# Spectral Analysis and Coarsening Rates for the Cahn–Hilliard Equation

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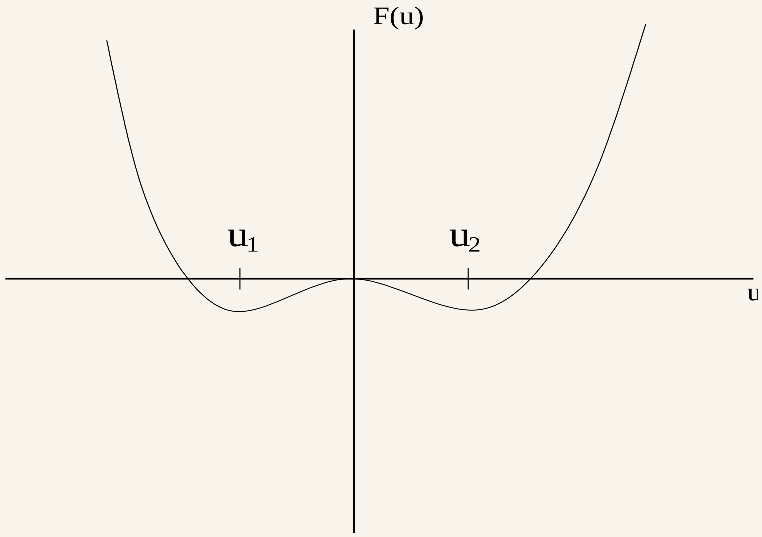
SIAM Conference on Applications of Dynamical Systems, May 18, 2009

# The Cahn–Hilliard Equation

We consider the Cahn–Hilliard equation on $\mathbb{R}^n$ (focus on $n = 1$)

$$u_t = \Delta(-\epsilon^2 \Delta u + F'(u)),$$

where we assume $F(u)$ has a double well form.



## The Physical Setting

One setting in which the Cahn–Hilliard equation arises is in the modeling of spinodal decomposition, a phenomenon in which the rapid cooling of a homogeneously mixed binary alloy causes separation to occur, resolving the mixture into regions in which one component or the other is dominant, with these regions separated by steep transition layers.

In this context, $u$ denotes the concentration of one component of the alloy (or a convenient affine transformation of this concentration), $F$ denotes the bulk free energy density of the alloy, and $\epsilon^2$ is a measure of interfacial energy.

Our emphasis will be on the rate at which this separation occurs.

# The Stationary Solutions

We focus on $n = 1$:

$$u_t = (-\epsilon^2 u_{xx} + F'(u))_{xx}.$$

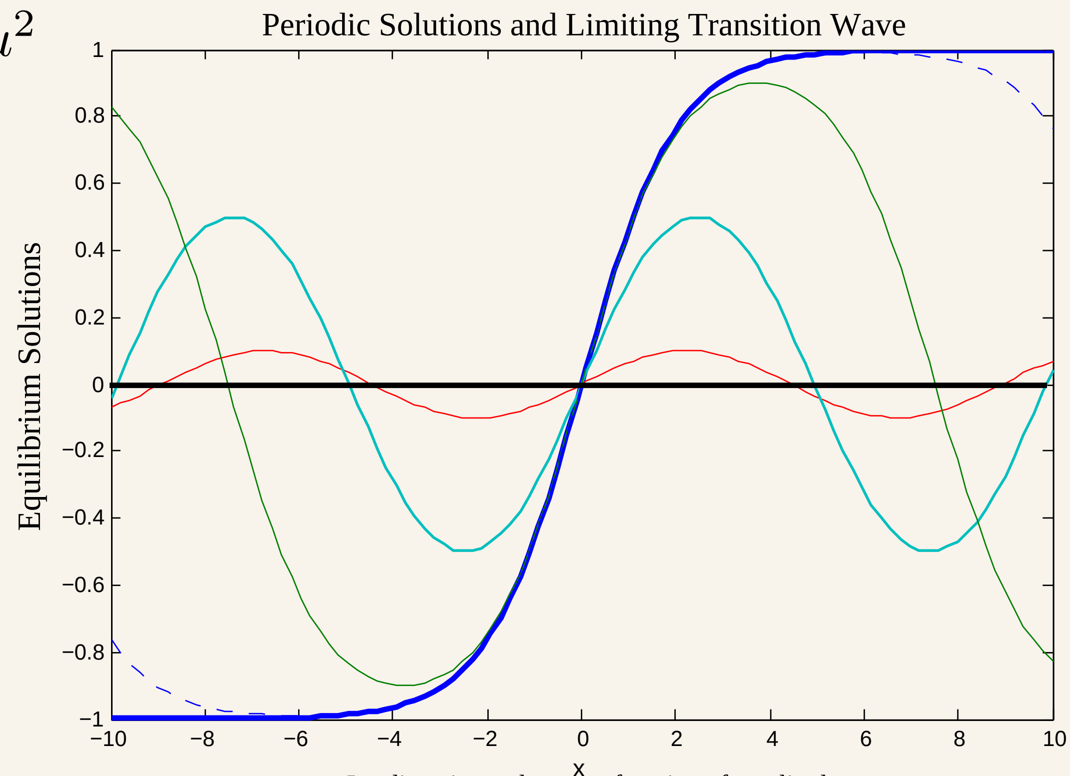
In this case, there are only three types of bounded non-constant stationary solutions $\bar{u}(x)$ to (CH).

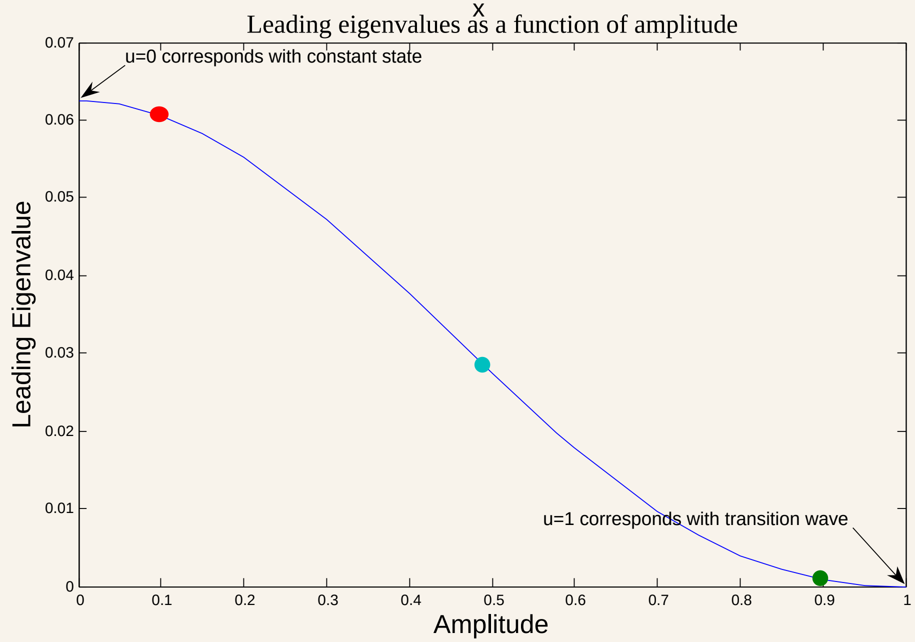
- Periodic solutions
- Pulse type ($reversal$) solutions $\bar{u}(\pm\infty) = u_{\pm}$, $u_- = u_+$
- Transition waves $\bar{u}(\pm\infty) = u_{\pm}$, $u_- \neq u_+$

The homogeneous state corresponds with a constant solution to $u(t, x) \equiv u_h$, which is typically in the spinodal region $\{u : F''(u) < 0\}$.

$$F(u) = \frac{1}{8}u^4 - \frac{1}{4}u^2$$

$$\epsilon^2 = 1$$



## Langer’s View of Coarsening

In the paper, *Theory of Spinodal Decomposition in Alloys* [Annals of Physics **65** (1971) 53–86], James Langer suggested the following view of coarsening:

*1. A decomposing alloy, at least during the late stages of coarsening, spends most of its time in configurations which are nearly stationary solutions of the Cahn–Hilliard equation.*

*2. The rate of decay of one of these almost stationary configurations is determined primarily by thermal fluctuations.*

*3. The rate of coarsening may be determined by using fluctuation theory to compute the rate of decay of exactly stationary solutions.*

## Langer's statistical model

Langer divides a finite volume $U$ into $N/\nu$ microregions, each containing $\nu$ lattice points. Let $\boldsymbol{\eta}$ denote a vector with component $\eta_j$ corresponding with the average composition of microregion $j$. Let $\rho(t, \boldsymbol{\eta})$ denote the probability distribution function over the states $\boldsymbol{\eta} \in \mathbb{R}^{N/\nu}$ at time $t$. Langer's model is

$$\rho_t + \nabla \cdot \mathbf{J} = 0.$$

Here, $\mathbf{J}$ is a vector with $N/\nu$ components

$$J_j = -\sum_k \Gamma_{jk} \Big( \frac{1}{\kappa T} \frac{\partial E}{\partial \eta_k} \rho + \frac{\partial \rho}{\partial \eta_k} \Big),$$

where $\Gamma_{jk}$ is a finite difference operator that measures the phenomenological fluctuation frequency, $E(\boldsymbol{\eta})$ denotes the total free energy of the system, $\kappa$ is Boltzmann's constant and $T$ is the system temperature.

# Connection to the Cahn–Hilliard Equation

Set

$$\langle \boldsymbol{\eta} \rangle = \int_{\mathbb{R}^{N/\nu}} \boldsymbol{\eta} \rho(t, \boldsymbol{\eta}) d\boldsymbol{\eta}.$$

Then $\langle \boldsymbol{\eta} \rangle$ is a discrete approximation to the solution $u$ of the Cahn–Hilliard equation

$$u_t = \frac{\Gamma h^{2+n}}{2\kappa T \nu^{1+2/n}} \Delta \Big( -\epsilon^2 \Delta u + F'(u) \Big).$$

Here, $h$ denotes distance between nearest microregions.

# Coarsening

Let $\bar{\boldsymbol{\eta}}$ denote a critical point for the system, $\nabla E(\bar{\boldsymbol{\eta}}) = 0$. This corresponds with a stationary solution of the Cahn–Hilliard equation, which we denote $\bar{u}(x)$.

For $t$ large, Langer derives

$$\rho(t, \bar{\boldsymbol{\eta}}) \approx C(\kappa T, h, \nu, \Gamma, \epsilon^2) e^{-\frac{t}{\tau}},$$

where

$$\frac{1}{\tau} = \sum_{\{n : \omega_n > 0\}} \omega_n,$$

and the $\{\omega_n\}_{n=1}^{N/\nu}$ are the eigenvalues of a finite difference discretization of the continuum eigenvalue problem

$$\frac{\Gamma h^{2+n}}{2\kappa T \nu^{1+2/n}} (-\epsilon^2 \Delta + F''(\bar{u}(x)))\phi = \lambda \phi. \tag{E}$$

# The Coarsening ODE

Physically, we view $\tau^{-1}$ as the rate at which transition layers are being eliminated by the coalescence of neighboring pockets of A-rich and B-rich regions. If $M(t)$ denotes the number of such regions, we find

$$\frac{dM}{dt} \approx -\frac{1}{\tau(M)}.$$

In the case $U = \mathbb{R}$ we take $\frac{1}{\tau} \approx \frac{\lambda_{\max}}{2}$, where $\lambda_{\max}$ denotes the leading eigenvalue of (E).

Let $X(t)$ denote the period of the solution at time $t$. We conclude

$$\frac{dX}{dt} = \frac{\lambda_{\max}(X)}{2} X.$$

## Spectral analysis

Let $\bar{u}(x)$ denote a stationary periodic solution of (CH) and consider the eigenvalue problem

$$L\phi = \lambda\phi, \tag{E}$$

where

$$L\phi := (-\phi_{xx} + F''(\bar{u})\phi)_{xx}.$$

Let $\{\phi_j\}_{j=1}^4$ be solutions of (E) initialized at $(0;\lambda)$ as

$$\begin{pmatrix} \phi_1 & \phi_2 & \phi_3 & \phi_4 \\ (b\phi_1)' & (b\phi_2)' & (b\phi_3)' & (b\phi_4)' \\ \phi_1'' & \phi_2'' & \phi_3'' & \phi_4'' \\ \phi_1''' & \phi_2''' & \phi_3''' & \phi_4''' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Here $b(x) = F''(\bar{u}(x))$.

## The Evans Function

We define the Evans function as

$$D(\lambda, \xi) := \det(M(\lambda, X) - e^{i\xi X} I),$$

where $M(\lambda; X)$ is the monodromy or Floquet matrix

$$M(\lambda; X) = \begin{pmatrix} \phi_1(X;\lambda) & \phi_2(X;\lambda) & \phi_3(X;\lambda) & \phi_4(X;\lambda) \\ (b\phi_1)'(X;\lambda) & (b\phi_2)'(X;\lambda) & (b\phi_3)'(X;\lambda) & (b\phi_4)'(X;\lambda) \\ \phi_1''(X;\lambda) & \phi_2''(X;\lambda) & \phi_3''(X;\lambda) & \phi_4''(X;\lambda) \\ \phi_1'''(X;\lambda) & \phi_2'''(X;\lambda) & \phi_3'''(X;\lambda) & \phi_4'''(X;\lambda) \end{pmatrix}.$$

The spectrum of $L$ consists precisely of the values $\lambda$ such that there exists $\xi \in \mathbb{R}$ so that $D(\lambda, \xi) = 0$.

# The Leading eigenvalue

We look for a curve $\lambda_*(\xi)$ such that

$$D(\lambda_*(\xi), \xi) = 0.$$

**Theorem** [H. 2008] Suppose $F$ is even and $\bar{u}(x)$ is a stationary periodic solution of the Cahn–Hilliard equation with minimum $-u_*$ and maximum $+u_*$ and period $X = X(u_*)$. Then for $|\xi|$ sufficiently small there is a solution curve

$$\lambda_*(\xi) = a_2\xi^2 + a_4\xi^4 + \mathbf{O}(\xi^6),$$

where $a_2$ and $a_4$ can be specified as explicit nonlinear functionals evaluated at $\bar{u}(x)$.

Here

$$a_2(X) = \frac{X}{\Phi_3(X)},$$

where

$$\Phi_3(X) = 4\int_0^{\frac{X}{4}} \frac{u_*^2 - \bar{u}(x)^2}{\bar{u}'(x)^2} dx - \frac{X'(u_*)}{F'(u_*)} u_*^2,$$

or equivalently

$$\Phi_3(X) = \sqrt{2}\int_0^{u_*} \frac{u_*^2 - x^2}{(F(x) - F(u_*))^{3/2}} dx - \frac{X'(u_*)}{F'(u_*)} u_*^2.$$

Our perturbation approximation to $\lambda_{max}(X)$ will be

$$\lambda_{max} \approx -\frac{a_2^2}{4a_4} > 0.$$

We will compare this with Langer's form

$$\lambda_{max} \approx \frac{A}{X} e^{-\omega X}.$$

# Large Eigenvalues

If the Cahn–Hilliard equation is linearized about the homogeneous solution $u_h = 0$, we obtain the eigenvalue problem

$$-\phi^{(4)} + F''(0)\phi''(x) = \lambda\phi,$$

with eigenvalues

$$\lambda(\xi) = -F''(0)\xi^2 - \xi^4.$$

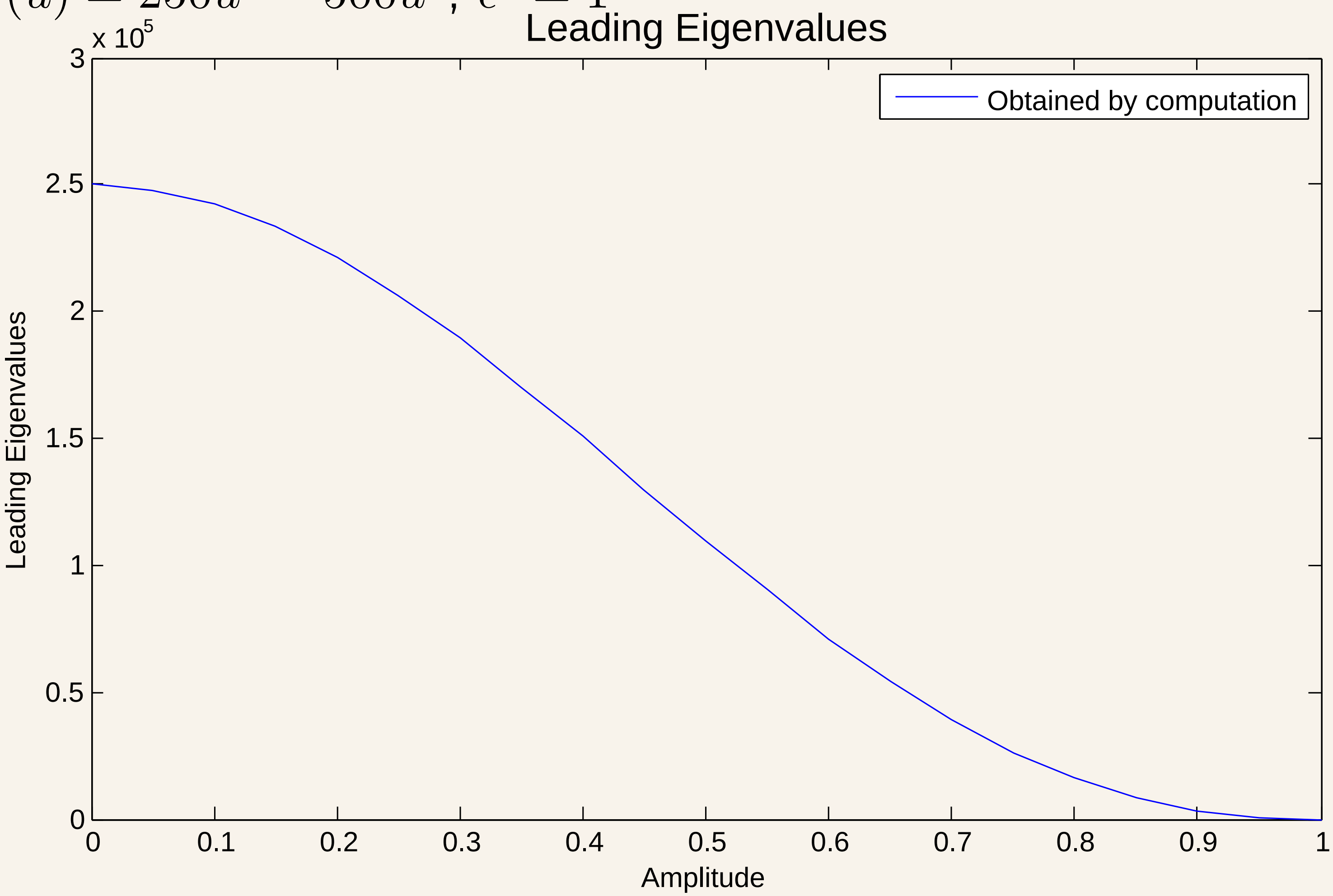
We have, as $u_* \to 0$

$$a_2 \to -F''(0)$$

$$a_4 \to -1.$$

# Leading Eigenvalues vs Amplitude

$F(u) = 250u^4 - 500u^2;\ \epsilon^2 = 1$



# Eigenvalues obtained by perturbation and numerics

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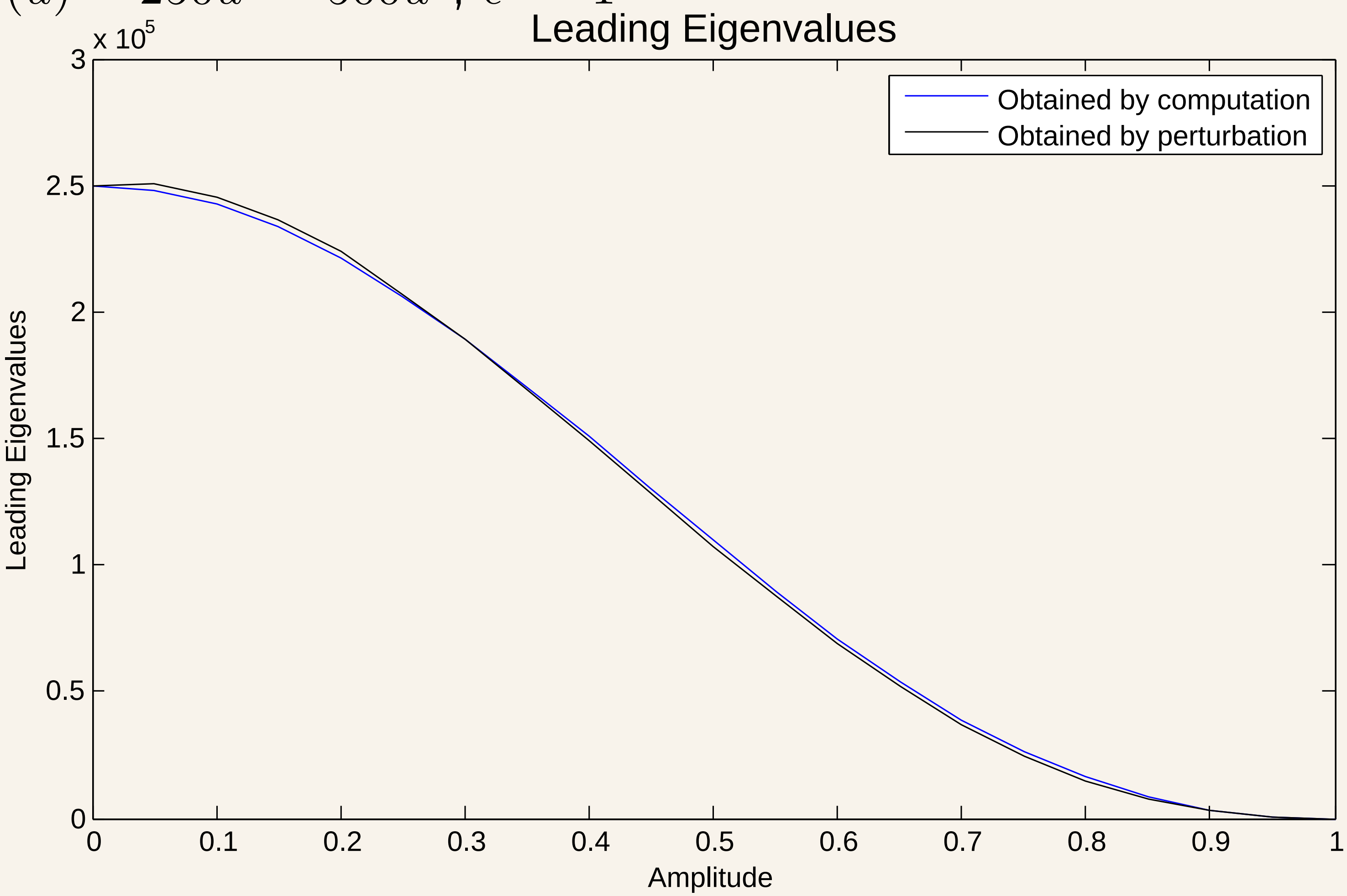

# Leading Eigenvalues vs Period

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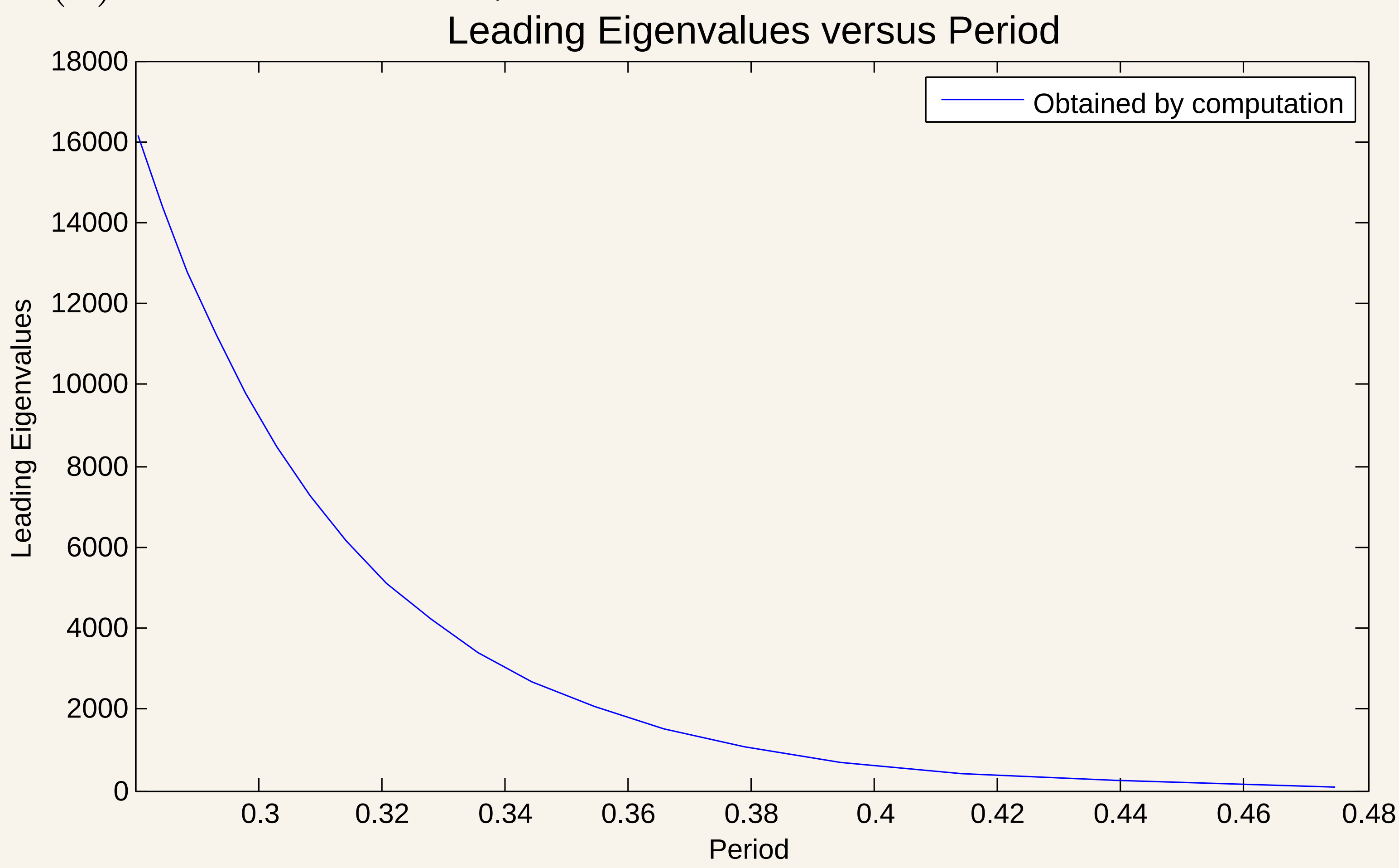

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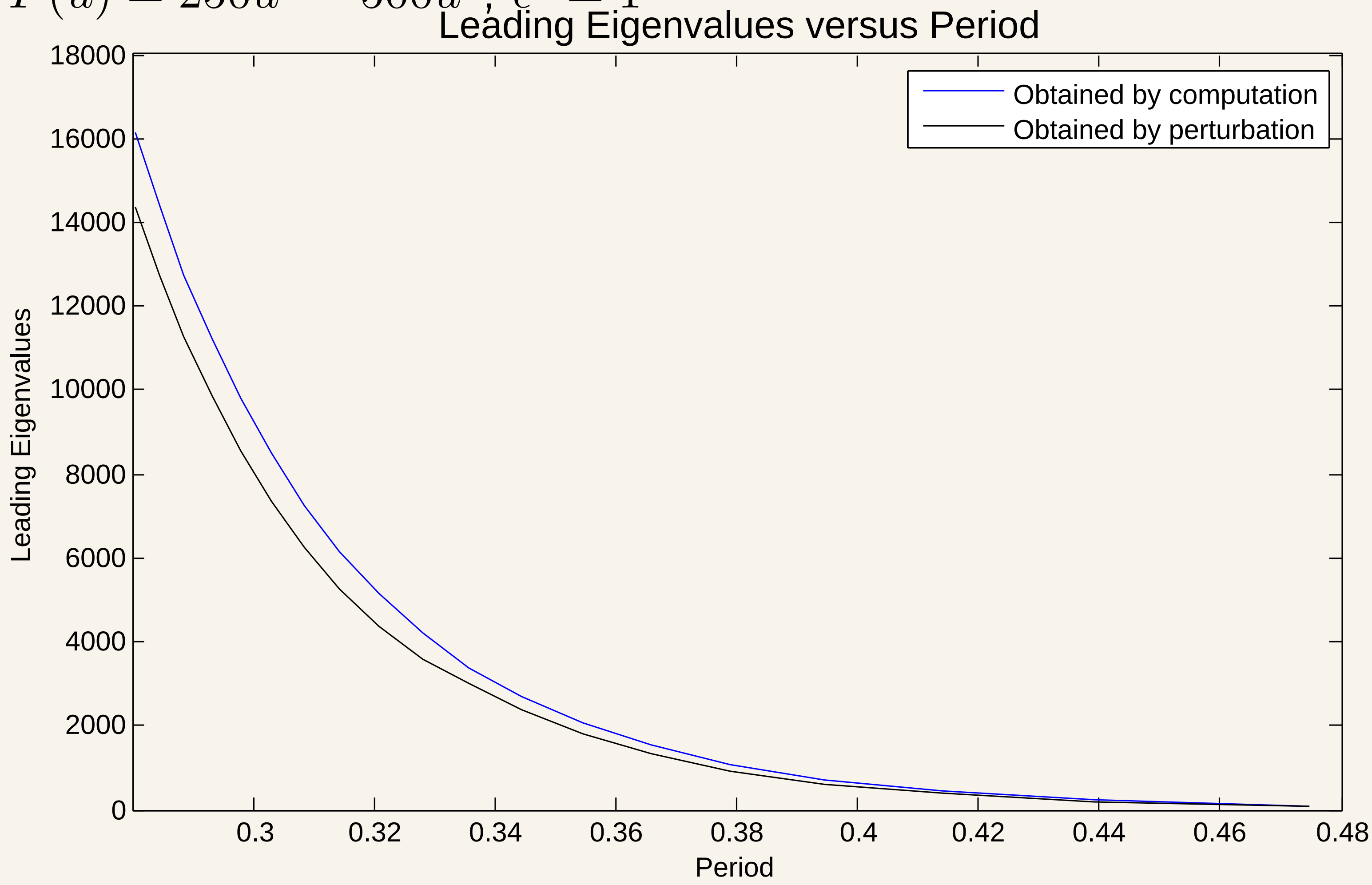

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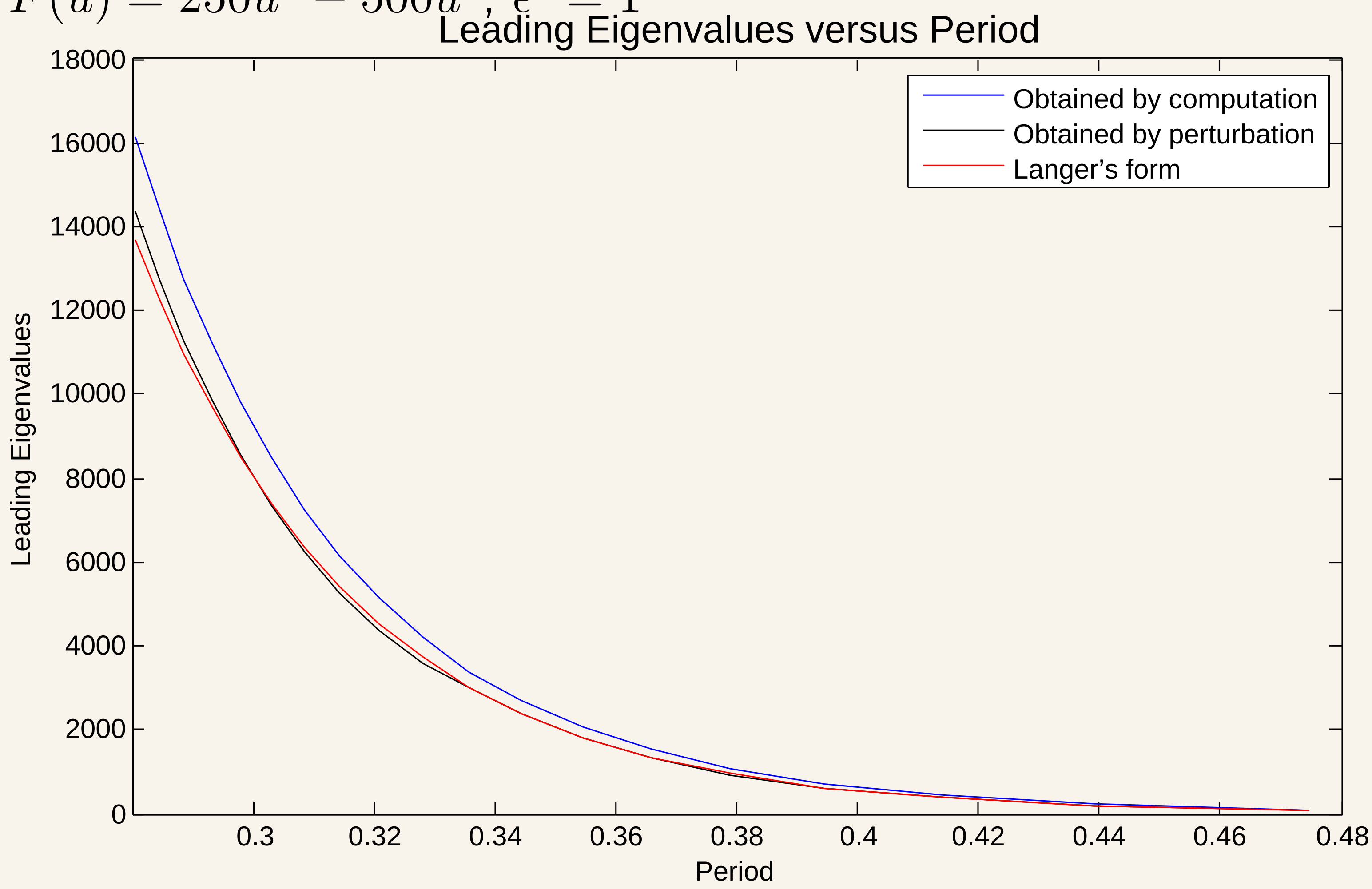
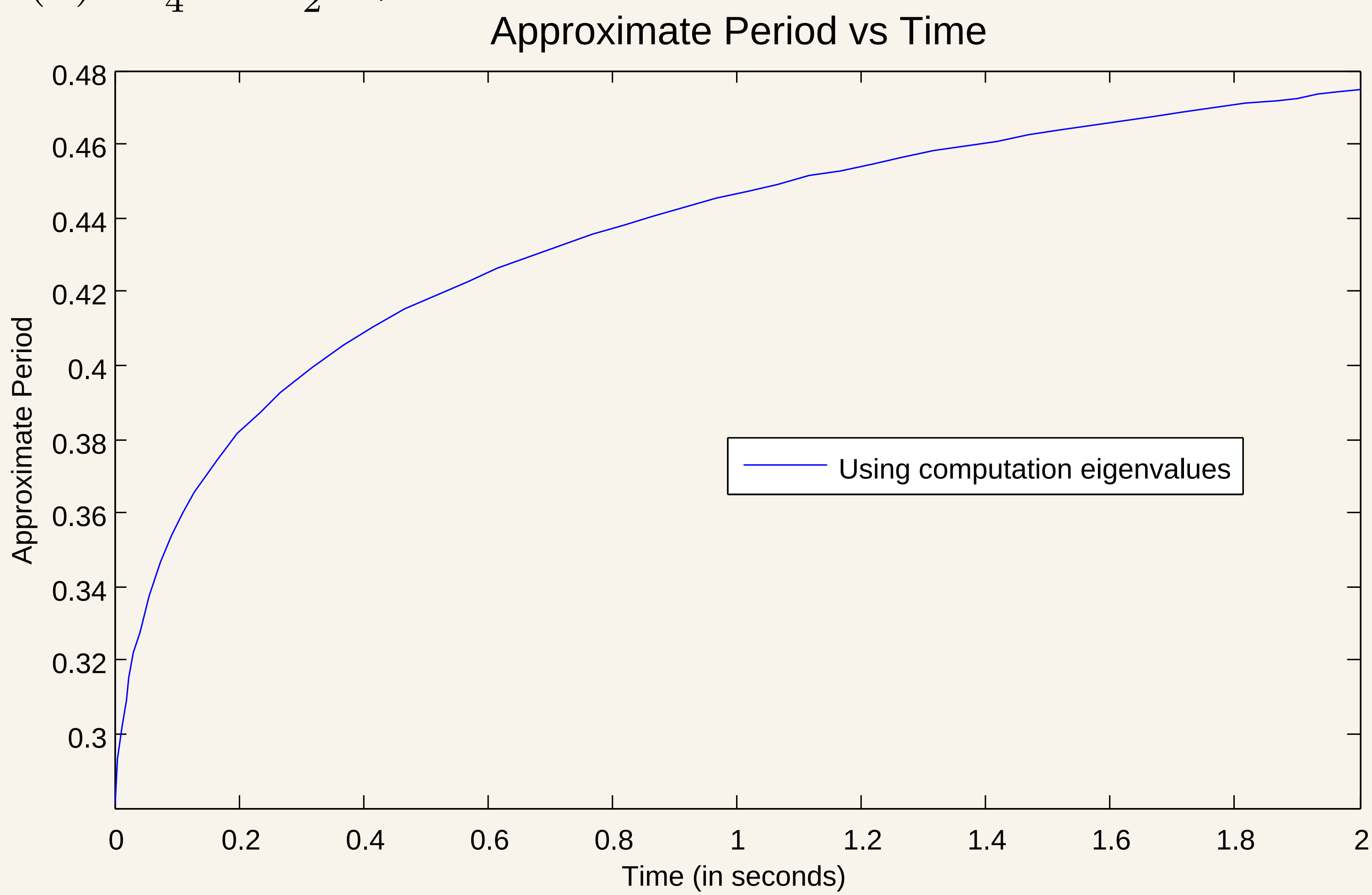


# Approximate Period

$F(u) = \frac{1}{4}u^4 - \frac{1}{2}u^2;\ \epsilon^2 = .001$



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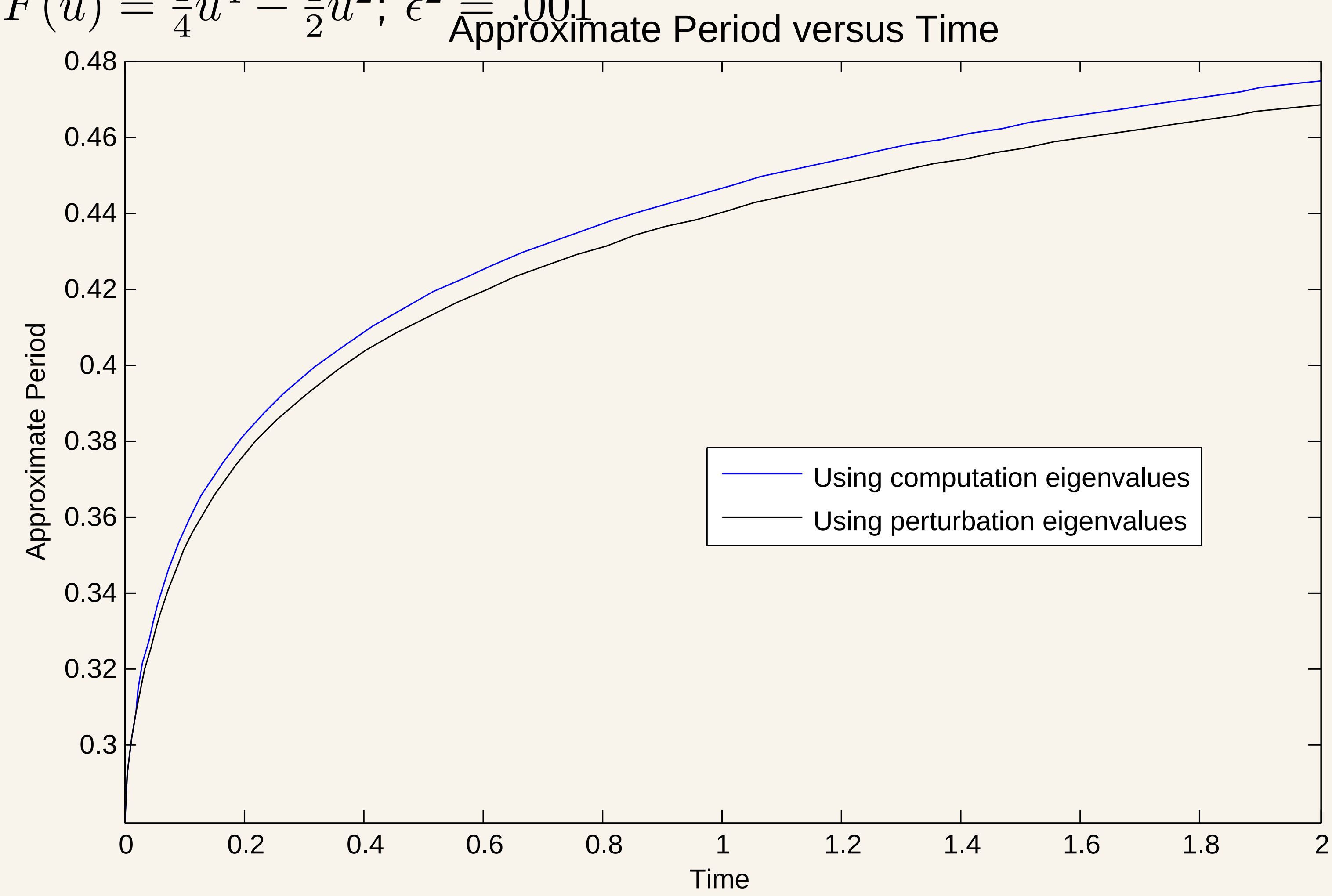

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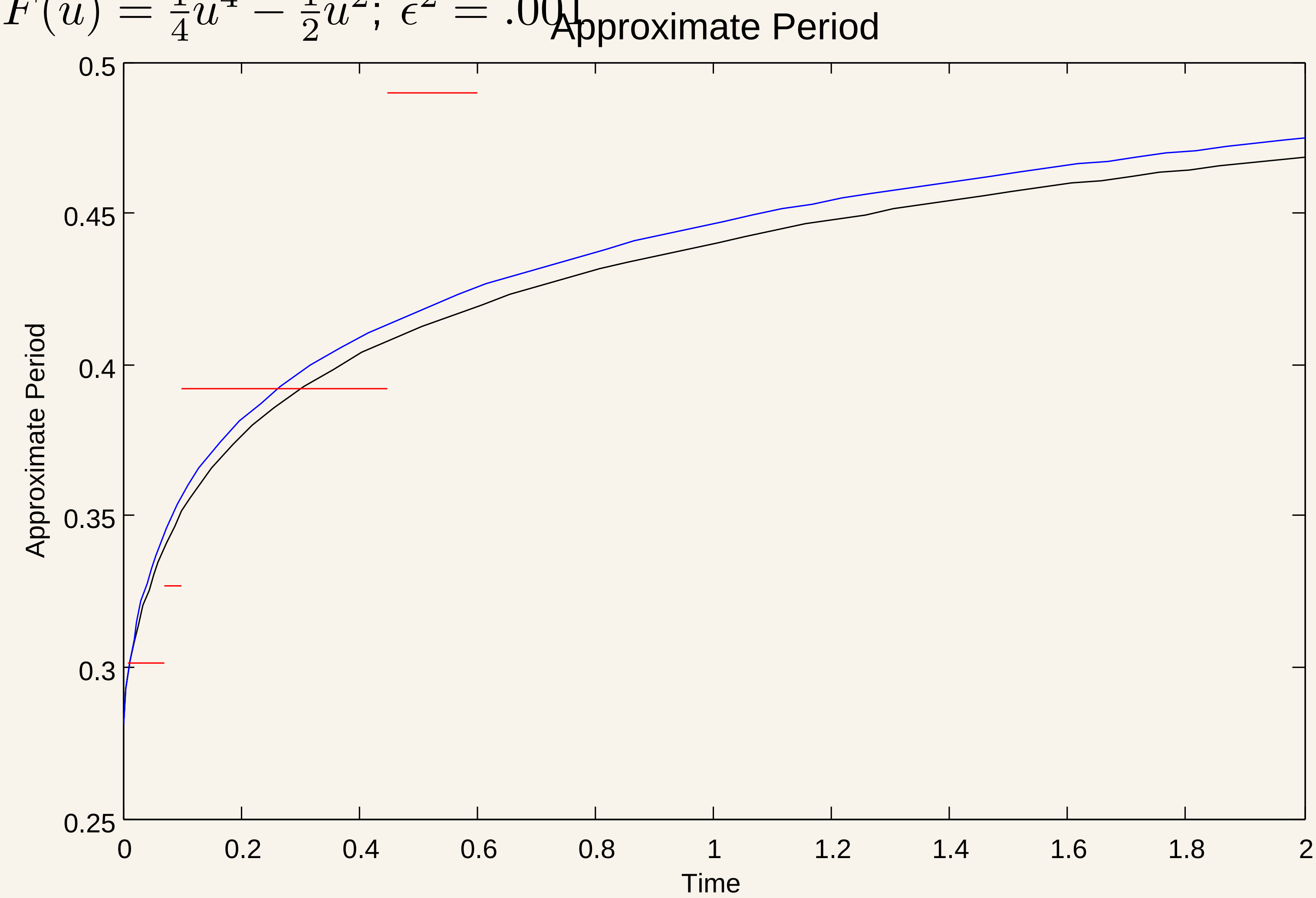

# Numerical Solution of the Cahn-Hilliard equation

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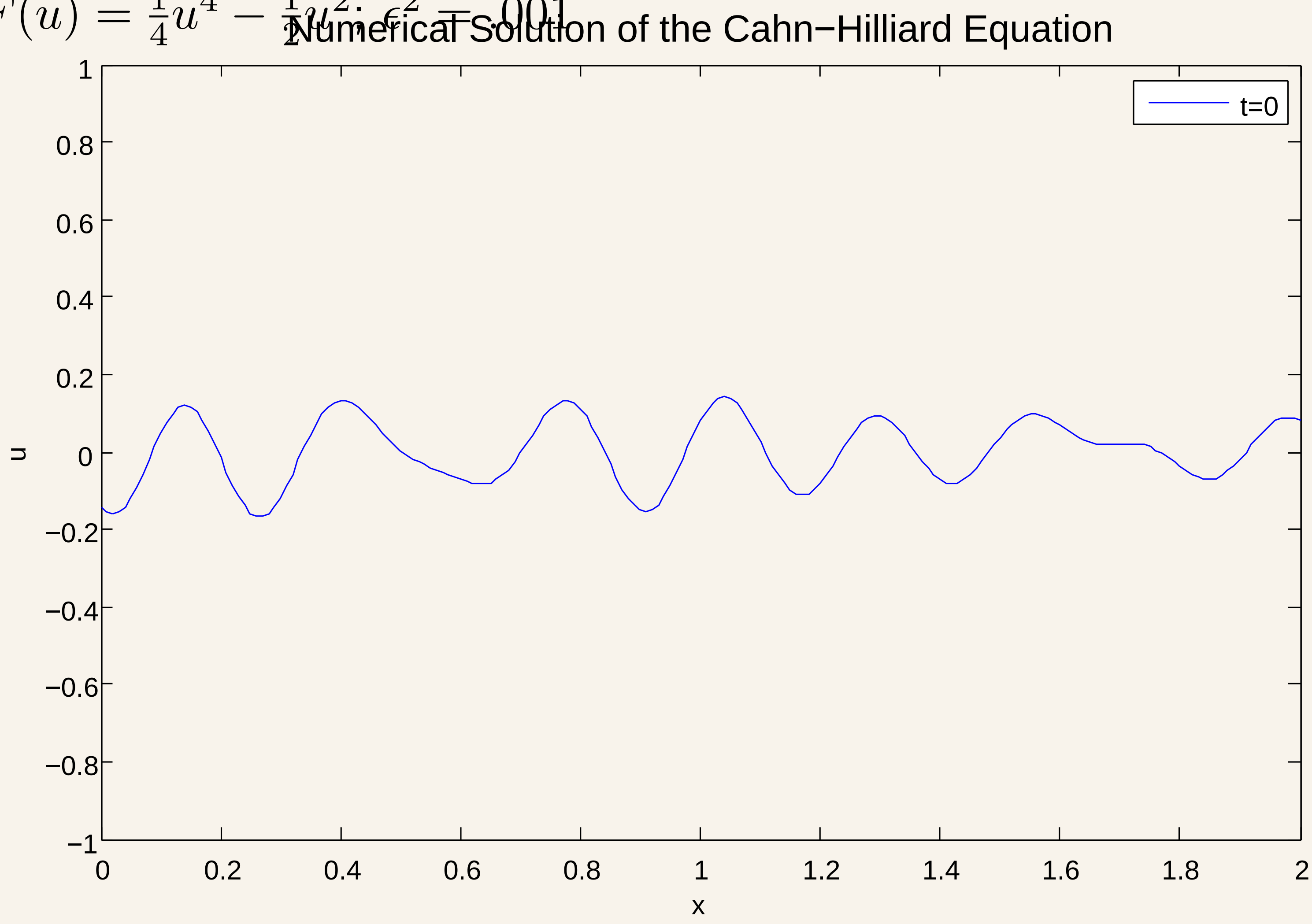

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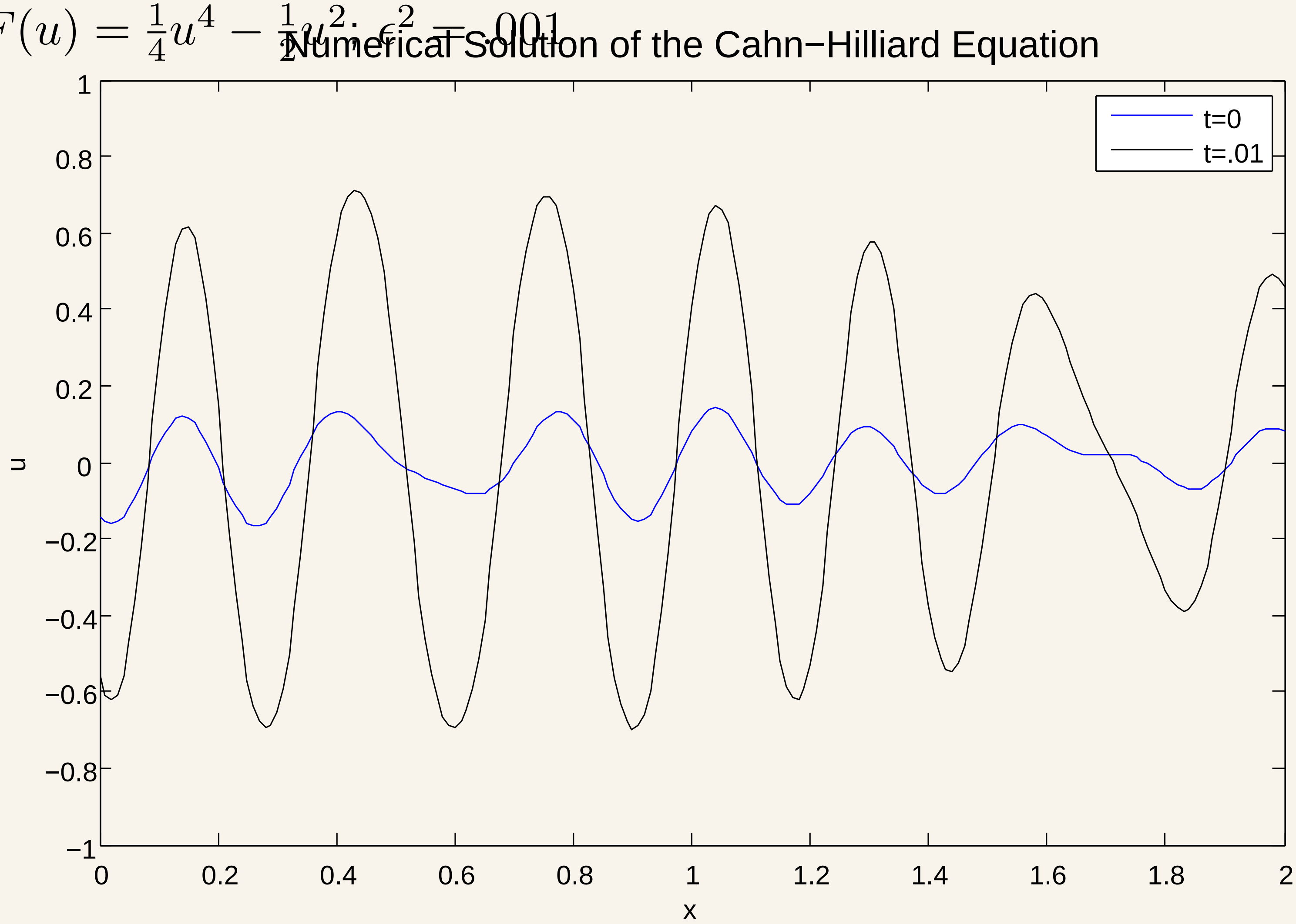

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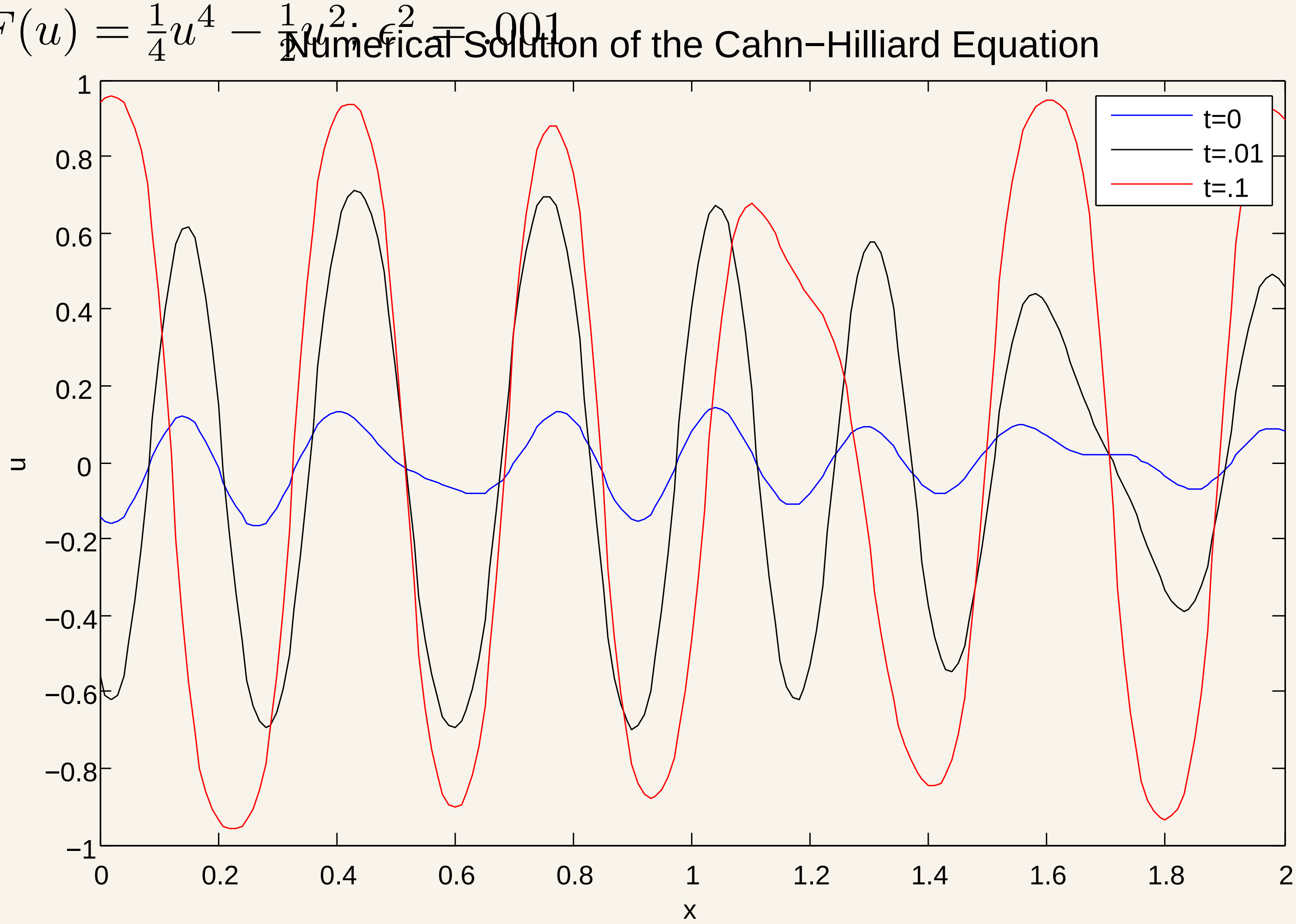


## Multiple Dimensions $u_t = \nabla \cdot \{M(u)\nabla(F'(u) - \kappa \triangle u)\}$

For $d \geq 2$, we have a broader cast of stationary solutions. For example, in the case $d = 2$, some of the players are:

1. Three types of planar solutions.

2. Radial solutions $\bar{u}(r)$ that satisfy $\bar{u}'(0) = 0$, $\bar{u}'(r) < 0$ for $r > 0$, and $\lim_{r\to\infty} \bar{u}(r) = u_\infty$.

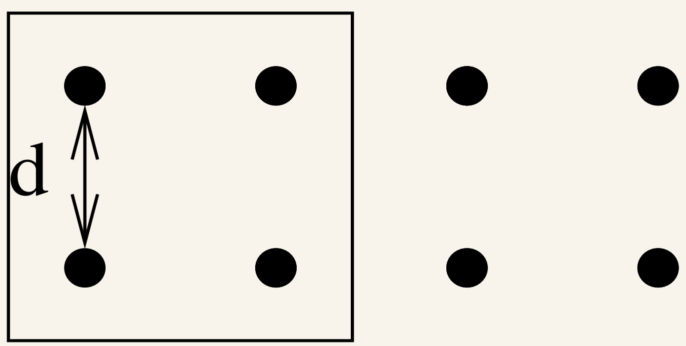
3. *Saddle* solutions, which have infimum $u_1$ and supremum $u_2$ (the binodal values), and which have the same sign as $xy$.

4. Doubly periodic solutions.

## Langer's statistical model

Assume the alloy under investigation is composed of two metals, $A$ and $B$, and that it is contained in a bounded volume $U$. We specify $N$ lattice sites on $U$, each separated from its nearest neighbor by distance $d$. We assume that at each lattice site there is either one atom of species $B$ (composition $+1$) or one atom of species $A$ (composition $-1$).

Now subdivide $U$ into $N/\nu$ microregions, each containing $\nu$ lattice points. Let $\boldsymbol{\eta}$ denote a vector with component $\eta_j$ corresponding with the average composition of microregion $j$.

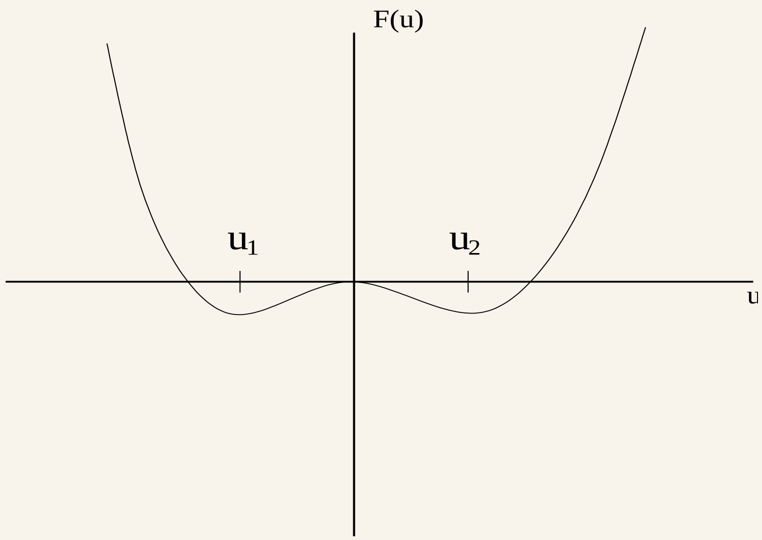


Working under the assumption that if a particular $\eta_j$ changes by some small $+\epsilon$ then a neigbhoring $\eta_{j'}$ must simultaneously change by a corresponding $-\epsilon$, Langer derives his $master$ equation

$$\rho_t + \nabla \cdot \mathbf{J} = 0.$$

## (CH): $u_t = \Delta(-\Delta u + F'(u))$

For any line $G(u) = Au + B$, we can replace $F$ with $F - G$, and we can also shift $F$ with a change of variable $w = u - c$. Without loss of generality, we can put $F$ in the (not necessarily even) standard form:




The values $u_1$ and $u_2$ are called the *binodal* values. This transformation places the generic homogeneous configuration at $u_h = 0$.

## Grant's Analysis

In the paper, *Spinodal decomposition for the Cahn–Hilliard equation* [Comm. PDE **18** (1993) 453–490], C. Grant showed that for $n = 1$, and for the case of a bounded interval domain (with natural boundary conditions), solutions initiated by small, random (in some sense) perturbations from $u_h = 0$ will evolve toward a particular, necessarily unstable, periodic solution.

This suggests that in some sense periodic solutions may be the correct stationary solutions to focus on in Langer's framework.

Loosely, we associate the end of Grant's evolution with the beginning of Langer's late-stage coarsening.

## The Continuum Model

For comparison with Langer's model, we recall that the Cahn–Hilliard is a conservation law

$$u_t + \nabla \cdot \vec{J} = 0,$$

where

$$\vec{J} = -\nabla \frac{\delta E}{\delta u},$$

and $E(u)$ has the form

$$E(u) = \int_U F(u) + \frac{\kappa}{2} |\nabla u|^2 dx.$$

Here

$$\frac{\delta E}{\delta u} = F'(u) - \kappa \Delta u.$$

## The discrete energy map

In Langer's setting the energy for a system in state $\boldsymbol{\eta}$ is

$$E(\boldsymbol{\eta}) := h^n \sum_{j=1}^{N/\nu} \Big( F(\eta_j) + \frac{1}{4} \sum_{j'}^{(j)} \frac{(\eta_{j'} - \eta_j)^2}{h^2} \Big).$$

Here, $\sum_{j'}^{(j)}$ denotes summation over the $2n$ nearest neighbors of microregion j, and $h$ denotes the distance between nearest microregions, $h = d\nu^{1/n}$.

Also,

$$\Gamma_{jk} := \frac{\Gamma h^2}{2\nu^{1+(2/n)}} \Big( 2n\delta_{jk} - \sum_{j'}^{(j)} \delta_{j'k} \Big) / h^2,$$

where the constant $\Gamma$ is a phenomenological fluctuation frequency, $\delta_{jk}$ denotes a standard Kronecker delta,