\sum_{\alpha=1}^{\tilde{N}} \phi_\alpha - 1 = \frac{1}{\tilde{N}} \sum_{\alpha=1}^{\tilde{N}} \left(\sum_{\beta=1}^{\tilde{N}} \psi_{\alpha\beta} + 1 \right) - 1 = \frac{1}{\tilde{N}} \sum_{\alpha=1}^{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \psi_{\alpha\beta} = 0 \quad (19)$$

because of the antisymmetry of the $\psi_{\alpha\beta}$.

Thus, the $N - 1$ dimensional subspace of the $\psi_{\alpha\beta}$ in the $\binom{N}{2}$ dimensional space can be left and the $\psi_{\alpha\beta}$ can be varied independently. Of course (12) is then no longer valid and an explicit rule for transforming the $\{\phi_\alpha\} \rightarrow \{\psi_{\alpha\beta}\}$ can no longer be given, as it would be (for $\tilde{N} > 2$) a transformation into a higher dimensional space. The reverse transformation $\{\psi_{\alpha\beta}\} \rightarrow \{\phi_\alpha\}$ (13) must then be interpreted as a projection from the $\binom{\tilde{N}}{2}$ dimensional space of the $\{\psi_{\alpha\beta}\}$ into the \tilde{N} dimensional space of the $\{\phi_\alpha\}$. This projection, by its definition, conserves the constraint (2).

Treating the $\psi_{\alpha\beta}$ linearly independent and using the antisymmetry of the $\psi_{\alpha\beta}$ we have

$$\frac{\delta\psi_{\alpha\beta}}{\delta\psi_{\gamma\delta}} = \delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma}, \quad (20)$$

$$\frac{\delta}{\delta\psi_{\alpha\beta}} = \sum_{\gamma} \frac{\delta\phi_\gamma}{\delta\psi_{\alpha\beta}} \frac{\delta}{\delta\phi_\gamma} = \frac{1}{\tilde{N}} \sum_{\gamma} \sum_{\delta} \frac{\delta\psi_{\gamma\delta}}{\delta\psi_{\alpha\beta}} \frac{\delta}{\delta\phi_\gamma} = \frac{1}{\tilde{N}} \left(\frac{\delta}{\delta\phi_\alpha} - \frac{\delta}{\delta\phi_\beta} \right). \quad (21)$$

The motion $\overset{\circ}{\psi}_{\alpha\beta}$ can be calculated as

$$\overset{\circ}{\psi}_{\alpha\beta} = -\frac{\delta\mathcal{L}}{\delta\psi_{\alpha\beta}} = \frac{1}{\tilde{N}} \left(-\frac{\delta F}{\delta\phi_\alpha} + \frac{\delta F}{\delta\phi_\beta} (+\lambda - \lambda) \right). \quad (22)$$

Comparing (22) and (18) we find that the motion $\overset{\circ}{\phi}_{\alpha\beta}$ and $\overset{\circ}{\psi}_{\alpha\beta}$ scales by a factor $1/\tilde{N}$. This scaling can be understood by two reasons. First

$$\overset{\circ}{\psi}_{\alpha\beta} = \left(\frac{\partial}{\partial\phi_\alpha} - \frac{\partial}{\partial\phi_\beta} \right) F \quad (23)$$

and

$$\overset{\circ}{\psi}_{\alpha\beta} = \frac{\partial}{\partial\psi_{\alpha\beta}} F \quad (24)$$

differ by a factor 2, as the definition range of values of the $\psi_{\alpha\beta}$ and ϕ_α differs by a factor 2. For $\tilde{N} = 2$ we have by the definition (12)

$$\delta\psi_{\alpha\beta} = 2\delta\phi_\alpha = -2\delta\phi_\beta. \tag{25}$$

For $\tilde{N} > 2$ we may put

$$\tilde{N} = 2 \binom{\tilde{N}}{2} = 2 \frac{\binom{\tilde{N}}{2}}{N-1}, \tag{26}$$

i.e. the motions $\overset{\circ}{\psi}_{\alpha\beta}$ and $\overset{\odot}{\psi}_{\alpha\beta}$ scale, besides the factor 2 due to the difference in definition range, according to the ratios of the dimensions of the spaces $\binom{\tilde{N}}{2}$ for $\{\psi_{\alpha\beta}\}$ and $(N-1)$ for $\{\phi_\alpha\}$, and we have

$$\overset{\odot}{\psi}_{\alpha\beta} = \frac{(\tilde{N}-1)}{2 \cdot \binom{\tilde{N}}{2}} \overset{\circ}{\psi}_{\alpha\beta} = \frac{1}{\tilde{N}} \overset{\circ}{\psi}_{\alpha\beta}. \tag{27}$$

The consistency of this result can easily be checked by comparing the equations of motion of the $\dot{\phi}_\alpha$ on the physical timescale τ set alike for all interfaces

$$\tau_{\alpha\beta} \equiv \tau. \tag{28}$$

The standard treatment via the Lagrange formalism (4) then gives

$$\dot{\phi}_\alpha = -\frac{\partial}{\partial\phi_\alpha} F + \lambda, \tag{29}$$

$$\lambda = \frac{1}{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \frac{\partial}{\partial\phi_\beta} F, \tag{30}$$

$$\tau\dot{\phi}_\alpha = -\frac{\partial}{\partial\phi_\alpha} F + \frac{1}{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \frac{\partial}{\partial\phi_\beta} F = -\frac{\tilde{N}-1}{\tilde{N}} \frac{\partial}{\partial\phi_\alpha} F + \frac{1}{\tilde{N}} \sum_{\beta \neq \alpha} \frac{\partial}{\partial\phi_\beta} F = -\frac{1}{\tilde{N}} \sum_{\beta \neq \alpha} \left(\frac{\partial}{\partial\phi_\alpha} - \frac{\partial}{\partial\phi_\beta} \right) F. \tag{31}$$

The same result is obtained from (18) using (13) or from (22) using (13) and (27):

$$\tau\dot{\phi}_\alpha = \overset{\circ}{\phi}_\alpha = \frac{1}{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \overset{\circ}{\psi}_{\alpha\beta} = \sum_{\beta=1}^{\tilde{N}} \overset{\odot}{\psi}_{\alpha\beta} = -\frac{1}{\tilde{N}} \sum_{\beta \neq \alpha} \left(\frac{\partial}{\partial\phi_\alpha} - \frac{\partial}{\partial\phi_\beta} \right) F. \tag{32}$$

In the general case, where the timescales $\tau_{\alpha\beta}$ differ for the different interfaces, we now can specify the total timescale

$$\dot{\phi}_\alpha = \frac{1}{\tilde{N}} \sum_{\beta \neq \alpha} \dot{\psi}_{\alpha\beta} = \frac{1}{\tilde{N}} \sum_{\beta \neq \alpha} \frac{1}{\tau_{\alpha\beta}} \overset{\circ}{\psi}_{\alpha\beta} = \sum_{\beta \neq \alpha} \frac{1}{\tau_{\alpha\beta}} \overset{\odot}{\psi}_{\alpha\beta}. \tag{33}$$

In the same way the energy scale can be fixed

$$\dot{q}_\alpha = \frac{1}{\tilde{N}} \sum_{\beta \neq \alpha} L_{\alpha\beta} \dot{\psi}_{\alpha\beta} = \sum_{\beta \neq \alpha} \frac{L_{\alpha\beta}}{\tau_{\alpha\beta}} \overset{\odot}{\psi}_{\alpha\beta}, \tag{34}$$

where \dot{q}_α is the release or consumption of latent heat associated with the phase change ϕ_α .

For the special model of the free energy functional (9) and (10) we may evaluate explicitly

$$\dot{\psi}_{\alpha\beta} = \frac{\sigma_{\alpha}\sigma_{\beta}}{\tau_{\alpha\beta}} \left[\sum_{\gamma \neq \alpha} \sigma_{\gamma} \left(-\frac{\varepsilon_{\alpha\gamma}}{2} \nabla^2 \phi_{\gamma} - \gamma_{\alpha\gamma} \phi_{\gamma} \right) - \sum_{\gamma \neq \beta} \sigma_{\gamma} \left(-\frac{\varepsilon_{\beta\gamma}}{2} \nabla^2 \phi_{\gamma} - \gamma_{\beta\gamma} \phi_{\gamma} \right) \right]. \quad (35)$$

4. Interpretation of the interface fields $\psi_{\alpha\beta}$

The interface fields $\psi_{\alpha\beta}$ are by their definition restricted to the finite interface regions $\overline{\mathcal{D}}_{\alpha} \cap \overline{\mathcal{D}}_{\beta}$.

At dual phase boundaries $\alpha \leftrightarrow \beta$ only one interface field $\psi_{\alpha\beta}$ is defined locally. At triple points $\alpha \leftrightarrow \beta \leftrightarrow \gamma$ three interface fields overlap $\psi_{\alpha\beta}$, $\psi_{\alpha\gamma}$, $\psi_{\beta\gamma}$, and at multiple points of order \tilde{N} , $\binom{\tilde{N}}{2}$ interface fields overlap.

The most remarkable feature of these fields is the fact that a variation $\delta\psi_{\alpha\beta}$ at a multiple point, where e.g. $0 < \phi_{\gamma}, \phi_{\alpha}, \phi_{\beta} < 1$, only affects the phases ϕ_{α} and ϕ_{β} , but is influenced by ϕ_{γ} . ϕ_{γ} itself, however, is not influenced by $\delta\psi_{\alpha\beta}$. ϕ_{γ} is only changed by $\delta\psi_{\alpha\gamma}$ or $\delta\psi_{\beta\gamma}$. The sum over all possible variations $\delta\psi_{\alpha\beta}$, $\delta\psi_{\alpha\gamma}$, $\delta\psi_{\beta\gamma}$ describes the whole variational problem. The timescale and the energy scale of the individual phase transformations can now be fixed in a unique way.

The release (or consumption) of latent heat \dot{q} of a multiple point of order \tilde{N} is then given by

$$\dot{q} = \sum_{\alpha=1}^{\tilde{N}} \dot{q}_{\alpha} = \sum_{\alpha=1}^{\tilde{N}} \sum_{\beta>\alpha}^{\tilde{N}} L_{\alpha\beta} \dot{\psi}_{\alpha\beta} = \sum_{\alpha=1}^{\tilde{N}} \sum_{\beta>\alpha}^{\tilde{N}} \frac{L_{\alpha\beta}}{\tau_{\alpha\beta}} \dot{\psi}_{\alpha\beta}, \quad (36)$$

where $\dot{\psi}_{\alpha\beta}$ in general is a nonlinear function of all present phases, and the $L_{\alpha\beta}$ and $\tau_{\alpha\beta}$ are the latent heat contributions and relaxation rates of the individual phase changes.

This is the desired decomposition of the multiple phase interactions at triple points into dual contributions. On the other hand, the static asymptotics of the multiphase theory is unchanged, i.e. the proof of stress balance at multiple points as given in [2,3] is still valid.

The derivation of the generalized model is possible in two ways: either treating the interface fields as linear transformations of the phase fields or treating them linearly independent in space of higher dimension $\binom{\tilde{N}}{2}$. Though both interpretations lead to the same result, we feel that the interpretation of $\psi_{\alpha\beta}$ being linearly independent is more general. Especially this interpretation removes the unaesthetic feature of the linear scheme, that the equations of motion depend on the order of the multiphase point (see Eqs. (33) and (34)). This is achieved by rescaling the time unit according to the ratios of the dimensions of the different spaces (27).

Additionally, the treatment is very general and not restricted to a certain free energy functional. We therefore feel that this scheme can have a wider application in many body theories besides the application to the multiphase change problem presented here.

In particular, the considered example indicates clearly that a relaxation ansatz in a field theory with multiple interacting fields is warranted only for a set of functionally independent fields and the Lagrange formalism has to be treated carefully with respect to the setting of time and energy scales.

5. Conclusion

A generalized field method for multiphase transformations is derived using interface fields. The interface fields $\psi_{\alpha\beta}$ may either be treated as linear transformations of the phase fields ϕ_{α} or as linear independent fields defined in

a $\binom{\tilde{N}}{2}$ dimensional space, in general being of higher dimension than the dimension $\tilde{N} - 1$ of the manifold of the phase fields ϕ_α . In both cases, the interface fields are seen to be generalized coordinates of the variational problem.

Not using these generalized coordinates, but using the Lagrange formalism and treating the basic variables ϕ_α independent is shown to mix time and energy scales.

The practical relevance of this model is that the time and energy scales of a multiphase change problem can be attributed uniquely to individual dual phase changes, and the whole multiphase problem is decomposed into a sum of dual phase changes.

References

- [1] I. Steinbach, F. Pezzolla, B. Nestler, M. Seeßelberg, R. Prieler, G.J. Schmitz, J.L.L. Rezende, *Physica D* 94 (1996) 135–147.
- [2] H. Garcke, B. Nestler, B. Stoth, *Physica D* 115 (1998) 87.
- [3] B. Nestler, A.A. Wheeler, *Phys. Rev. E* 57(3) (1998) 2602.
- [4] G. Fix, in: A. Fasano, M. Primicero (Eds.), *Free Boundary Problems, Research Notes in Mathematics*, vol. 2, Pitman, New York, 1983.
- [5] G. Caginalp, P.C. Fife, *Phys. Rev. B* 33 (1986) 7792.