Cahn-Hilliard Equation Analysis

Jinghao Chen
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Introduction

Notes: in the following context, [A] represents Anguige's paper, while [W] represents Witelski's thesis. Also, we let the viscosity/perturbation $\varepsilon \sim h$ on the same level as the spatial discretization size.

Recall in [A], we derived the continuum limit from our original discrete model:

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2 K(\rho)}{\partial x^2} + \mathrm{O}(h^2)$$

where

$$K(\rho) \coloneqq \rho(1 - 2\alpha\rho + \alpha\rho^2) = \rho - 2\alpha\rho^2 + \alpha\rho^3$$

was called reduced chemical potential in [W].

From higher order Taylor expansion, we got higher accuracy limit:

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2}{\partial x^2}\left(K(\rho) + h^2 \left(\alpha\rho(\rho-1)\frac{\partial^2 \rho}{\partial x^2} - \alpha\rho\left(\frac{\partial \rho}{\partial x}\right)^2 + \frac{1}{12}\frac{\partial^2 K(\rho)}{\partial x^2} \right) \right) + O(h^4)$$

Here we have our modified equation:

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2}{\partial x^2}\left(K(\rho) + h^2 G_\alpha(\rho)\right)$$

with

$$G_\alpha(\rho) \coloneqq \alpha\rho(\rho-1)\frac{\partial^2 \rho}{\partial x^2} - \alpha\rho\left(\frac{\partial \rho}{\partial x}\right)^2 + \frac{1}{12}\frac{\partial^2 K(\rho)}{\partial x^2}$$

In the stability analysis, we found the diffusion term becomes negative in a determined interval I_α when $\alpha \geq \frac{3}{4}$, so our modified equation can be categorized as a Cahn-Hilliard equation, which is the same type in [W].

The equilibrium problem

Consider the steady state:

$$\frac{\partial^2}{\partial x^2}\left(K(\rho) + h^2 G_\alpha(\rho)\right) = 0$$

([A] theorem 2, page 400) Initial condition $\rho(x,0) = \rho_I(x)$ with $0 \leq \rho_I(x) \leq 1$ (reasonable density representation) and $\int_0^1 \rho_I(x)dx = M$ (mass conservation). Notice that there is a similar but different initial condition in [W]: $\rho(0) = 1$ and $\rho(1) = 0$. Additionally, we have homogeneous Neumann boundary condition at $x = 0, 1$, i.e. $\frac{\partial \rho}{\partial x}(0,t) = \frac{\partial \rho}{\partial x}(1,t) = 0$.

Integrating the steady state equation twice yields

$$K(\rho) + h^2 G_\alpha(\rho) = ax + b$$

Where a and b are integration constants.

Here we see h as ε in the perturbation theory, then the leading order equation in the outer expansion is the following:

$$K(\rho) = ax + b$$

Assume in the steady state, $\rho(0,t)=\rho_0,\ \rho(1,t)=\rho_1$ (this is outside of jumps/oscillation, so can be determined). Take into the equation above:

$$K(\rho_0)=b$$
$$K(\rho_1)=a+b$$

So

$$a=K(\rho_1)-K(\rho_0),\qquad b=K(\rho_0)$$

Here we get the multi-valued implicit outer solution for the leading order equation:

$$x(\rho)=\frac{K(\rho)-K(\rho_0)}{K(\rho_1)-K(\rho_0)}$$

Return back to the full problem, we have

$$K(\rho)+h^2G_\alpha(\rho)=\big(K(\rho_1)-K(\rho_0)\big)x+K(\rho_0)$$

Plug $x(\rho)=\frac{K(\rho)-K(\rho_0)}{K(\rho_1)-K(\rho_0)}$ into the equation above, we see that the outer solution cannot satisfy the full problem for any $h>0$, so we insert a shock layer, assume the existence of a sharp interface of width $\mathrm{O}(h)$ at some position x_s (the width of this interface can be set as ε at first and determined later to be exactly h). The corresponding stretched variable (inner variable) is

$$\tilde{x}\coloneqq\frac{x-x_s}{h}\quad\Rightarrow\quad x=h\tilde{x}+x_s,\qquad\frac{d\tilde{x}}{dx}=\frac{1}{h}$$

Correspondingly

$$\begin{aligned}G_\alpha(\rho)&=\alpha\rho(\rho-1)\frac{\partial^2\rho}{\partial x^2}-\alpha\rho\left(\frac{\partial\rho}{\partial x}\right)^2+\frac{1}{12}\frac{\partial^2K(\rho)}{\partial x^2}\\&=\alpha\rho(\rho-1)\frac{\partial^2\rho}{\partial\tilde{x}^2}\cdot\frac{1}{h^2}-\alpha\rho\left(\frac{\partial\rho}{\partial\tilde{x}}\right)^2\cdot\frac{1}{h^2}+\frac{1}{12}\frac{\partial^2K(\rho)}{\partial\tilde{x}^2}\cdot\frac{1}{h^2}\\&=\frac{1}{h^2}G_\alpha(\tilde{\rho})\end{aligned}$$

The notation $\tilde{\rho}=\tilde{\rho}(\tilde{x},t)=\rho(x,t)$. So

$$K(\rho)+h^2G_\alpha(\rho)\Rightarrow K(\tilde{\rho})+G_\alpha(\tilde{\rho})$$

We get

$$K(\tilde{\rho})+G_\alpha(\tilde{\rho})=c+\mathrm{O}(h)$$

With

$$c \coloneqq ax_s + b = \big(K(\rho_1) - K(\rho_0)\big)x_s + K(\rho_0)$$

And $O(h)$ is $\big(K(\rho_1) - K(\rho_0)\big)\tilde{x}h$ comes from $x = h\tilde{x} + x_s$ on the RHS of the full problem. Now check $O(1)$ level equation $K(\tilde{\rho}) + G_\alpha(\tilde{\rho}) = c$, the general solution (leading order solution) is ([W] (3.19))

$$\tilde{x} - \tilde{x}_0 = -\int_{\tilde{\rho}_0}^{\tilde{\rho}} \frac{dP}{\sqrt{2(F(\rho) - c\rho)}}$$

where $\tilde{x}_0$ and $\tilde{\rho}_0$ are constants of integration, and

$$F(\rho) = \int_0^\rho K(P)dP\,, \qquad \tilde{\rho}(\tilde{x}_0) = \tilde{\rho}_0$$

Recall $K(\rho) \coloneqq \rho(1 - 2\alpha\rho + \alpha\rho^2) = \rho - 2\alpha\rho^2 + \alpha\rho^3$, so we can explicitly define

$$F(\rho) = \frac{\rho^2}{2} - \frac{2\alpha\rho^3}{3} + \frac{\alpha\rho^4}{4}$$

This was called free energy density in [W].

Now take a look at the jump through the interface. The density right on the left of this interface is $\bar{\rho}_1$, while right on the right of this interface is $\bar{\rho}_2$, so we have

$$\lim_{\tilde{x}\to-\infty} \tilde{\rho} = \bar{\rho}_1, \qquad \lim_{\tilde{x}\to+\infty} \tilde{\rho} = \bar{\rho}_2$$

The left side $K(\bar{\rho}_1) = ax_s + b = \big(K(\rho_1) - K(\rho_0)\big)x_s + K(\rho_0) = c$, the same as the right side, $K(\bar{\rho}_2) = ax_s + b = \big(K(\rho_1) - K(\rho_0)\big)x_s + K(\rho_0) = c$, so

$$K(\bar{\rho}_1) = K(\bar{\rho}_2) = c$$

Then back to our general leading order solution

$$\tilde{x} - \tilde{x}_0 = -\int_{\tilde{\rho}_0}^{\tilde{\rho}} \frac{dP}{\sqrt{2(F(\rho) - c\rho)}}$$

Either $\tilde{x} \to -\infty$ or $\tilde{x} \to +\infty$, requiring the denominator $F(\rho) - c\rho \to 0$ in the corresponding cases, which means

$$F\big(\bar{\rho}_j\big) - c\bar{\rho}_j = 0, \qquad j = 1, 2$$

So

$$\int_0^{\bar{\rho}_j} K(P)dP - c\int_0^{\bar{\rho}_j} 1\, dP = 0 \Rightarrow \int_0^{\bar{\rho}_j} (K(P) - c)dP = 0, \qquad j = 1,2$$

which implies a necessary condition:

$$\int_{\bar{\rho}_1}^{\bar{\rho}_2} (K(P) - c)dP = 0$$

This is so called equal area rule in [W], and this equation with 2 of $F(\bar{\rho}_j) - c\bar{\rho}_j = 0$ forms a system yields the shock position x_s as

$$x_s = \frac{c - K(\rho_0)}{K(\rho_1) - K(\rho_0)} = x(\rho_s)$$

Where ρ_s is the one on the middle branch of our multi-valued outer solution $x(\rho) = \frac{K(\rho) - K(\rho_0)}{K(\rho_1) - K(\rho_0)}$ such that $x(\rho_s) = x_s$. From here we get $c = K(\rho_s)$.

The dynamic problem

Consider time-dependent Cahn-Hilliard equation:

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2}{\partial x^2}\big(K(\rho) + h^2 G_\alpha(\rho)\big)$$

The dynamic shock layer should be similar to the equilibrium case. In fact, in this section, we will derive their connection. Set the moving shock position $x_s \coloneqq s(t)$, which will be determined later by the outer solution. Consider an inner expansion

$$\tilde{x} \coloneqq \frac{x - s(t)}{h} \quad \Rightarrow \quad x = h\tilde{x} + s(t), \qquad \frac{\partial \tilde{x}}{\partial x} = \frac{1}{h}, \qquad \frac{\partial \tilde{x}}{\partial t} = -\frac{s'(t)}{h}$$

So, the RHS (inside is the same as the equilibrium case):

$$\frac{\partial^2}{\partial x^2}\big(K(\rho) + h^2 G_\alpha(\rho)\big) = \frac{\partial^2}{\partial x^2}\big(K(\tilde{\rho}) + G_\alpha(\tilde{\rho})\big) = \frac{1}{h^2} \cdot \frac{\partial^2}{\partial \tilde{x}^2}\big(K(\tilde{\rho}) + G_\alpha(\tilde{\rho})\big)$$

And the LHS by the chain rule:

$$\frac{\partial \rho}{\partial t} = \frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial \tilde{\rho}}{\partial \tilde{x}} \cdot \frac{\partial \tilde{x}}{\partial t} = \frac{\partial \tilde{\rho}}{\partial t} - \frac{s'(t)}{h} \cdot \frac{\partial \tilde{\rho}}{\partial \tilde{x}}$$

Here $\frac{\partial \tilde{\rho}}{\partial t}$ represents the partial derivative w.r.t t position, not w.r.t t variable for overall expression of $\tilde{\rho}$.

Now combine LHS and RHS, we get

$$h^2 \frac{\partial \tilde{\rho}}{\partial t} - hs'(t) \frac{\partial \tilde{\rho}}{\partial \tilde{x}} = \frac{\partial^2}{\partial \tilde{x}^2} \left(K(\tilde{\rho}) + G_\alpha(\tilde{\rho}) \right)$$

From the leading order expansion ($\frac{\partial^2}{\partial \tilde{x}^2} \left(K(\tilde{\rho}) + G_\alpha(\tilde{\rho}) \right) = 0$) we get

$$K(\tilde{\rho}) + G_\alpha(\tilde{\rho}) = A\tilde{x} + B$$

A and B are integration "constants" which are possibly functions of time. To match with outer solution, check $\tilde{x} \to \infty$ with equilibrium data (finite, smooth), we conclude that $A \equiv 0$ to avoid blowing up on the RHS. So, we have

$$K(\tilde{\rho}) + G_\alpha(\tilde{\rho}) = B$$

Which is the same equation as steady state shock $K(\tilde{\rho}) + G_\alpha(\tilde{\rho}) = c$, and therefore we obtain the same equal area rule for shock placement to leading order.

Similarity solutions and multivalued solutions

[W] mentioned "by specifying the conserved quantity in the system, a unique shock equation is determined", here in our system, mass is conserved so the density function ρ should be considered as that conserved quantity. Let's rewrite our nonlinear diffusion equation into conservation form:

$$\frac{\partial \rho}{\partial t} + \frac{\partial q}{\partial x} = 0$$

Where the flux is given by

$$q \coloneqq -\frac{\partial K(\rho)}{\partial x} = -D(\rho) \cdot \frac{\partial \rho}{\partial x}$$

In this form we can derive the motion of the shock ([W] (3.49)):

$$\frac{ds}{dt} = \frac{[q]}{[\rho]} = -\frac{[K(\rho)_x]}{[\rho]}$$

To determine the location, let's introduce similarity solution in the following form:

$$\rho(x,t) = \hat{\rho}(z), \qquad z = \frac{x}{\sqrt{t}}$$

This will reduce our equation into an ODE as the following (justified in the manuscript):

$$\frac{1}{2} z\hat{\rho}'(z) = -\big(D(z)\hat{\rho}'(z)\big)' = -K''\big(\hat{\rho}(z)\big)$$

so back to the shock condition, we have (justified in the manuscript):

$$\frac{1}{2} z_s = -\frac{[D(\hat{\rho})\hat{\rho}'(z)]}{[\hat{\rho}(z)]}$$

On the other hand, the solution of $\frac{1}{2} z\hat{\rho}'(z) = -K''\big(\hat{\rho}(z)\big)$ is in the form

$$\hat{\rho}(z) = \begin{cases} \bar{\rho}_1, & 0 \le z < z_s \\ \bar{\rho}_2, & z > z_s \end{cases}$$

which implies $[K(\hat{\rho})] = 0$, i.e. C^0 continuous at the shock position z_s. To see this, let's take this step function $\hat{\rho}(z)$ into the LHS of our reduced ODE. Its derivative contains Dirac delta function, so in order to balance this singularity, the RHS of our reduced ODE, which is $-K''(\hat{\rho})$, must act like a delta function. Hence, $K'(\hat{\rho})$ is like step function, implying that $K(\hat{\rho})$ must be C^0 continuous at the shock position z_s, i.e. $[K(\hat{\rho})] = 0$.

The following 5 restrictions determine the shock position x_s from $x_s = z_s\sqrt{t}$:

- $[K(\hat{\rho})] = 0$ (C^0 condition)
- $\frac{1}{2} z_s = -\frac{[D(\hat{\rho})\hat{\rho}\prime(z)]}{[\hat{\rho}(z)]}$ (shock condition)
- $\rho(0,t) = \rho_0,\ \rho(1,t) = \rho_1$ (boundary conditions)
- $\int_{\bar{\rho}_1}^{\bar{\rho}_2} (K(P) - c)dP = 0$ (equal area rule)

Implicit reduced ODE

Just like what we did in the equilibrium problem, we can also derive the implicit form for our reduced Cahn-Hilliard equation

$$\frac{1}{2} z\hat{\rho}'(z) = Q'(z) = -\big(D(z)\hat{\rho}'(z)\big)'$$

where $Q(z) \equiv -D(z)\hat{\rho}'(z)$ is the similarity flux, and its relation with the original flux is $q(x,t) = t^{-\frac{1}{2}} \cdot Q(z)$.

$$\frac{1}{2} z\hat{\rho}'(z) = Q'(z) \;\Leftrightarrow\; \frac{1}{2} z \frac{d\hat{\rho}}{dz} = \frac{dQ}{dz} \;\Rightarrow\; \frac{1}{2} z = \frac{dQ}{dz} \cdot \frac{dz}{d\hat{\rho}} = \frac{dQ}{d\hat{\rho}}$$

So we have the problem in inverse variables:

$$\frac{1}{2} z(\hat{\rho}) = \frac{dQ}{d\hat{\rho}}$$

Introduce the inverse-flux to derive our final alternative equation

$$J(\hat{\rho}) \coloneqq -\frac{1}{D(\hat{\rho})} \cdot \frac{dz}{d\hat{\rho}} \equiv \frac{1}{Q(z)}$$

Now

$$\begin{aligned}
\frac{1}{2} z(\hat{\rho}) &= \frac{dQ}{d\hat{\rho}} \\
&= \frac{d}{d\hat{\rho}} \left(\frac{1}{J(\hat{\rho})} \right) \\
&= -\frac{1}{J^2} \cdot J' \\
&= -\frac{1}{\frac{z'^2}{D^2}} \cdot \left(-\frac{z''D - z'D'}{D^2} \right) \\
&= \frac{D^2}{z'^2} \cdot \frac{z''D - z'D'}{D^2} \\
&= \frac{z''D - z'D'}{z'^2}
\end{aligned}$$

So we got the alternative form of ODE for similarity solutions:

$$\frac{1}{2} z z'^2 = D(\hat{\rho}) z'' - D'(\hat{\rho}) z'$$

For the diffusion equation of porous media type, this form is easier to solve as shown in [W]. However, recall our diffusion term $D(\rho) = K'(\rho) = 3\alpha \left(\rho - \frac{2}{3} \right)^2 + 1 - \frac{4}{3}\alpha$, so $D(0) = 1 \neq 0$. This is not porous media type. Hence the similarity solutions do not have compact support and the leading edge of the region $z_* \to \infty$.

Summary

(1) The equal-area rule also holds for [A]’s model on both equilibrium problem and dynamic problem, which is an important condition to determine the shock position.

(2) [W]'s similarity solutions can be derived from [A]'s model, as both models share the same leading order equation.

(3) The complex inside of the modified equation affects the shock layer analysis, but width = h scale works well for building the interface on the jump.

(4) $D'(0) = 1 \neq 0$ in [A]'s model, which means it's not a porous media type so similarity solutions have no compact support, and those subsequent results from [W] need to be further modified.