

# The Whitham principle for multikink solutions of reaction-diffusion equations

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In this text we discuss how equations for interface motion can be calculated for some special reaction-diffusion systems with small diffusion coefficients.

## 1 Introduction

An useful strategy for the study of nonlinear partial differential equations (PDE) arising in pattern formation is to consider asymptotic solutions containing one or several localized defects and to simplify the dynamics by finding the equations of motion of the system of interacting defects. The great advantage of this approach is that we are dealing with ordinary differential equations (ODEs) instead PDEs. This type of approach has been successfully applied to solitons in continuous and discrete sine-Gordon equation [16, 17, 10, 13, 12],  $\phi^4$  classical field theory [14], Korteweg-de Vries equation [11], non-linear Schrödinger, Klein-Gordon [11, 8, 9], and Frenkel-Kontorova [2] lattices, Fisher-Kolmogorov-Petrovsky-Piscounoff (FKPP) equation [5], to bubbles in Cahn-Hilliard equation [3].

## 2 Kink and multi-kink solutions of PDEs

Kinks are interface-like solutions of non-linear PDEs, representing smooth transitions between regions where the solutions are constants. A particular class of PDEs, relevant to the problem we study are the reaction-diffusion equations (FKPP also belongs to this class). The existence of kinks is a well studied problem for a single reaction diffusion equation. For the space homogeneous 1D case, a typical reaction-diffusion equation admitting kink solutions reads:

$$u_t = du_{xx} + f(u), \quad t > 0, \quad x \in (-\infty, \infty) \quad (S1)$$

Physically, travelling wave solutions  $U(x - VT)$  (kinks) exist, for example, if the function  $f(u)$  has three roots, one root corresponds to a saddle point of the shorted (where diffusion is removed) equation  $du/dt = f(u)$  (unstable root), and two roots  $u_{\pm}$  are local attractors of  $du/dt = f(u)$  (stable roots). This case was studied in detail by P.C. Fife and J. B. Macleod [7]. The condition for kink existence can be also formulated by using the potential

$$\Phi(u) = \int_0^u f(s)ds.$$

*A sufficient kink existence condition by potential:* The kink exists if  $\Phi(u)$  has two local non-degenerate maxima and a single local minimum.

*Energetic relation for kink velocity:* Suppose eq. (S1) has a kink solution of the form  $U(x - Vt)$  such that  $U(\pm\infty) = u_{\pm}$ . Let us multiply eq. (S1) by  $u_x$  and integrating over  $x$  one has

$$Vd \int_{-\infty}^{+\infty} u_x^2 dx = \Phi(u_+) - \Phi(u_-). \quad (S2)$$

The system energy  $F[u]$  for the  $u$ -pattern is defined by

$$F = \int_{-\infty}^{+\infty} \left( \frac{d}{2} u_x^2 - \Phi(u) \right) dx.$$

Then, eq. (S2) means that in a bistable medium the interface (kink) moves in direction of the stable state with the minimal energy.

In the space inhomogeneous case, the reaction term depends on  $x$ :

$$u_t = \epsilon^2 u_{xx} + f(u, x). \quad (S3)$$

The well localized kink solutions exist if  $\epsilon$  is small enough and if the potential  $\Phi(u, q)$ , depending on kink position parameter  $q$ ,

$$\Phi(u, q) = \int_0^u f(s, q) ds,$$

satisfies the above sufficient kink existence condition for each  $q$ .

One can assume that there holds an asymptotic analogue of eq. (S2)

$$V(q)\epsilon^2 \int_{-L_k}^{L_k} U(x, q, \epsilon)_x^2 dx = \Phi(u_+(q)) - \Phi(u_-(q)) + \text{small corrections}, \quad (S4)$$

where  $U(x, q)$  is an asymptotic solution describing a kink localized in a small  $\epsilon$  neighborhood of the point  $q = q(t)$ ,  $L_k \gg \epsilon$  (one can even take formally  $L_k = \infty$ , a change of  $L_k$  gives an exponentially small error, since  $U_x$  decreases exponentially as  $\exp(-c|x - q|/\epsilon)$ ,  $c = c(q) > 0$ ).

### 3 The Whitham principle

For some complicated problems from condensed matter theory, pattern formation and wave propagation, the formal asymptotic methods, lead to complex mathematical relations. G.B. Whitham proposed a principle [19] which, when applied to periodic waves, simplifies these computations. This principle has been generalized to dissipative systems by one of us [15, 18, 1]. In this case, it leads to ordinary differential equations for interface positions (see [1] for a review).

The Whitham principle applies to equations that admit a variational formulation

$$\frac{\delta D[u]}{\delta u_t} = - \frac{\delta F[u]}{\delta u}, \quad (S5)$$

where  $u$  is an order parameter,  $u = u(x, t)$ ,  $F$  is a functional that defines a free energy of the system, and  $D$  is a functional that defines a dissipative function (which depends on the time derivative  $u_t$ ).

Suppose we have found some asymptotic **ansatz**, i.e., some approximation  $U(x, q)$  of our solution, depending on some unknown parameters  $q = (q_1, q_2, \dots, q_n)$ . If we describe a layered pattern consisting of narrow interfaces, then  $q_i$  are interface positions.

By the Whitham principle, we can obtain differential equations for time evolution of  $q_i$  straightforwardly. Namely, we substitute  $U(x, q)$  in  $D$  and  $F$  and we obtain "Whitham averaged functionals"

$$\bar{D}(q) = D[U(x, q)], \quad \bar{F}(q) = F[U(x, q)].$$

Then, we write Whitham averaged equations

$$\frac{\partial \bar{D}}{\partial q_{it}} = -\frac{\partial \bar{F}}{\partial q_i}. \quad (S6)$$

Eqs. (S6) give the time evolution of  $q_i$ .

An elementary analysis shows that for kink motion problem (see eq. (S3)), this equation reduces to eq. (S4). In turn, eq. (S4) leads to the main equations of our paper.

The complete mathematical justification of this approach is, sometimes, a difficult task, however, it is done for some cases [6, 4, 18, 1].

## 4 Equations of motion of kinks for the gene circuit model

We obtain first the equation of motion of a single kink in a slowly varying external field. Then, we add the effect of other kinks to the external field.

### 4.1 One kink equation of motion

We start with the equation

$$u_t = du_{xx} + R\sigma(Tu + M(x)) - \lambda u, \quad (S7)$$

where  $M(x)$  is the slowly varying external field.

In order to obtain a variational formulation of eq. (S7) we define the potential  $\Phi$  as the antiderivative of  $-f$ ,  $\Phi_u = -R\sigma(Tu + M(x)) + \lambda u$ . Considering  $\sigma$  to be a step function, we get

$$\Phi = \begin{cases} \Phi^-(u) = RM/T + \lambda u^2/2, & u < -M/T \\ \Phi^+(u) = -Ru + \lambda u^2/2, & u > -M/T. \end{cases} \quad (S8)$$

Then, we define  $D$  and  $F$  as the dissipation and energy functionals

$$D = \frac{1}{2} \int u_t^2 dx, \quad F = \int [\frac{1}{2} du_x^2 + \Phi(u, x)] dx. \quad (S9)$$

From  $\delta D = \int u_t \delta u_t dx$ , and  $\delta F = \int [du_x \delta(u_x) + \frac{\partial \Phi}{\partial u} \delta u] dx = \int [-du_{xx} \delta u - f \delta u] dx$  we get the Fréchet derivative of  $D$  and  $F$ , respectively

$$\frac{\delta D}{\delta u_t} = u_t, \quad \frac{\delta F}{\delta u} = -du_{xx} - f. \quad (S10)$$

The variational form of eq. (S7) is as follows:

$$\frac{\delta D[u_t]}{\delta u_t} = -\frac{\delta F[u]}{\delta u}. \quad (S11)$$

A kink solution (right border of an expression domain) of eq. (S7) has the form

$$U(x; q) = \frac{R}{\lambda} \begin{cases} 1 - \frac{1}{2} \exp(\gamma(x - q)), & x < q, \\ \frac{1}{2} \exp(-\gamma(x - q)), & x > q, \end{cases} \quad (S12)$$

where  $\gamma = \sqrt{\lambda/d}$  is the kink tail parameter,  $q$  is the kink position. Antikink solutions, i.e. (left borders of expression domains) are obtained by symmetry (change  $x - q$  in  $q - x$  in eq. (S12)).

The *Whitham averaged* functionals  $\bar{D}, \bar{F}$  for a kink depend on  $q$  through  $U$  according to  $\bar{D} = D[U]$ ,  $\bar{F} = F[U]$ . The *Whitham principle* reads:

$$\frac{d\bar{D}(q_t)}{dq_t} = -\frac{d\bar{F}(q)}{dq}. \quad (S13)$$

Next we compute  $\bar{D}(q_t), \bar{F}(q)$ .

From  $\bar{D}(q_t) = \frac{1}{2} \int u_t^2 dx = \frac{1}{2} q_t^2 \int U_x^2 dx$  (here we have used  $u(x, t) = U(x - q(t))$ ) we get

$$\frac{d\bar{D}(q_t)}{dq_t} = q_t \int U_x^2 dx. \quad (S14)$$

From  $\bar{F}(q) = \int \frac{1}{2} dU_x^2 + \int^q \Phi^+(U(x; q)) dx + \int_q \Phi^-(U(x; q)) dx$  we get

$$d\bar{F}(q)/dq = \Phi^+(U(q; q)) - \Phi^-(U(q; q)) = -R^2[M(RT)^{-1} + (2\lambda)^{-1}]. \quad (S15)$$

Using eqs. (S13), (S14), (S15) we get

$$r \frac{dq}{dt} = \frac{M(q)}{RT} + \frac{1}{2\lambda}, \quad (S16)$$

where  $r = \frac{1}{R^2} \int U_x^2 dx$ .

For an antikink,  $d\bar{F}(q)/dq = \Phi^-(U(q; q)) - \Phi^+(U(q; q))$  is just the opposite of the similar expression for a kink, which leads to the following equation of motion

$$r \frac{dq}{dt} = -\frac{M(q)}{RT} - \frac{1}{2\lambda}. \quad (S17)$$

### Computing $\int U_x^2 dx$

We do this using the asymptotic solution eq. (S12). The limits of the integral correspond to the size of the egg. As this size is much larger compared to  $\gamma^{-1}$ , we can safely integrate from  $-\infty$  to  $\infty$  and we obtain

$$\int_{-\infty}^{\infty} U_x^2 dx = \frac{R^2 \gamma^2}{4\lambda^2} \left[ \int_{-\infty}^0 e^{2\gamma x} dx + \int_0^{\infty} e^{-2\gamma x} dx \right] = \frac{R^2 \gamma}{4\lambda^2}.$$

It follows that  $r = \frac{1}{4} \frac{\gamma}{\lambda^2}$ .

## 4.2 Multikink equations of motion

The Whitham principle also allows us to obtain multi-kink equations of motion, in the case of a single gene (one reaction-diffusion equation).

For instance, to study forces between a kink and an antikink, one should define double kinks solutions  $U^{(2)}(x; q_1, q_2)$  as approximate steady states of eq. (S7):

$$U^{(2)}(x; q_1, q_2) = \frac{R}{2\lambda} \begin{cases} e^{\gamma(x-q_1)}(1 - e^{\gamma(q_1-q_2)}), & x < q_1, \\ e^{-\gamma(x-q_2)}(1 - e^{\gamma(q_1-q_2)}), & x > q_2, \\ 2[1 - e^{-\gamma(q_2-q_1)/2} \cosh \gamma(x - \bar{q})], & q_1 < x < q_2, \end{cases}, \quad (S19)$$

where  $q_1, q_2$  are the kink and the anti-kink positions, and  $\bar{q} = (q_1 + q_2)/2$ .

By using  $u = U^{(2)}$  to define averaged Whitham functionals and applying Whitham principle (eq. (S6)) we find the equations of motion of the kink-antikink pair.

First, notice that

$$u(x, t) = U^{(2)}(x; q_1(t), q_2(t)) \approx U(x; q_2(t)) + U(x; q_1(t)) - R/\lambda,$$

also

$$u_t^2 \approx (q_2')^2 U_x^2(x; q_2(t)) + (q_1')^2 U_x^2(x; q_1(t)),$$

where  $U$  is defined by eq. (S12). It follows that

$$\frac{\partial \bar{D}}{\partial q_1'} \approx \frac{dq_1}{dt} \int U_x^2 dx, \quad \frac{\partial \bar{D}}{\partial q_2'} \approx \frac{dq_2}{dt} \int U_x^2 dx.$$

Also, from

$$\begin{aligned} \bar{F}(q_1, q_2) &= \int \frac{1}{2} du_x^2 + \int^{q_1} \Phi^-(U^{(2)}(x; q_1, q_2)) dx + \\ &+ \int_{q_1}^{q_2} \Phi^+(U^{(2)}(x; q_1, q_2)) dx + \int_{q_2} \Phi^-(U^{(2)}(x; q_1, q_2)) dx \end{aligned}$$

it follows

$$\partial \bar{F} / \partial q_1 = \Phi^-(U^{(2)}(q_1; q_1, q_2)) - \Phi^+(U^{(2)}(q_1; q_1, q_2)) = R^2 [M/(RT) + (2\lambda)^{-1} (1 - e^{-\gamma(q_2-q_1)})],$$

and

$$\partial \bar{F} / \partial q_2 = \Phi^+(U^{(2)}(q_2; q_1, q_2)) - \Phi^-(U^{(2)}(q_2; q_1, q_2)) = -R^2 [M/(RT) + (2\lambda)^{-1} (1 - e^{-\gamma(q_2-q_1)})].$$

The equations of motion resulting from the application of the Whitham's principle (eq. (S6)) are

$$r \frac{dq_1}{dt} = - \frac{M(q_1) - \frac{RT}{2\lambda} e^{-\gamma(q_2-q_1)}}{RT} - \frac{1}{2\lambda}, \quad (S20)$$

for the antikink, and

$$r \frac{dq_2}{dt} = \frac{M(q_2) - \frac{RT}{2\lambda} e^{-\gamma(q_2-q_1)}}{RT} + \frac{1}{2\lambda}, \quad (S21)$$

for the kink.

Eqs. (S20), (S21) can be formally obtained from eqs. (S16), (S17) by adding the contribution (attraction) of opposite kink to the external field  $M$ . The constant parts of these contributions have to be discarded in order to avoid counting twice the kink self-interaction energy. When  $\gamma(q_2 - q_1) \gg 1$ , the kink-antikink attraction interaction can be neglected.

The multi-component gene circuit model generalizes eq. (S7) by considering that  $u$  is a vector. It corresponds to a system of reaction-diffusion equations, that reads:

$$\frac{\partial u_i}{\partial t} = d_i \frac{\partial^2 u_i}{\partial x^2} + R_i \sigma \left( \sum_{j=1}^m T_{ij} u_j + m_i \mu(x) + h_i \right) - \lambda_i u_i. \quad (S22)$$

Whitham's method is not applicable in general to the multi-component case, eq. (S22). The problem arises from the fact that, in general, the reaction vector field  $f_i = R_i \sigma \left( \sum_{j=1}^m T_{ij} u_j + m_i \mu(x) + h_i \right) - \lambda_i u_i$  is not the gradient of a scalar potential as a function of  $u$ . If  $f$  has a nonzero rotational (for instance if the rescaled gene interaction matrix  $\tilde{T}_{ij} = R_i T_{ij}$  is not symmetric), one can not find a variational formulation of the problem.

However, in the case of small diffusion, we can use the result for one component obtained above, to get the multikink equations of motion. The ansatz is to add to the field  $M(x)$  the contributions of the other genes, considering that

$$M_i(x) = \sum_{j \neq i}^m T_{ij} U_j(x) + m_i \mu(x) + h_i, \quad (S23)$$

where  $U_j$  is the asymptotic solution (kink or kink-antikink pair) for gene  $j$ .

The above sum (eq. (S23)) does not consider the single component kink-antikink interaction. This interaction can be neglected when the expression domains are large enough.

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