# A nonlocal phase-field model with nonconstant specific heat


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EXAMPLE. $k$= the Newton potential $\longrightarrow k(|x|) = \kappa |x|^{-1}$ in 3D.

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$$\int_\Omega m^{N+2} k(|m(x-y)|^2)\,|\chi(x)-\chi(y)|^2\,dy$$

$$= \int_{\Omega_m(x)} k(|z|^2) \left| \frac{\chi\left(x+\frac{z}{m}\right)-\chi(x)}{\frac{1}{m}} \right|^2 dz$$

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for a sufficiently regular $\chi$, where $\nu = 2 \int_{\mathbb{R}^N} k(|z|^2)|z|^2 \, dz$ and $\Omega_m(x) = m(\Omega - x)$.

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- e.g., in solid-liquid phase transitions it may be $c_V(\chi) = c_V^0 + \chi(c_V^1 - c_V^0)$, where $c_V^0$ is the specific heat in the solid and $c_V^1$ in the liquid;

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- $\sigma$ and $\lambda$ are smooth functions;
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- e.g., $G(\chi(x) - \chi(y)) = |\chi(x) - \chi(y)|^2$ if $\varphi = I_{[-1,1]}$.

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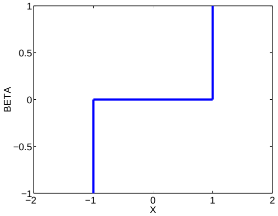
Subdifferential case: $\partial\varphi := \partial I_{[-1,1]} = \mathcal{H}^{-1}$:



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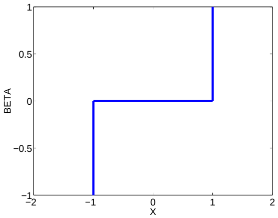
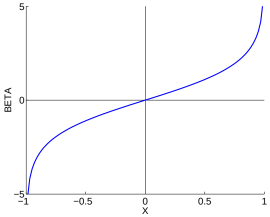



Logarithmic case: $\partial\varphi = \log(1+\chi) - \log(1-\chi)$:



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- the phase equation, which follows from the tendency of the system to move towards local minima of the free energy with speed proportional to $1/\mu(\vartheta)$

$$\mu(\vartheta)\frac{\partial \chi}{\partial t} \in -\delta_{\chi}\mathcal{F}[\vartheta,\chi].$$

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$$\Psi(\Omega') = \int_{\Omega'} (-b[\chi]\chi_t + B[\chi]_t)\, dx, \quad \text{where}$$

$$B[\chi](x,t) := \int_\Omega K(x,y)\, G(\chi(x,t) - \chi(y,t))\, dy,$$

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($\Rightarrow$ the entropy does not decrease along the solution paths).

# The equation for $\vartheta$

With these choices the internal energy balance becomes

$$\left(c_V(\chi(x))\vartheta(x) + \lambda(\chi(x)) + \beta\varphi(\chi(x))\right)_t$$
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coupled with the initial-boundary conditions

$$\vartheta(x,0) = \vartheta_0(x) \quad \text{in } \Omega,$$
$$\partial_{\mathbf{n}}\vartheta(s,t) = \gamma(s)(\vartheta_\Gamma(s,t) - \vartheta(s,t)) \quad \text{on } \Sigma_\infty := \partial\Omega \times (0,\infty),$$

where $\Delta$ is the Laplace operator, $\gamma$, $\vartheta_\Gamma \geq 0$ bounded. Let $\kappa = 1$ in the following.

# The inclusion for $\chi$

$$\mu(\vartheta(x))\chi_t(x) + \vartheta(x)\sigma'(\chi(x)) + \lambda'(\chi(x))$$
$$+ 2\int_\Omega K(x,y)G'(\chi(x) - \chi(y))\,dy + (\beta + \vartheta(x))\partial\varphi(\chi(x))$$
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which we couple with the initial condition

$$\chi(x,0) = \chi_0(x) \quad \text{in } \Omega,$$

where $\chi_0$ is a given initial configuration.

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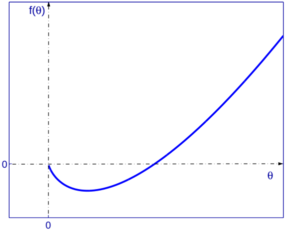
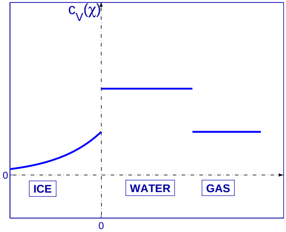
Then, $c_V'(\chi) := c_V^1 - c_V^0$ must have a positive sign, otherwise $\chi = -1$ would be the only stable equilibrium both for low and high $\vartheta$.



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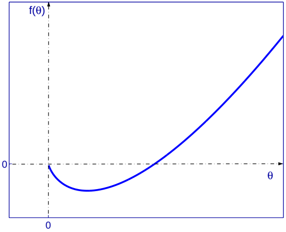


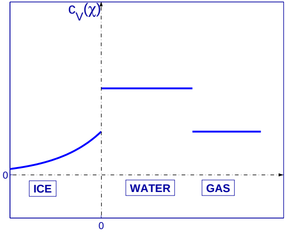


Hence, the model is appropriate for ice-water phase transitions (and also phase changes in alloys), but not, e.g., for water-vapour phase changes (where $c_V^1 < c_V^0$).

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(vi) There exist constants $\psi^* > \psi_* > 0$ such that $\psi^* \geq \psi_1(x) \geq \psi_*$ a. e., where $\psi_1 \in H^1$ is the eigenfunction with unit $H$-norm corresponding to the smallest eigenvalue $\lambda_1 \geq 0$ of

$$-\Delta\psi_1 = \lambda_1\psi_1 \quad \text{in } \Omega, \quad \partial_{\mathbf{n}}\psi_1 + \gamma\psi_1 = 0 \quad \text{on } \partial\Omega\,.$$

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(iv) $c_V \in W^{2,\infty}(\mathcal{D}(\varphi))$ such that $c_V(z) \geq c_0 > 0$ for all $z \in \mathcal{D}(\varphi)$;

(v) $\gamma \in L^\infty(\partial\Omega)$ is non-negative and $\vartheta_\Gamma \in L^\infty(\Sigma_\infty)$, $(\vartheta_\Gamma)_t \in L^2_{loc}(\Sigma_\infty)$, $\vartheta_\Gamma \geq \bar{\vartheta}_\Gamma > 0$ a.e. in $\Sigma_\infty$;

(vi) There exist constants $\psi^* > \psi_* > 0$ such that $\psi^* \geq \psi_1(x) \geq \psi_*$ a. e., where $\psi_1 \in H^1$ is the eigenfunction with unit $H$-norm corresponding to the smallest eigenvalue $\lambda_1 \geq 0$ of

$$-\Delta\psi_1 = \lambda_1\psi_1 \quad \text{in } \Omega, \quad \partial_{\mathbf{n}}\psi_1 + \gamma\psi_1 = 0 \quad \text{on } \partial\Omega\,.$$

(vii) $\mu$ is locally Lipschitz, $\mu_*(1+\tau) \leq \mu(\tau)\ \forall\, \tau \in \mathbb{R}^+$.

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$$\chi_0 \in L^\infty(\Omega)\,,\ \exists\, C_0 > 0\ :\ \chi_0(x) \in \mathcal{D}_{C_0}(\varphi)\ \text{ a.e. in } \Omega\,,$$

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$$\vartheta \in L^\infty(Q_\infty)\,,\ \vartheta_t, \Delta\vartheta \in L^2_{\text{loc}}(0,\infty\,;\, L^2(\Omega))\,,$$
$$\vartheta(x,t) > 0 \quad \text{a.e. in } Q_\infty := \Omega \times (0,\infty)\,,$$
$$\chi \in L^\infty_{\text{loc}}(Q_\infty),\ \chi_t \in L^\infty(Q_\infty);$$
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Moreover, there exist two positive constants $\overline{\vartheta}$ and $\underline{\vartheta}$ (independent of $t$) such that:

$$\underline{\vartheta} < \vartheta(x,t) < \overline{\vartheta} \quad \text{for a.e. } (x,t) \in Q_\infty.$$

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Let the same Hypotheses hold, and let $(\vartheta_1, \chi_1)$, $(\vartheta_2, \chi_2)$ be solutions to our problem associated with respective boundary and initial data $\vartheta_{\Gamma 1}, \vartheta_{01}, \chi_{01}$ and $\vartheta_{\Gamma 2}, \vartheta_{02}, \chi_{02}$.

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$$\int_0^T \int_\Omega |\hat{\theta}(x,t)|^2 \, dx \, dt + \max_{t \in [0,T]} \int_\Omega |\hat{\chi}(x,t)|^2 \, dx$$

$$\leq C_T \left( |\hat{\theta}_0|_H^2 + |\hat{\chi}_0|_H^2 + \int_0^T \int_{\partial\Omega} \gamma \hat{\theta}_\Gamma^2(x,t) \, ds \, dt \right) .$$

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- Prove uniqueness using a $L^1$-Lipschitz continuity of the solution operator associated to the differential inclusion related to the phase variable

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such that $\chi(x, t) \in \mathcal{D}_C(\varphi)$ a.e. in $Q_T$, $\chi_t \in L^\infty(Q_T)$, and

$$|f[\chi, \vartheta](x, t) - \alpha(\vartheta(x, t))\, \chi_t(x, t)| \le C \quad \text{a. e. in } Q_T\, .$$

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- Strong continuity $L^1(Q_T) \to L^p(Q_T)$ of the solution mapping for $p < \infty$ follows however from the uniform $L^\infty$-bound.

# MAXIMUM PRINCIPLE RESULT.

# Maximum principle result.

Fix a final time $T > 0$ and sufficiently regular and bdd $r$, $h_1$, $h_2$, $\gamma$, $u_\Gamma$, $u_0$ : $\gamma, r, u_\Gamma \geq 0$, $a(x,t) \geq a_* > 0$, and $u_*\psi_* < u_*\psi_1(x) \leq u_0(x) \leq u^*$ a. e.

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Then the following PROBLEM in $Q_T$ (for all $w \in H^1$)

$$\begin{cases} \int_\Omega a u_t w\,dx + \int_\Omega \langle \nabla u, \nabla w \rangle\,dx + \int_{\partial\Omega} \gamma(u - u_\Gamma) w\,ds \\ = \int_\Omega (r(x,t) + h_1(x,t)\,u \,+ h_2(x,t)\,u\,|\log|u||)\,w\,dx\,, \\ u(x,0) = u_0(x) \quad \text{a. e.} \end{cases}$$

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$$u_*\psi_1(x) e^{-H(t)} \leq u(x,t) \leq K \, e^{H(t)} \text{ a. e. },$$

where $H(t) = \frac{A}{a_*} \int_0^t \left(1 + e^{B\tau}\right) d\tau$, and $K$, $A$, and $B$ depend only on the data (not on T).

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Then there exists $C^* > 0$, depending on the data (but not on $a_1$, $H_0$, $H_1$, $E_0$) such that, for a. e. $t > 0$, it holds:

$$|u(t)|_{L^\infty(\Omega)} \le C^*\,(1 + H_0 + a_1)^{1+N/2}\,(1 + H_1 + E_0).$$

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$$\mu_\varrho(\vartheta) = \begin{cases} \mu(|\vartheta|) & \text{for } |\vartheta| \le \varrho\,, \\ \mu(\varrho) + \mu_*(|\vartheta| - \varrho) & \text{for } |\vartheta| > \varrho\,; \end{cases}$$

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Then, via Faedo-Galerkin method, for $T > 0$, we find a pair $(\vartheta, \chi)$ solving a. e. in $Q_T$ the system coupling the same equations as before for $\vartheta$, the same I.B.C. with

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$$\mu_\varrho(\vartheta) = \begin{cases} \mu(|\vartheta|) & \text{for } |\vartheta| \le \varrho\,, \\ \mu(\varrho) + \mu_*(|\vartheta| - \varrho) & \text{for } |\vartheta| > \varrho\,; \end{cases}$$

$$f_\varrho(\vartheta) = \begin{cases} 1 & \text{for } \vartheta \le 0\,, \\ 1 - \log\vartheta & \text{for } 0 < \vartheta < \varrho\,, \\ 1 - \log\varrho & \text{for } \vartheta \ge \varrho\,, \end{cases}$$

Then, via Faedo-Galerkin method, for $T > 0$, we find a pair $(\vartheta, \chi)$ solving a. e. in $Q_T$ the system coupling the same equations as before for $\vartheta$, the same I.B.C. with

$$\mu_\varrho(\vartheta)\chi_t + c_V'(\chi)\vartheta f_\varrho(\vartheta) + \lambda'(\chi) + \vartheta\sigma'(\chi) + (\beta + |\vartheta|)\partial\varphi(\chi)$$
$$+ \int_\Omega K(x,y)G'(\chi(x) - \chi(y))\,dy \ni 0.$$

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By Hypothesis $f[\vartheta, \chi]$ is bdd for all $\vartheta$, $\chi \in L^1(Q_T)$, $\chi \in \mathcal{D}(\varphi)$. Hence, the assumptions of PROPOSITION (DI) are satisfied. We thus may define the solution mapping

$$A_\varrho : L^1(Q_T) \to L^\infty(Q_T) : \vartheta \mapsto \chi,$$

which with each $\vartheta \in L^1(Q_T)$ associates the solution $\chi$ to (**??**) with fixed initial condition $\chi_0$.

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We may test with $\vartheta_t$ the equation for $\vartheta$ and integrate over $(0, t)$ with $t \in (0, T]$, obtaining

$$|\vartheta_t|_{L^2(0,T;L^2(\Omega))} + |\vartheta|_{L^\infty(0,T;H^1(\Omega))} \ \leq \ c(1 + \log \varrho),$$

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with $c$ independent of $\varrho$. It remains to prove the positivity and a uniform upper bound for the $\vartheta$-component of the solution to the approximating problem.

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Choosing in the Maximum principle result $u = \vartheta$, and

$$a(x,t) = c_V(\chi), \quad r(x,t) = \frac{\mu_\varrho(\vartheta)}{1+|\vartheta|}\chi_t^2,$$

$$h_1(x,t) = \sigma(\chi)_t + \mathrm{sign}(\vartheta)\left(\varphi(\chi)_t + \frac{\mu_\varrho(\vartheta)}{1+|\vartheta|}\chi_t^2\right),$$

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we get $\vartheta > 0$ a. e. in $Q_T$, hence we can remove the absolute value from the truncated problem.

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Apply the MOSER ITERATION SCHEME to

$$c_V(\chi)\vartheta_t - \Delta\vartheta = -c_V'(\chi)\chi_t\vartheta - b[\chi]\chi_t - (\lambda(\chi) + \beta\varphi(\chi))_t\,,$$

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$$\varrho > \bar{c}(1 + \log\varrho)^{2+N/2},$$

it follows that $\vartheta, \chi$ are also solutions of the starting equations.

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