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On Global Minimizers for a Variational Problem with non-local effect related to micro-phase separation

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1 Introduction

In this note we consider the following functional

$$F_{\varepsilon,\sigma}(u) := \int_\Omega \{\frac{\varepsilon^2}{2}|\nabla u|^2 + W(u) + \frac{\sigma}{2}|(-\triangle_N)^{-\frac{1}{2}}(u-\overline{u})|^2\}dx, \tag{1}$$

$$\overline{u} := \frac{1}{|\Omega|}\int_\Omega u dx, \qquad u \in H^1(\Omega),$$

where Ω is a smooth bounded domain in $\mathbf{R}^n$, $W(u)$ is a double-well potential with global minima $u = \pm 1$, typically of the form $\frac{1}{4}(u^2-1)^2$, ε and σ are positive constants, $H^1(\Omega)$ is the usual Sobolev space, and $(-\triangle_N)^{-\frac{1}{2}}$ is a fractional power of the Laplace operator under the zero flux boundary condition. (The underlying space for the Laplace operator is the subspace of $L^2(\Omega)$ orthogonal to constants. See Henry [6] for details.) The third term is of nonlocal, since $(-\triangle_N)^{-\frac{1}{2}}$ is, roughly speaking, an integral operator in Ω. Without this term, (1) becomes a well-known functional from which we can derive the Allen-Cahn (non-conserved) and the Cahn-Hilliard (conserved) equations.

The functional (1) was first introduced in a different form by [11] and [1], then formulated like (1) in [10] in order to describe the micro-phase separation of diblock copolymer where two different homopolymers are connected and this connectivity is responsible for introducing the long range interaction, i.e., the nonlocal term of (1). The parameter σ is inversely proportional to the square of the total chain length N of the copolymer, and ε represents the interfacial thickness at the bonding point assumed to be sufficiently small, and the average $\overline{u}$ $(-1 < \overline{u} < 1)$ stands for the ratio of components of two homopolymers. In this note we focus on a scaling regime $0 < \varepsilon \ll 1$. The above micro constraint (connectivity) prevents copolymer from forming a large domain and hence usual coarsening process stops at certain stage of mesoscopic level. Namely, (1) has a potential to have a variety of metastable states (local minimizers) with fine structures, which is not the case for the usual Cahn-Hilliard dynamics, although it has a long and interesting coarsening process. When one tries to minimize the functional (1), one easily see that there is a competition between the first gradient term and the third nonlocal term, assuming that u is close to 1 or -1 off the interface. The first term wants to minimize the area of interface, however the nonlocal term does not become small if u takes 1 or -1 in a large domain. In order to make the third term small, u has to oscillate rapidly around $\overline{u}$ (which increases the area of interface), in other words if $u - \overline{u}$ converges to zero in weak sense in $L^2(\Omega)$, it goes to zero because of the compactness of the operator $(-\triangle_N)^{-\frac{1}{2}}$. Thus there should be an optimal domain size compromizing these two opposite tendencies. The main problems in [10] were the following:

(I) Scaling law: Characterize the domain size in terms of ε and σ.

(II) Morphology: Find a governing system of equations for the morphology of final states.

(III) Stability and selection mechanism of morphology.

The aim of this note is to answer the question (I) in one-dimensional space rigorously. Experimentally and numerically it is well-known in copolymer problems that the final asymptotic states prefer periodic structures such as lamellar, spherical, double-diamond geometries and so on (see, for instance [3], [4], [5], and [1]). Once one of the periodic structures is specified, it is not so difficult to determine the size of periodic cell which minimizes the functional (1) within the specified class (see [11]). Moreover, it is even possible at least fomally to derive a scaling law without specifying the periodic structure via dimensional analysis (see [1]). Those arguments may be physically convincing, however, it is still unclear mathematically why such scale is preferred independent of the precise structures. Our result in the next section determines completely the principal part of asymptotic expansion of the period and the free energy for the global minimizers in terms of ε and σ.

2 Main Results and Discussions

The evolutional equation associated with the functional of (1) can be obtaind by taking a gradient operator in some function space. However in order to make the resulting equation a conserved one of local operator form, the usual $L^2(\Omega)$ is not an appropriate space. According to Fife [2], $H^{-1}(\Omega)$ is a nice space for our purpose and the resulting equation becomes

$$
\begin{aligned}
(2) \qquad u_t &= \triangle\{-\varepsilon^2\triangle u - f(u) + \sigma(-\triangle_N)^{-1}(u-\overline{u_0})\} && \text{in } \Omega,\\
&= \triangle\{-\varepsilon^2\triangle u - f(u)\} - \sigma(u-\overline{u_0}) && \text{in } \Omega,\\
u(x,0) &= u_0(x) &&\\
\tfrac{\partial u}{\partial n} &= \tfrac{\partial \triangle u}{\partial n} = 0 && \text{on } \partial\Omega,\\
\tfrac{1}{|\Omega|}\textstyle\int_\Omega u_0(x)dx &= \overline{u_0}: && \text{a given constant,}
\end{aligned}
$$

where we define $f(u)$ by $f(u) := -W'(u)$ and n is the unit outward normal to $\partial\Omega$. It is clear that (2) is a conservative equation under the above boundary conditions.

Let $w(x)$ be a stationary solution of (2), i.e., a solution of

$$
\begin{aligned}
(3) \qquad \varepsilon^2\triangle w + f(w) - \sigma(-\triangle_N)^{-1}(w-\overline{u_0}) &= \text{ const. }, && \text{in } \Omega,\\
\tfrac{\partial w}{\partial n} &= 0, && \text{on } \partial\Omega,\\
\tfrac{1}{|\Omega|}\textstyle\int_\Omega w(x)dx &= \overline{u_0}. &&
\end{aligned}
$$

We define $q(x)$ as $f'(w(x))$. Then the linearized eigenvalue problem of (2) about $w(x)$ is

$$
\begin{aligned}
(4) \qquad -\triangle\{-\varepsilon^2\triangle - q(x)I + \sigma(-\triangle_N)^{-1}\}\phi &= \lambda\phi, && \text{in } \Omega,\\
\tfrac{\partial\phi}{\partial n} &= \tfrac{\partial\triangle\phi}{\partial n} = 0, && \text{on } \partial\Omega,\\
\textstyle\int_\Omega \phi dx &= 0. &&
\end{aligned}
$$

We now state our main results about the structure of global minimizers. We assume that the domain Ω is the one-dimensional unit interval $(0,1)$ in what follows.

Theorem 2.1 *Let ε be small enough and $0 < \sigma \le \sigma_0$ for any fixed positive constant σ_0. Assume moreover that $\frac{\varepsilon}{\sigma}$ is also small enough, and that $W(u)$ is symmetric and that $\overline{u} = 0$. Then we have*

(1) There exist at most four global minimizers (up to folding up) of $F_{\varepsilon,\sigma}(u)$.

(2) A global minimizer $\underline{u_{\varepsilon,\sigma}}$ is spatially periodic and its period $P_{\varepsilon,\sigma}$ has the following form;

$$P_{\varepsilon,\sigma} = 2\left(6\sqrt{2}A_0\frac{\varepsilon}{\sigma}\right)^{1/3} + O\left(\left(\frac{\varepsilon}{\sigma}\right)^{2/3}\right),$$

(3) The free energy of $\underline{u_{\varepsilon,\sigma}}$ satisfies the following equality;

$$\frac{2}{\sigma}F_{\varepsilon,\sigma}(\underline{u_{\varepsilon,\sigma}}) = \frac{1}{4}\left(6\sqrt{2}A_0\frac{\varepsilon}{\sigma}\right)^{2/3} + O\left(\left(\frac{\varepsilon}{\sigma}\right)^{4/3}\right),$$

where

$$A_0 = 2\int_{-1}^{1}\sqrt{W(\tau)}d\tau.$$

The proof of the above theorem is based on the idea of S. Müller [12], who treats a different problem related to solid-solid phase transition. We first construct a periodic candidate for the minimizer and then show that it is optimal and that any other minimizer has to be periodic as well. For this purpose we prove that the candidate is approximated by the adequately rescaled solution of the following ordinary differential equation:

$$\begin{aligned} -2q'' + W'(q) &= 0, \\ q(0) &= 0, \\ q'(0) &= \sqrt{W(0)}. \end{aligned} \tag{5}$$

Then, we estimate the precise order of its approximation in terms of ε and σ.

So far we have concentrated on global minimizers. What about local minimizers of (1)? For this purpose it is more convenient to rewrite (3) in the following system:

$$\begin{aligned} \varepsilon\triangle w + f(w) &= y, && \text{in } \Omega, \\ \triangle y + \sigma(w - \overline{u_0}) &= 0, && \text{in } \Omega, \\ \frac{\partial y}{\partial n} = \frac{\partial w}{\partial n} &= 0, && \text{on } \partial\Omega, \\ \int_\Omega w dx &= \overline{u_0}. \end{aligned} \tag{6}$$

This is quite similar to the stationary problem of activator-inhibitor system (see, for instance, [7]). It can be proved for each fixed $n \in \mathbf{N}$, (6) has a n-layered solution for small ε. The SLEP method developped in [7] and [9] seems to work out to prove the following conjecture;

Conjecture 2.2 *For any natural number n and any $\sigma \in (0, \sigma_0]$, there exists a constant $\varepsilon_0 = \varepsilon_0(n, \sigma_0)$ such that, if $0 < \varepsilon < \varepsilon_0$, the n-layered solution of (3) is exponentially stable.*

The linearized problem (4) at an n-layered solution takes the following form:

$$
(7) \qquad \begin{aligned}
\triangle\psi + (\lambda - \sigma)\,\phi &= 0, && \text{in } \Omega, \\
(\varepsilon^2 \triangle + q(x) I)\,\phi + \psi &= 0, && \text{in } \Omega, \\
\tfrac{\partial \phi}{\partial n} &= 0, && \text{on } \partial\Omega, \\
\tfrac{\partial \psi}{\partial n} &= 0, && \text{on } \partial\Omega, \\
\textstyle\int_\Omega \phi dx &= 0.
\end{aligned}
$$

This seems to fit the framework of the SLEP method. The conjecture claims that there are many small valleys (local minimizers) besides the deepest valleys (global minimizers), hence the profile of the functional looks like a *rugged landscape.*

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