

# Clustered Spots In The FitzHugh-Nagumo System

Juncheng Wei <sup>\*</sup> and Matthias Winter <sup>†</sup>

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## Abstract

We construct **clustered** spots for the following FitzHugh-Nagumo system:

$$\begin{cases} \epsilon^2 \Delta u + f(u) - \delta v = 0 & \text{in } \Omega, \\ \Delta v + u = 0 & \text{in } \Omega, \\ u = v = 0 & \text{on } \partial\Omega, \end{cases}$$

where  $\Omega$  is a smooth and bounded domain in  $R^2$ . More precisely, we show that for any given integer  $K$ , there exists an  $\epsilon_K > 0$  such that for  $0 < \epsilon < \epsilon_K$ ,  $\epsilon^{m'}$   $\leq \delta \leq \epsilon^m$  for some positive numbers  $m', m$ , there exists a solution  $(u_\epsilon, v_\epsilon)$  to the FitzHugh-Nagumo system with the property that  $u_\epsilon$  has  $K$  spikes  $Q_1^\epsilon, \dots, Q_K^\epsilon$  and the following holds:

(i) The center of the cluster  $\frac{1}{K} \sum_{i=1}^K Q_i^\epsilon$  approaches a hotspot point  $Q_0 \in \Omega$ .

(ii) Set  $l^\epsilon = \min_{i \neq j} |Q_i^\epsilon - Q_j^\epsilon| = \frac{1}{\sqrt{a}} \log\left(\frac{1}{\delta \epsilon^2}\right) \epsilon(1 + o(1))$ . Then  $(\frac{1}{l^\epsilon} Q_1^\epsilon, \dots, \frac{1}{l^\epsilon} Q_K^\epsilon)$  approaches an optimal configuration of the following problem:

(\*) *Given  $K$  points  $Q_1, \dots, Q_K \in R^2$  with minimum distance 1, find out the optimal configuration that minimizes the functional  $\sum_{i \neq j} \log |Q_i - Q_j|$ .*

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## 1 Introduction

In this paper, we study the steady-states for the FitzHugh-Nagumo system [14], [22]. This is a two-variable reaction-diffusion system derived from the Hodgkin-Huxley model for nerve-impulse propagation [18]. In a suitably rescaled fashion it can be written as follows:

$$(FN) \quad \begin{cases} u_t = \epsilon^2 \Delta u + f(u) - v & \text{in } \Omega, \\ v_t = \Delta v - \delta \gamma v + \delta u & \text{in } \Omega, \\ u = v = 0 & \text{on } \partial\Omega. \end{cases}$$

The unknowns  $u = u(x, t)$  and  $v = v(x, t)$  represent the electric potential and the ion concentration across the cell membrane at a point  $x \in \Omega \subset R^N$  ( $N = 1, 2, \dots$ ) and at a time  $t > 0$ , respectively;  $\epsilon > 0$ ,  $\delta > 0$ , and  $\gamma > 0$  are real constants;  $\Delta := \sum_{j=1}^N \frac{\partial^2}{\partial x_j^2}$  is the Laplace operator in  $R^N$ ;  $\Omega$  is a smooth bounded domain in  $R^N$ ;  $f(u) = u(1-u)(u-a)$  with  $a \in (0, \frac{1}{2})$ .

<sup>\*</sup>Department of Mathematics, The Chinese University of Hong Kong, Shatin, Hong Kong, e-mail: wei@math.cuhk.edu.hk

<sup>†</sup>Fachbereich Mathematik, Universität Stuttgart, D-70511 Stuttgart, Germany, e-mail: winter@mathematik.uni-stuttgart.de

In this paper, we consider steady-states of (FN), namely we study the following elliptic system:

$$\begin{cases} \epsilon^2 \Delta u + f(u) - \delta v = 0 & \text{in } \Omega, \\ \Delta v - \delta \gamma v + \delta u = 0 & \text{in } \Omega, \\ u = v = 0 & \text{on } \partial\Omega. \end{cases} \quad (1.1)$$

For simplicity, from now on we assume that  $\gamma = 0$ . (With slight modifications, the results also hold for fixed  $\gamma > 0$ .) Setting  $v = \delta \tilde{v}$  and dropping the tilde we get the system

$$\begin{cases} \epsilon^2 \Delta u + f(u) - \delta v = 0 & \text{in } \Omega, \\ \Delta v + u = 0 & \text{in } \Omega, \\ u = v = 0 & \text{on } \partial\Omega. \end{cases} \quad (1.2)$$

This is the final form of the system which we will study in the rest of the paper.

In the investigation of the system (1.1) we make use of the fact that it arises as the Euler-Lagrange equation to the energy functional  $E_\epsilon : H_0^1(\Omega) \rightarrow \mathbb{R}$  given by

$$E_\epsilon[u] = \frac{\epsilon^2}{2} \int_\Omega |\nabla u|^2 - \int_\Omega F(u) + \frac{\delta}{2} \int_\Omega uT[u], \quad (1.3)$$

where  $F(u) = \int_0^u f(s)ds$ . Here  $v = T[u]$  for given  $u \in L^2(\Omega)$  is defined as the unique solution  $v \in H^2(\Omega)$  of the linear problem

$$\Delta v + u = 0 \quad \text{in } \Omega, \quad v = 0 \quad \text{on } \partial\Omega. \quad (1.4)$$

Let  $w$  be the unique solution of

$$\Delta w + f(w) = 0, \quad w > 0 \quad \text{in } \mathbb{R}^N, \quad w(0) = \max_{y \in \mathbb{R}^N} w(y), \quad w(y) \rightarrow 0 \quad \text{as } |y| \rightarrow \infty. \quad (1.5)$$

It is well-known that  $w$  is radially symmetric:  $w(y) = w(|y|)$  and strictly decreasing:  $w'(r) < 0$  for  $r > 0, r = |y|$ . Moreover, we have the following asymptotic behavior of  $w$ :

$$w(r) = A_N r^{-\frac{N-1}{2}} e^{-\sqrt{a}r} (1 + O(\frac{1}{r})), \quad w'(r) = -A_N \sqrt{a} r^{-\frac{N-1}{2}} e^{-\sqrt{a}r} (1 + O(\frac{1}{r})), \quad (1.6)$$

for  $r$  large, where  $A_N > 0$  is a generic constant.

For the uniqueness of problem (1.5), we refer to [2], [4] and [29]. Furthermore,  $w$  is nondegenerate, i.e.,

$$\text{Kernel} (\Delta - 1 + f'(w)) = \text{span} \left\{ \frac{\partial w}{\partial y_1}, \dots, \frac{\partial w}{\partial y_N} \right\}. \quad (1.7)$$

We denote the energy of  $w$  as

$$I[w] = \frac{1}{2} \int_{\mathbb{R}^N} |\nabla w|^2 - \int_{\mathbb{R}^N} F(w). \quad (1.8)$$

System (1.1) has been studied among others by DeFigueiredo-Mitidieri [12], Klaasen-Mitidieri [19], Klaasen-Troy [20], Lazer-McKenna [21], Reinecke and Sweers ([33], [34], [35], [36]).

Note that our regime  $0 < \beta^2 = \gamma\delta < a$  is complementary to [36] and the references therein and so a different behavior is expected. Our results show that this is actually the case.

Many of the existence results are analogies of the results for the scalar case  $\delta = 0$  in [3]. However, numerical results in one and two-dimensional domains of Sweers and Troy [32] suggest that problem (1.1) admits a rich

solution structure. In this regard, the papers [36] and [8] show very interesting behavior of minimizers of (1.1) which are completely different from the single equation case [3]. The system (1.1) with Neumann boundary conditions has been studied in [27], [28], and [30]. Certain spot-like solutions have been constructed in [31]. Recently (multi)peaks in the interior and near the boundary have been constructed for the Dirichlet case [9]. Multipesaks for the Neumann problem have been derived in [10]. Clusters for the Neumann problem have been constructed in [11].

In this study, we introduce a new type of spot-like solution, namely a **cluster**. More precisely, we rigorously construct a solution of (1.2) which for a given positive integer  $K$  is concentrated in  $K$  spots for  $\epsilon, \delta$  small enough. Further, these spots converge to the same point in the limit  $\epsilon, \delta \rightarrow 0$ . This is **new** for the FitzHugh-Nagumo system. It shows that the solutions of (1.2) have a rich structure.

They are derived by the so-called “**localized energy method**” based on Liapunov-Schmidt reduction and variational techniques. This poses a restriction on the location of the spots. Namely, we prove the existence of clusters whose limiting spot locations satisfy the following conditions:

- (1) the center of the cluster approaches a hotspot point of  $\Omega$ ,
- (2) the rescaled cluster (by making the minimum distance between spots to 1) approaches an optimal configuration of the following geometric problem in  $R^2$ :

(\*) *Given  $K$  points  $Q_1, \dots, Q_K \in R^2$  with shortest distance 1, find the optimal configuration which minimizes the functional  $\sum_{i \neq j} \log |Q_i - Q_j|$ .*

We denote the minimum in (\*) by  $m(K)$ .

We remark that, using the same method, also solutions with multiple (separated) spots or clusters can be constructed. To keep notation and proofs simple, we restrict ourselves to the single-cluster case.

Note that for  $\delta = 0$  the system (1.1) decouples. The first equation of (1.1) for  $\delta = 0$  becomes

$$\epsilon^2 \Delta u + u(u - a)(1 - u) = 0, \quad u > 0 \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \partial\Omega, \tag{1.9}$$

which has been studied by numerous authors. It is known that this equation has interior spike solutions, see [5], [7], [26], [25], [37]. It is also known that there are no clusters to (1.9) with the Dirichlet boundary condition. However, if we replace in (1.9) the Dirichlet by the Neumann boundary condition then there are cluster solutions with spikes at the boundary, [6], [17]. In the present paper we show that interior clusters do occur for a **coupled** elliptic system even with the **Dirichlet** boundary condition.

We now state our main assumptions. We first assume that  $N = 2$ . (It may be possible to generalize the results to higher-dimensional domains.) Our second assumption is as follows: There exist two positive numbers  $m'$  and  $m$  such that

$$\epsilon^{m'} \leq \delta \leq \epsilon^m. \tag{1.10}$$

(This condition on  $\delta$  is needed for our computations.)

Let  $G$  be the Green's function  $-\Delta = \delta$  in  $\Omega$  with the Dirichlet boundary condition. Then equation (1.4) is equivalent to

$$v(x) = \int_{\Omega} G(x, z) u(z) dz.$$

We decompose

$$G(Q, x) = K(|x - Q|) - H(Q, x), \tag{1.11}$$

where  $H(Q, x)$  is the regular part which is  $C^2$  in  $\Omega$  and

$$K(|x - Q|) = \frac{1}{2\pi} \log \frac{1}{|x - Q|}. \quad (1.12)$$

We denote by  $H(Q) := H(Q, Q)$  the Robin function. Let  $H_0$  be the minimal value of  $H(Q)$ . The set  $\{Q_0 \in \Omega : H(Q_0) = H_0 = \min_{Q \in \Omega} H(Q)\}$  is called the set of hotspots of  $\Omega$ . For the properties of hot-spots, we refer to [1].

The main result of this paper is stated as follows:

**Theorem 1.1** *Let  $K > 0$  be a fixed positive integer. Suppose (1.10) holds. Then, for  $\epsilon$  sufficiently small, problem (1.2) admits a solution  $(u_\epsilon, v_\epsilon)$  with the following properties:*

(1)  $u_\epsilon(x) = \sum_{i=1}^K \left( w \left( \frac{x - Q_i^\epsilon}{\epsilon} \right) + o(1) \right)$  uniformly for  $x \in \bar{\Omega}$ , where  $w$  is the unique solution of the problem (1.5) and the points  $Q_1^\epsilon, \dots, Q_K^\epsilon$  approach the same point  $Q_0 \in \Omega$ .

(2) the center of the cluster  $\frac{1}{K} \sum_{i=1}^K Q_i^\epsilon \rightarrow Q_0$ , where  $H(Q_0) = H_0$ .

(3)  $\frac{1}{l^\epsilon} (Q_1^\epsilon, \dots, Q_K^\epsilon)$  approaches an optimal configuration of the problem (\*), where  $l^\epsilon = \min_{i \neq j} |Q_i^\epsilon - Q_j^\epsilon| = \left( \frac{1}{\sqrt{a}} + o(1) \right) \epsilon \log \frac{1}{\delta \epsilon^2} \rightarrow 0$ .

(3)  $v_\epsilon(x) = \epsilon^2 K G(x, Q_0) (1 + o(1)) \int_{\mathbb{R}^2} w dy$  uniformly for any compact subset of  $\bar{\Omega} \setminus \{Q_0\}$ .

**Remarks:** 1. In the same way one can prove the existence of multiple clusters at the maximum of

$$F(\mathbf{Q}) = \sum_{i,j=1,\dots,K,i \neq j} G(Q_i, Q_j) - \sum_{k=1}^K H(Q_k, Q_k). \quad (1.13)$$

where  $\mathbf{Q} = (Q_1, Q_2, \dots, Q_K) \in \Omega^K$ ,  $Q_i \neq Q_j$  for  $i \neq j$ . We omit the details.

2. Condition (1.10) implies  $\delta$  is of algebraic order of  $\epsilon$ . If  $\delta$  is exponentially small with respect to  $\epsilon$ , i.e.,  $\delta = e^{-d/\epsilon}$  for some positive number  $d$ , then the existence of multiple spots depends on  $d$ . We believe if  $d$  is small, clustered spots become separated multiple spots. If  $d$  is large, the existence of multiple spots depends on the geometry of the domain. It is an interesting problem to investigate the critical threshold of  $\delta$  for which multiple interior spots exists (even for simple domains like balls).

Let us now summarize the proof of Theorem 1.1.

We define a configuration space:

$$\Gamma := \left\{ (Q_1, \dots, Q_K) \in \Omega^K \mid H(\bar{Q}) \leq H_0 + \eta, \quad \frac{1 - \eta}{\sqrt{a}} \log \frac{1}{\delta \epsilon^2} \leq \frac{|Q_i - Q_j|}{\epsilon} \leq \left( \log \frac{1}{\delta \epsilon^2} \right)^2 \right\} \quad (1.14)$$

where  $\bar{Q} = \frac{1}{K} \sum_{j=1}^K Q_j$  and  $\eta > 0$  is such that

$$\eta = \frac{1}{40} \min(1, m). \quad (1.15)$$

Let  $\mathbf{Q} = (Q_1, \dots, Q_K) \in \bar{\Gamma}$ .

Theorem 1.1 is proved by the so-called “**localized energy method**”, a combination of the Liapunov-Schmidt reduction method and the variational principle. The Liapunov-Schmidt reduction method has been introduced and used in a lot of papers. See [16], [38] and the references therein. A combination of the Liapunov-Schmidt reduction method and the variational principle was used in [2], [8], [6], [16], and [17]. We shall follow the procedure

in [16]. This enables us to reduce the energy  $E_\delta$  to finite dimensions. Then local maxima for the reduced energy are found by maximizing  $E_\delta$  over  $\bar{\Gamma}$  and showing that this maximum actually belongs to the interior of  $\Gamma$ .

As far as we know, this is the first study on steady-state clusters for reaction-diffusions in the interior of a higher-dimensional bounded domain. For clusters which are supported by the boundary see [6], [17]. The one-dimensional case has been solved in [39] for the Gierer-Meinhardt system. Cluster ground states for the Gierer-Meinhardt system in the whole  $R^2$  have been constructed in [13].

Let us now give an outline of the paper. In Section 2 we study the geometric problem (\*). In Section 3 we derive the key energy estimates. In Section 4 we reduce the problem to finite dimensions by the Liapunov-Schmidt reduction method. In Section 5, we compute the reduced energy and show that a critical point for the reduced energy gives rise to a solution to (1.2). In Section 6 we solve the reduced problem by energy maximization in the set  $\bar{\Gamma}$  defined in (1.14) and derive Theorem 1.1.

Throughout this paper, the constants  $c_1, c_2, \dots$  are generic constants depending on  $N$  and  $w$  only.

We write

$$f(u) = -au + (a+1)u^2 - u^3 = -au + g(u), \quad \text{where } g(u) = (a+1)u^2 - u^3.$$

Let  $G[u] = \int_0^u g(s)ds$ .

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## 2 Optimal Configurations For Problem (\*)

Since problem (\*) plays an important role in the formation of the cluster, we study the properties of (\*) in this section.

To begin with, let us fix  $K$  points  $(Q_1, \dots, Q_K) \in R^{2K}$  and define

$$R[Q_1, \dots, Q_K] = \sum_{i \neq j} \log |Q_i - Q_j|. \quad (2.1)$$

Set

$$\Sigma := \{(Q_1, \dots, Q_K) \in R^{2K} \mid \sum_{j=1}^K Q_j = 0, \min_{i \neq j} |Q_i - Q_j| = 1\}. \quad (2.2)$$

Then Problem (\*) can be restated as the following minimization problem:

$$m(K) := \inf_{(Q_1, \dots, Q_K) \in \Sigma} R[Q_1, \dots, Q_K]. \quad (2.3)$$

The task is to determine this number  $m(K)$  and also characterize the configurations for which such an optimal number is achieved.

We state the following simple lemma.

**Lemma 2.1** *The minimum in problem (2.3) is always attained by some optimal configuration.*

**Proof:** Let  $Q_1^n, \dots, Q_K^n$  be a minimizing sequence. Without loss of generality, we may assume that  $|Q_1^n - Q_2^n| = 1$ . We claim that there exists a  $C(K)$  such that  $|Q_i^n - Q_j^n| \leq C(K)$ . In fact, since the number  $m(K) < +\infty$ , we have for  $n$  large,  $R[Q_1, \dots, Q_K] \leq m(K) + 1$ , which implies that  $|Q_i^n - Q_j^n| \leq e^{m(K)+1}$ . Therefore we have to minimize the continuous function  $R[Q_1, \dots, Q_K]$  on a compact set which implies that the minimum is attained. ■

We know  $m(3) = 0$  which is attained by a regular triangle.  $m(4) = \frac{1}{2} \log 3$  and  $m(4)$  is attained by two equal triangles with a common side. In general, it is difficult to find the number  $m(K)$ . This is an interesting geometric problem.

### 3 Key Energy Estimates

In this section, we derive some key energy estimates.

Let  $w$  be the ground state solution defined in (1.5). For  $z \in R^2$  let  $\Psi(z)$  be defined as

$$\Psi(z) = \int_{R^2} \left[ \frac{1}{2\pi} \log \frac{1}{|z-y|} \right] w(y) dy. \quad (3.1)$$

Then it is easy to see that

$$\Psi(z) = \frac{1}{2\pi} \log \frac{1}{|z|} \int_{R^2} w(y) dy + O\left(\frac{1}{|z|}\right). \quad (3.2)$$

Let  $\mathbf{Q} = (Q_1, \dots, Q_K) \in \Gamma$ . We denote the center of  $\mathbf{Q}$  as  $\bar{Q} = \frac{1}{K} \sum_{j=1}^K Q_j$ . Without loss of generality, we may assume that  $0 \in \Omega$  and let

$$\Omega_\epsilon = \{y | \epsilon y \in \Omega\}, \quad \Omega_{\epsilon,i} = \{y | \epsilon y + Q_i \in \Omega\}, \quad (3.3)$$

We define

$$w_{\epsilon,i} = w(y - Q_i) \chi(\epsilon y), \quad \Psi_i = \Psi(y - Q_i), \quad w_{\epsilon,\mathbf{Q}} = \sum_{i=1}^K w_{\epsilon,i}, \quad (3.4)$$

where  $\chi(x)$  is a smooth cut-off function such that  $\chi(x) = 1$  for  $d(x, \partial\Omega) > d_0$  and  $\chi(x) = 0$  for  $d(x, \partial\Omega) < \frac{d_0}{2}$  and  $d_0 = \min_{j=1, \dots, K} d(Q_j, \partial\Omega)$ .

Note that  $\|w_{\epsilon,i}(y) - w(\epsilon y)\|_\infty = O(e^{-d_0 \sqrt{a}/(2\epsilon)})$ . There is a better way of changing the function  $w$  to a function with Dirichlet boundary condition (and which gives a better error estimate) than using this cutoff, namely by defining a suitable projection as in [25]. By our choice of  $\delta$  in (1.10), this estimate is not part of the main terms in our problem and to keep the presentation simple we choose the cutoff.

We first compute  $T[w_{\epsilon,\mathbf{Q}}]$  near  $Q_j$ :

For  $\epsilon|z| < \kappa$  ( $\kappa > 0$  small enough), we compute

$$\begin{aligned} T[w_{\epsilon,\mathbf{Q}}](Q_j + \epsilon z) &= \int_{\Omega} G(Q_j + \epsilon z, \xi) \left( \sum_{i=1}^K w_{\epsilon,i} \right) d\xi \\ &= \int_{\Omega} G(Q_j + \epsilon z, \xi) w \left( \frac{\xi - Q_j}{\epsilon} \right) d\xi + \sum_{i \neq j} \int_{\Omega} G(Q_j + \epsilon z, \xi) w \left( \frac{\xi - Q_i}{\epsilon} \right) d\xi + O(e^{-\sqrt{a}d_0/(2\epsilon)}) \\ &= \epsilon^2 \int_{\Omega_{\epsilon,j}} \left[ \frac{1}{2\pi} \log \frac{1}{\epsilon|z-y|} - H(Q_j + \epsilon z, Q_j + \epsilon y) \right] w(y) dy \end{aligned}$$

$$\begin{aligned}
& +\epsilon^2 \sum_{i \neq j} \int_{R^2} G(Q_j + \epsilon z, Q_i + \epsilon y) w(y) dy + O(\epsilon^3) \\
& = \epsilon^2 \left( \frac{1}{2\pi} \log \frac{1}{\epsilon} \right) \int_{R^2} w(y) dy + \epsilon^2 \frac{1}{2\pi} \int_{R^2} \log \frac{1}{|z-y|} w(y) dy \\
& \quad + \epsilon^2 \left( \sum_{i \neq j} G(Q_j, Q_i) - H(Q_j, Q_j) \right) \int_{R^2} w(y) dy + o(\epsilon^2) \\
& \quad = \epsilon^2 \left( \frac{1}{2\pi} \log \frac{1}{\epsilon} \right) \int_{R^2} w(y) dy + \epsilon^2 \Psi(z) \\
& + \epsilon^2 \left( \sum_{i \neq j} K(|Q_i - Q_j|) - \epsilon^2 \sum_{i=1}^K H(Q_i, Q_j) \right) \int_{R^2} w(y) dy + o(\epsilon^2). \tag{3.5}
\end{aligned}$$

The following lemma is an easy consequence of Lebesgue's Dominated Convergence Theorem.

**Lemma 3.1** *Let  $g \in C(R^2) \cap L^\infty(R^2)$ ,  $h \in C(R^2)$  be radially symmetric and satisfy for some  $\alpha > 0, \beta, c_0 \in R$*

$$\begin{aligned}
& g(x) \exp(\alpha|x|)|x|^\beta \rightarrow c_0 \text{ as } |x| \rightarrow \infty \\
& \int_{R^2} |h(x)| \exp(\alpha|x|)(1 + |x|^\beta) dx < \infty.
\end{aligned}$$

Then

$$\exp(\alpha|y|)|y|^\beta \int_{R^2} h(x+y)g(x) dx \rightarrow c_0 \int_{R^2} h(x) \exp(-\alpha x_1) dx \text{ as } |y| \rightarrow \infty.$$

From Lemma 3.1, we then have the following estimate.

**Lemma 3.2** *It holds that*

$$\frac{1}{\epsilon^2 w \left( \frac{|Q_1 - Q_2|}{\epsilon} \right)} \int_{R^2} g \left( w \left( \frac{x - Q_1}{\epsilon} \right) \right) w \left( \frac{x - Q_2}{\epsilon} \right) dx \rightarrow \gamma_0 > 0 \text{ as } \epsilon \rightarrow 0, \tag{3.6}$$

where

$$\gamma_0 = \int_{R^2} g(w) e^{-\sqrt{a}y_1} dy. \tag{3.7}$$

Moreover, the function

$$\int_{R^2} g \left( w \left( \frac{x - Q_1}{\epsilon} \right) \right) w \left( \frac{x - Q_2}{\epsilon} \right) dx$$

is a  $C^2$  function in  $\frac{|Q_1 - Q_2|}{\epsilon}$  and (3.6) holds in the  $C^2$  sense.

Let us set

$$\alpha \left( \frac{|Q_i - Q_j|}{\epsilon} \right) = \int_{R^2} g \left( w \left( y - \frac{Q_i}{\epsilon} \right) \right) w \left( y - \frac{Q_j}{\epsilon} \right) dy. \tag{3.8}$$

Note that for  $\mathbf{Q} = (Q_1, \dots, Q_K) \in \Gamma$ ,

$$\alpha \left( \frac{|Q_i - Q_j|}{\epsilon} \right) = \gamma_0 w \left( \frac{|Q_i - Q_j|}{\epsilon} \right) (1 + o(1)) \leq C e^{-\sqrt{a} \frac{|Q_i - Q_j|}{\epsilon}} \leq C (\delta \epsilon^2)^{1-\eta} \tag{3.9}$$

by (1.14).

Using the previous results we will prove the next lemma which is the key energy estimate.

**Lemma 3.3** For any  $\mathbf{Q} = (Q_1, \dots, Q_K) \in \bar{\Gamma}$  and  $\epsilon, \delta$  sufficiently small

$$\begin{aligned} E_\epsilon(w_{\epsilon, \mathbf{Q}}) &= \epsilon^2 \left[ KI[w] + c_1 \delta \epsilon^2 \log \frac{1}{\epsilon} + c_2 \delta \epsilon^2 - \frac{1}{2} \sum_{i \neq j} \alpha \left( \frac{|Q_i - Q_j|}{\epsilon} \right) \right. \\ &\quad \left. + c_3 \delta \epsilon^2 \sum_{i \neq j} K \left( \frac{|Q_i - Q_j|}{\epsilon} \right) - c_4 \delta \epsilon^2 H(\bar{Q}) + o(\delta \epsilon^2) \right]. \end{aligned} \quad (3.10)$$

**Proof:** We compute

$$\begin{aligned} E_\epsilon[w_{\epsilon, \mathbf{Q}}] &= \frac{1}{2} \int_{\Omega} |\nabla w_{\epsilon, \mathbf{Q}}|^2 - \int_{\Omega} F(w_{\epsilon, \mathbf{Q}}) + \frac{\delta}{2} \int_{\Omega} \left( \sum_{j=1}^K w_{\epsilon, j} \right) T[w_{\epsilon, \mathbf{Q}}] \\ &=: I_1 + I_2, \end{aligned} \quad (3.11)$$

where

$$I_1 = \frac{1}{2} \int_{\Omega} |\nabla w_{\epsilon, \mathbf{Q}}|^2 - \int_{R^N} F(w_{\epsilon, \mathbf{Q}}), \quad I_2 = \frac{\delta}{2} \sum_{j=1}^K \int_{\Omega} w_{\epsilon, j} T[w_{\epsilon, \mathbf{Q}}].$$

For  $I_1$ , we compute using Lemma 3.2 in the case  $K = 2$

$$\begin{aligned} &\int_{\Omega} \frac{1}{2} |\nabla(w_{\epsilon, 1} + w_{\epsilon, 2})|^2 - \int_{\Omega} F(w_{\epsilon, 1} + w_{\epsilon, 2}) \\ &= \epsilon^2 2I[w] + \int_{\Omega} 2\nabla w_{\epsilon, 1} \cdot \nabla w_{\epsilon, 2} - \int_{\Omega} (f(w_{\epsilon, 1})w_{\epsilon, 2} + f(w_{\epsilon, 2})w_{\epsilon, 1}) + O(e^{-d_0 \sqrt{a}/(2\epsilon)}) + O((\delta \epsilon^2)^{3/2-\eta}) \\ &= \epsilon^2 2I[w] + \frac{1}{2} \int_{\Omega} (-w_{\epsilon, 1} \Delta w_{\epsilon, 2} - w_{\epsilon, 2} \Delta w_{\epsilon, 1}) - \int_{\Omega} (f(w_{\epsilon, 1})w_{\epsilon, 2} + f(w_{\epsilon, 2})w_{\epsilon, 1}) \\ &\quad + O((\delta \epsilon^2)^{3/2-\eta}) \\ &= \epsilon^2 2I[w] + \frac{1}{2} \int_{\Omega} (w_{\epsilon, 1} f(w_{\epsilon, 2}) + w_{\epsilon, 2} f(w_{\epsilon, 1})) \\ &\quad - \int_{\Omega} (f(w_{\epsilon, 1})w_{\epsilon, 2} + f(w_{\epsilon, 2})w_{\epsilon, 1}) + O((\delta \epsilon^2)^{3/2-\eta}) \\ &= \epsilon^2 \left[ 2I[w] - \frac{1}{2} \alpha \left( \frac{|Q_1 - Q_2|}{\epsilon} \right) + O((\delta \epsilon^2)^{3/2-\eta}) \right]. \end{aligned}$$

Note that  $e^{-d_0 \sqrt{a}/(2\epsilon)} \leq (\delta \epsilon^2)^\alpha$  for all  $\alpha > 0$  if  $\epsilon$  is small enough.

For  $K = 3, 4, \dots$  the proof is similar. See the proof of Lemma 2.6 of [15]. We get

$$\epsilon^{-2} I_1 = KI[w] - \frac{1}{2} \sum_{i \neq j} \alpha \left( \frac{|Q_i - Q_j|}{\epsilon} \right) + O((\delta \epsilon^2)^{3/2-\eta})$$

By (3.9) and (1.10), we have

$$\epsilon^{-2} I_1 = KI[w] - \frac{1}{2} \sum_{i \neq j} \alpha \left( \frac{|Q_i - Q_j|}{\epsilon} \right) + o(\delta \epsilon^2). \quad (3.12)$$

For  $I_2$ , we calculate, using (3.5),

$$\int_{\Omega} w_{\epsilon, \mathbf{Q}} T[w_{\epsilon, \mathbf{Q}}] dx = \int_{\Omega} \left( \sum_{j=1}^K w \left( \frac{x - Q_j}{\epsilon} \right) \right) T[w_{\epsilon, \mathbf{Q}}](x) dx + o(\epsilon^4)$$



$$\begin{aligned}
&= \sum_{j=1}^K \int_{\Omega} w \left( \frac{x - Q_j}{\epsilon} \right) T[w_{\epsilon, \mathbf{Q}}](x) dx + o(\epsilon^4) \\
&= \epsilon^2 \int_{R^2} w(z) \left[ \frac{K}{2\pi} \epsilon^2 \log \frac{1}{\epsilon} \int_{R^2} w(z) dz + \frac{K}{2\pi} \epsilon^2 \int_{R^2} \log \frac{1}{|z - \bar{z}|} w(\bar{z}) d\bar{z} \right. \\
&\quad \left. + \epsilon^2 \left( \sum_{i \neq j} K(|Q_j - Q_i|) - \sum_{i,j} H(Q_i, Q_j) \right) \int_{R^2} w(z) dz \right] dz + o(\epsilon^4) \\
&= \epsilon^4 \left( c_1 \log \frac{1}{\epsilon} + c_2 + c_3 \left( \sum_{i \neq j} K \left( \frac{|Q_i - Q_j|}{\epsilon} \right) - \sum_{i,j} H(Q_i, Q_j) \right) \right) + o(\epsilon^4)
\end{aligned}$$

where

$$c_1 = \frac{K}{2\pi} \left( \int_{R^2} w(z) dz \right)^2, \quad c_2 = \frac{K}{2\pi} \int_{R^2 \times R^2} w(z) w(\bar{z}) \log \frac{1}{|z - \bar{z}|} d\bar{z} dz, \quad c_3 = \left( \int_{R^2} w(z) dz \right)^2.$$

Note that for  $(Q_1, \dots, Q_K) \in \Gamma$ , we have  $Q_j - \frac{1}{K}(\sum_{i=1}^K Q_i) = O(\epsilon(\log \frac{1}{\delta \epsilon^2})^2)$ . Hence

$$H(Q_i, Q_j) = H(\bar{Q}) + O(\epsilon(\log \frac{1}{\delta \epsilon^2})^2). \quad (3.13)$$

So we obtain

$$I_2 = \delta \epsilon^4 \left( c_1 \log \frac{1}{\epsilon} + c_2 + c_3 \sum_{i \neq j} K \left( \frac{|Q_i - Q_j|}{\epsilon} \right) - c_4 H(\bar{Q}) + o(1) \right), \quad (3.14)$$

where  $c_4 = K(K-1)c_2 > 0$ .

Summarizing the results for  $I_1$  and  $I_2$ , the proof is finished. ■

Our last lemma contains the estimates for the error

**Lemma 3.4** *Let  $\mathbf{Q} = (Q_1, \dots, Q_K) \in \Gamma$ . Then we have*

$$\left| \Delta w_{\epsilon, \mathbf{Q}} + f(w_{\epsilon, \mathbf{Q}}) - \delta T[w_{\epsilon, \mathbf{Q}}] \right|_{L^\infty(\Omega_\epsilon)} \leq C((\delta \epsilon^2)^{1-\frac{\eta}{2}} + \delta \epsilon^2 |\log \epsilon|). \quad (3.15)$$

**Proof:** For the local term, we have

$$\left| \Delta w_{\epsilon, \mathbf{Q}} + f(w_{\epsilon, \mathbf{Q}}) \right| \leq C \sum_{i \neq j} w \left( \frac{|Q_i - Q_j|}{\epsilon} \right) \leq C(\delta \epsilon^2)^{1-\frac{\eta}{2}}. \quad (3.16)$$

See the proof of Lemma 3.3 in [16].

For the nonlocal term, we have from (3.5) that

$$\delta |T[w_{\epsilon, \mathbf{Q}}]| \leq C \delta \epsilon^2 |\log \epsilon|. \quad \blacksquare$$

## 4 Liapunov-Schmidt Reduction

Let

$$S_\epsilon[u] := \Delta u - au + g(u) - \delta T[u]. \quad (4.1)$$

We now introduce the functional-analytic framework. For  $u, v \in H_0^1(\Omega_\epsilon)$ , we equip it with the following scalar product:

$$(u, v) = \int_{\Omega_\epsilon} [\nabla u \nabla v + auv]. \quad (4.2)$$

Then orthogonality to the function  $\frac{\partial w_{\epsilon,i}}{\partial Q_{i,j}}$  in  $H_0^1(\Omega_\epsilon)$  is equivalent to orthogonality to the function

$$Z_{i,j} = (\Delta - a) \frac{\partial w_{\epsilon,i}}{\partial Q_{i,j}} \quad (4.3)$$

in  $L^2(\Omega_\epsilon)$  equipped with the usual scalar product

$$\langle u, v \rangle = \int_{\Omega_\epsilon} uv \, dy. \quad (4.4)$$

This section is devoted to the study of the following system in  $(\phi, \beta)$ :

$$S_\epsilon[w_{\epsilon, \mathbf{Q}} + \phi] = \sum_{i,j} \beta_{ij} Z_{i,j}, \quad \langle \phi, Z_{i,j} \rangle = 0, \quad i = 1, \dots, K, \quad j = 1, \dots, N. \quad (4.5)$$

To this end, we introduce the following norm for a function defined on  $\Omega_\epsilon$ : For  $(Q_1, \dots, Q_K) \in \bar{\Gamma}$  we define

$$\|\phi\|_\infty := \sup_{y \in \Omega_\epsilon} |\phi(y)|. \quad (4.6)$$

We first consider a linear problem:  $h \in L^\infty(\Omega_\epsilon)$  being given, find a function  $\phi$  satisfying

$$\begin{cases} L_\epsilon[\phi] := \Delta \phi - a\phi + g'(w_{\epsilon, \mathbf{Q}})\phi - \delta T[\phi] = h + \sum_{i,j} \beta_{ij} Z_{i,j}, \\ \langle \phi, Z_{i,j} \rangle = 0 \end{cases} \quad (4.7)$$

for some real constants  $\beta_{i,j}$ .

The following Lemma provides an a priori estimate for (4.7).

**Lemma 4.1** *Let  $(\phi, \beta)$  satisfy (4.7). Then for  $\epsilon$  sufficiently small, we have*

$$\|\phi\|_\infty \leq C \|h\|_\infty. \quad (4.8)$$

**Proof:** We prove it by contradiction. Suppose not. Then there exists a sequence  $\epsilon_k \rightarrow 0$  and a sequence of functions  $\phi_k$  satisfying (4.7) such that the following holds:

$$\|\phi_k\|_\infty = 1, \quad \|h_k\|_\infty = o(1), \quad \langle \phi_k, Z_{i,j} \rangle = 0, \quad i = 1, \dots, K, \quad j = 1, \dots, N.$$

For simplicity of notation, we drop the dependence on  $k$ .

Multiplying (4.7) by  $\frac{\partial w_{\epsilon,k}}{\partial Q_{k,l}}$  and integrating over  $\Omega_\epsilon$ , we obtain that

$$\sum_{i,j} \beta_{ij} \langle Z_{ij}, \frac{\partial w_{\epsilon,k}}{\partial Q_{k,l}} \rangle = - \langle h, \frac{\partial w_{\epsilon,k}}{\partial Q_{k,l}} \rangle + O(\delta) = O(\|h\|_\infty) + O(\delta)$$

Hence we obtain that

$$|\beta| = O(\|h\|_\infty) + O(\delta) = o(1), \quad \|h + \sum_{i,j} \beta_{ij} Z_{ij}\|_\infty = o(1). \quad (4.9)$$

Note also that

$$\|T[\phi]\|_\infty = O(1).$$

Therefore we have

$$\|\Delta\phi - a\phi + g'(w_{\epsilon, \mathbf{Q}})\phi\|_\infty = o(1). \quad (4.10)$$

Since

$$\|(g'(w_{\epsilon, \mathbf{Q}}) - \sum_{j=1}^K g'(w_{\epsilon, j}))\phi\|_\infty = o(1),$$

(4.10) is equivalent to

$$\|\Delta\phi - a\phi + \sum_{j=1}^K g'(w_{\epsilon, j})\phi\|_\infty = o(1). \quad (4.11)$$

Fix an  $R > 0$ . We claim that  $\|\phi\|_{L^\infty(\cup_{j=1}^K B_R(Q_j))} = o(1)$ . In fact, suppose not, we may assume that  $\|\phi\|_{L^\infty(B_R(Q_1))} \geq c_0 > 0$ . Then as  $\epsilon \rightarrow 0$ , we have  $\phi(y - Q_1) \rightarrow \phi_0$  in  $C_{loc}^2(\mathbb{R}^N)$ , where  $\phi_0$  satisfies

$$\Delta\phi_0 - a\phi_0 + g'(w)\phi_0 = 0, \quad |\phi_0(y)| \leq C. \quad (4.12)$$

By Lemma 6.4 of [25],  $\phi_0 = \sum_{j=1}^N a_j \frac{\partial w}{\partial y_j}$ . But  $\int_{\mathbb{R}^N} \phi_0 g'(w) \frac{\partial w}{\partial y_j} = 0$  for  $j = 1, \dots, N$ . So  $a_j = 0, j = 1, \dots, N$ . A contradiction.

Since  $\|\phi\|_{L^\infty(\cup_{j=1}^K B_R(Q_j))} = o(1)$ , we obtain

$$\|\sum_{j=1}^K g'(w_{\epsilon, j})\phi\|_\infty = o(1)$$

and

$$\|\Delta\phi - a\phi\|_\infty = o(1) \quad (4.13)$$

By the Maximum Principle,  $\|\phi\|_\infty = o(1)$ . A contradiction. ■

Next we consider the existence problem for (4.7).

**Lemma 4.2** *There exists an  $\epsilon_0 > 0$  such that for any  $\epsilon < \epsilon_0$ , given any  $h \in L^\infty(\Omega_\epsilon)$ , there exists a unique pair  $(\phi, \beta)$  such that the following hold:*

$$L_\epsilon[\phi] = h + \sum_{i,j} \beta_{i,j} Z_{i,j}, \quad (4.14)$$

$$\langle \phi, Z_{i,j} \rangle = 0. \quad (4.15)$$

Moreover, we have

$$\|\phi\|_\infty \leq C\|h\|_\infty. \quad (4.16)$$

**Proof:** The existence follows from Fredholm's alternative. To this end, let

$$\mathcal{H} = \{u \in H_0^1(\Omega_\epsilon) \mid \langle u, Z_{i,j} \rangle = 0, i = 1, \dots, K, j = 1, \dots, N\}.$$

Observe that  $\phi$  solves (4.14) and (4.15) if and only if  $\phi \in H^1(\Omega_\epsilon)$  satisfies

$$\begin{aligned} \int_{R^N} (\nabla\phi\nabla\psi + a\phi\psi) - \langle g'(w_{\epsilon,\mathbf{Q}})\phi + \delta T[\phi], \psi \rangle \\ = \langle h, \psi \rangle, \quad \forall \psi \in H_0^1(\Omega_\epsilon). \end{aligned}$$

This equation can be rewritten in the following form

$$\phi + \mathcal{S}(\phi) = \bar{h}, \quad (4.17)$$

where  $\mathcal{S}$  is a linear compact operator from  $\mathcal{H}$  to  $\mathcal{H}$ ,  $\bar{h} \in \mathcal{H}$  and  $\phi \in \mathcal{H}$ .

Using Fredholm's alternative, to show equation (4.17) has a uniquely solvable solution for each  $\bar{h}$ , it is enough to show that the equation has a unique solution for  $\bar{h} = 0$ . To this end, we assume the contrary. That is, there exists  $(\phi, \beta)$  such that

$$L_\epsilon[\phi] = \sum_{i,j} \beta_{ij} Z_{i,j}, \quad (4.18)$$

$$\langle \phi, Z_{i,j} \rangle = 0, i = 1, \dots, K, j = 1, \dots, N. \quad (4.19)$$

From (4.18), it is easy to see that  $\|\phi\|_\infty < +\infty$ . So without loss of generality, we may assume that  $\|\phi\|_\infty = 1$ . But then this contradicts to (4.8). ■

Finally, we solve (4.5) for  $(\phi, \beta)$ . The following is the main result of this section.

**Lemma 4.3** *For  $(Q_1, \dots, Q_K) \in \bar{\Gamma}$  and  $\epsilon$  sufficiently small, there exists a unique pair  $(\phi_{\epsilon,\mathbf{Q}}, \beta_\epsilon(\mathbf{Q}))$  satisfying (4.5). Furthermore,  $(\phi_{\epsilon,\mathbf{Q}}, \beta_\epsilon(\mathbf{Q}))$  is continuous in  $\mathbf{Q}$  and we have the following estimate*

$$\|\phi_{\epsilon,\mathbf{Q}}\|_\infty \leq C((\delta\epsilon^2)^{1-\eta} + \delta\epsilon^2 |\log \epsilon|^2). \quad (4.20)$$

**Proof:** We write (4.5) in the following form:

$$L_\epsilon[\phi] = -S_\epsilon[w_{\epsilon,\mathbf{Q}}] - N_\epsilon[\phi] + \sum_{ij} \beta_{ij} Z_{i,j} \quad (4.21)$$

and use contraction mapping theorem. Here  $N_\epsilon[\phi]$  is given by

$$N_\epsilon[\phi] = g(w_{\epsilon,\mathbf{Q}} + \phi) - g(w_{\epsilon,\mathbf{Q}}) - g'(w_{\epsilon,\mathbf{Q}})\phi. \quad (4.22)$$

It is easy to see that

$$\|N_\epsilon[\phi]\|_\infty \leq C \left( \|\phi\|_\infty^2 \right). \quad (4.23)$$

Set  $\mathcal{B} = \{\|\phi\|_\infty < \delta\epsilon^2 |\log \epsilon|^2 + (\delta\epsilon^2)^{1-\eta}\}$ . Fix  $\phi \in \mathcal{B}$  and we consider the map  $\mathcal{A}_\epsilon$  to be the unique solution given by Lemma 4.2 with  $h = -S_\epsilon[w_{\epsilon,\mathbf{Q}}] - N_\epsilon[\phi]$ . Then by Lemma 4.2, we have

$$\|\mathcal{A}_\epsilon[\phi]\|_\infty \leq C \| -S_\epsilon[w_{\epsilon,\mathbf{Q}}] - N_\epsilon[\phi] \|_\infty \leq C \delta\epsilon^2 |\log \epsilon| + (\delta\epsilon^2)^{1-\eta} \quad (4.24)$$

and hence  $\mathcal{A}_\epsilon[\phi] \in \mathcal{B}$ . Moreover, we also have that

$$\|\mathcal{A}_\epsilon[\phi_1] - \mathcal{A}_\epsilon[\phi_2]\|_\infty \leq C\|N_\epsilon[\phi_1] - N_\epsilon[\phi_2]\|_\infty \leq (\delta\epsilon^2|\log \epsilon|^2 + (\delta\epsilon^2)^{1-\eta})\|\phi_1 - \phi_2\|_\infty. \quad (4.25)$$

(4.24) and (4.25) show that the map  $\mathcal{A}_\epsilon$  is a contraction map from  $\mathcal{B}$  to  $\mathcal{B}$ . By the contraction mapping theorem, (4.21) has a unique solution  $\phi \in B$ , called  $\phi_{\epsilon, \mathbf{Q}}$ .

The continuity of  $\phi_{\epsilon, \mathbf{Q}}, \beta_\epsilon(\mathbf{Q})$  follows from the uniqueness of  $(\phi_{\epsilon, \mathbf{Q}}, \beta_\epsilon(\mathbf{Q}))$  and the continuity of  $w_{\epsilon, i}, \frac{\partial w_{\epsilon, i}}{\partial Q_{k, l}}$ .  $\blacksquare$

The last lemma shows the  $C^1$ -smoothness of  $\phi_{\epsilon, \mathbf{Q}}$ .

**Lemma 4.4** *The map  $\mathbf{Q} : \bar{\Gamma} \rightarrow \phi_{\epsilon, \mathbf{Q}}$  is actually  $C^1$ .*

**Proof:**

Consider the following map  $H : \bar{\Gamma} \times H_0^1(\Omega_\epsilon) \times R^{2K} \rightarrow H_0^1(\Omega_\epsilon) \times R^{2K}$  of class  $C^1$

$$H(\mathbf{Q}, \phi, \beta) = \begin{pmatrix} (\Delta - a)^{-1}(S_\epsilon[w_{\epsilon, \mathbf{Q}} + \phi]) - \sum_{i, j} \beta_{ij} \frac{\partial w_{\epsilon, i}}{\partial Q_{i, j}} \\ (\phi, \frac{\partial w_{\epsilon, i}}{\partial Q_{i, j}}) \end{pmatrix}. \quad (4.26)$$

The equations (4.5) are equivalent to  $H[\mathbf{Q}, \phi, \beta] = 0$ . We know that, given  $\mathbf{Q} \in \bar{\Gamma}$ , there is a unique local solution  $(\phi_{\epsilon, \mathbf{Q}}, \beta_\epsilon(\mathbf{Q}))$  obtained with the above procedure. We prove that the linear operator

$$\frac{\partial H(\mathbf{Q}, \phi, \beta)}{\partial(\phi, \beta)} \Big|_{(\mathbf{Q}, \phi_{\epsilon, \mathbf{Q}}, \beta_\epsilon(\mathbf{Q}))} : H_0^1(\Omega_\epsilon) \times R^{2K} \rightarrow H_0^1(\Omega_\epsilon) \times R^{2K}$$

is invertible for  $\epsilon$  small. Then the  $C^1$ -regularity of  $s \mapsto \phi_{\epsilon, \mathbf{Q}}$  follows from the Implicit Function Theorem. Indeed we have

$$\frac{\partial H(\mathbf{Q}, \phi, \beta)}{\partial(\phi, \beta)} \Big|_{(\mathbf{Q}, \phi_{\epsilon, \mathbf{Q}}, \beta_\epsilon(\mathbf{Q}))} [\hat{\phi}, \hat{\beta}] = \begin{pmatrix} (\Delta - a)^{-1}(S'_\epsilon[w_{\epsilon, \mathbf{Q}} + \phi_{\epsilon, \mathbf{Q}}](\hat{\phi})) - \sum_{i, j} \hat{\beta}_{ij} \frac{\partial w_{\epsilon, i}}{\partial Q_{i, j}} \\ (\hat{\phi}, \frac{\partial w_{\epsilon, i}}{\partial Q_{i, j}}) \end{pmatrix}.$$

Since  $\|\phi_{\epsilon, \mathbf{Q}}\|_\infty$  is small, the same proof as in that of Lemma 4.1 shows that  $\frac{\partial H(\mathbf{Q}, \phi, \beta)}{\partial(\phi, \beta)} \Big|_{(\mathbf{Q}, \phi_{\epsilon, \mathbf{Q}}, \beta_\epsilon(\mathbf{Q}))}$  is invertible for  $\epsilon$  small.

This concludes the proof of Lemma 4.4.  $\blacksquare$

## 5 Reduced Energy functional

In this section we expand the quantity

$$M_\epsilon(\mathbf{Q}) := \epsilon^{-2} \left[ E_\epsilon[w_{\epsilon, \mathbf{Q}} + \phi_{\epsilon, \mathbf{Q}}] - \epsilon^2 KI[w] \right] - c_1 \delta \epsilon^2 \log \frac{1}{\epsilon} - c_2 \delta \epsilon^2 : \bar{\Gamma} \rightarrow R \quad (5.1)$$

in  $\epsilon, \delta$  and  $\mathbf{Q}$ , where  $\phi_{\epsilon, \mathbf{Q}}$  is given by Lemma 4.3.

We proceed by using Lemma 3.3 and estimating the error caused by adding  $\phi_{\epsilon, \mathbf{Q}}$ .

**Lemma 5.1** *Let  $\phi_{\epsilon, \mathbf{Q}}$  be defined by Lemma 4.3. Then for any  $\mathbf{Q} = (Q_1, \dots, Q_K) \in \bar{\Gamma}$  and  $\epsilon$  sufficiently small we have*

$$M_\epsilon(\mathbf{Q}) = \delta\epsilon^2 c_3 \sum_{i \neq j} K\left(\frac{|Q_i - Q_j|}{\epsilon}\right) - \frac{1}{2} \sum_{i \neq j} \alpha\left(\frac{|Q_i - Q_j|}{\epsilon}\right) - c_4 \delta\epsilon^2 H(\bar{Q}) + o(\delta\epsilon^2) \quad (5.2)$$

where  $c_2, c_4$  are positive constants, the function  $K$  is defined in (1.12), and the function  $\alpha$  is defined in (3.8).

**Proof.** In fact, for any  $\mathbf{Q} \in \bar{\Gamma}$ , we have

$$E_\epsilon(w_{\epsilon, \mathbf{Q}} + \phi_{\epsilon, \mathbf{Q}}) = E_\epsilon(w_{\epsilon, \mathbf{Q}}) + J_\epsilon(\phi_{\epsilon, \mathbf{Q}}) + O(\|\phi_{\epsilon, \mathbf{Q}}\|_\infty^2), \quad (5.3)$$

Note that

$$\|\phi_{\epsilon, \mathbf{Q}}\|_\infty^2 = O(\delta^2 \epsilon^4 |\log \epsilon|^4 + (\delta\epsilon^2)^{2-2\eta}) = o(\delta\epsilon^4)$$

by (1.10) and (1.15). Observe also that

$$J_\epsilon(\phi_{\epsilon, \mathbf{Q}}) = \epsilon^2 \int_{\Omega_\epsilon} S_\epsilon(w_{\epsilon, \mathbf{Q}}) \phi_{\epsilon, \mathbf{Q}} dy.$$

We compute

$$\begin{aligned} |J_\epsilon(\phi_{\epsilon, \mathbf{Q}})| &= \left| \int_{\Omega_\epsilon} S_\epsilon(w_{\epsilon, \mathbf{Q}}) \phi_{\epsilon, \mathbf{Q}} dx \right| \\ &\leq C\epsilon^{-2} ((\delta\epsilon^2)^{1-\frac{\eta}{2}} + \delta\epsilon^2 |\log \epsilon|) ((\delta\epsilon^2)^{1-\eta} + \delta\epsilon^2 |\log \epsilon|^2) = o(\delta\epsilon^2) \end{aligned}$$

by Lemma 3.4 and Lemma 4.3.

The proof of Lemma 5.1 is completed. ■

The second and the last lemma in this section concerns the relation between the critical points of  $M_\epsilon(\mathbf{Q})$  and those of energy function  $E_\epsilon[u]$ .

**Lemma 5.2** *Suppose  $\mathbf{Q}^\epsilon \in \text{int}(\Gamma)$  is a critical point of  $M_\epsilon(\mathbf{Q})$ . Then the corresponding function  $u_\epsilon = w_{\epsilon, \mathbf{Q}^\epsilon} + \phi_{\epsilon, \mathbf{Q}^\epsilon}$  is also a critical point of  $E_\epsilon[u] : H_0^1(\Omega) \rightarrow \mathbb{R}$  and hence a solution of (1.2).*

**Proof:** By Lemma 4.3 and Lemma 4.4, there exists an  $\epsilon_0 > 0$  such that for  $0 < \epsilon < \epsilon_0$  we have a  $C^1$  map which, to any  $\mathbf{Q} \in \bar{\Gamma}$ , associates  $\phi_{\epsilon, \mathbf{Q}}$  such that

$$S_\epsilon(w_{\epsilon, \mathbf{Q}} + \phi_{\epsilon, \mathbf{Q}}) = \sum_{i,j} \beta_{ij} Z_{i,j} \quad (5.4)$$

for some constants  $\beta_{ij} \in \mathbb{R}^{NK}$ .

Let  $\mathbf{Q}^\epsilon \in \Gamma$  be a critical point of  $M_\epsilon(\mathbf{Q})$ . Let  $u_\epsilon = w_{\epsilon, \mathbf{Q}^\epsilon} + \phi_{\epsilon, \mathbf{Q}^\epsilon}$ . Then we have

$$\frac{\partial}{\partial Q_{i,j}} \Big|_{\mathbf{Q}=\mathbf{Q}^\epsilon} M_\epsilon(\mathbf{Q}^\epsilon) = 0, \quad i = 1, \dots, K, \quad j = 1, \dots, N.$$

Hence we have

$$\int_{\Omega_\epsilon} [\nabla u_\epsilon \nabla \frac{\partial(w_{\epsilon, \mathbf{Q}} + \phi_{\epsilon, \mathbf{Q}})}{\partial Q_{i,j}}] \Big|_{\mathbf{Q}=\mathbf{Q}^\epsilon}$$

$$+(-au_\epsilon + g(u_\epsilon) - \delta T[u_\epsilon]) \frac{\partial(w_{\epsilon, \mathbf{Q}} + \phi_{\epsilon, \mathbf{Q}})}{\partial Q_{k,l}} \Big|_{\mathbf{Q}=\mathbf{Q}^\epsilon} = 0$$

which is equivalent to

$$\int_{\Omega_\epsilon} S_\epsilon(u_\epsilon) \frac{\partial(w_{\epsilon, \mathbf{Q}} + \phi_{\epsilon, \mathbf{Q}})}{\partial Q_{k,l}} \Big|_{\mathbf{Q}=\mathbf{Q}^\epsilon} = 0.$$

Thus we have from (5.4)

$$\sum_{i,j} \beta_{ij} \int_{\Omega_\epsilon} Z_{i,j} \left( \frac{\partial(w_{\epsilon, \mathbf{Q}} + \phi_{\epsilon, \mathbf{Q}})}{\partial Q_{k,l}} \right) \Big|_{\mathbf{Q}=\mathbf{Q}^\epsilon} = 0. \quad (5.5)$$

Since  $\langle Z_{i,j}, \phi_{\epsilon, \mathbf{Q}} \rangle > 0$ , we have for  $\mathbf{Q} = \mathbf{Q}^\epsilon$  that

$$\int_{\Omega_\epsilon} Z_{i,j} \frac{\partial \phi_{\epsilon, \mathbf{Q}}}{\partial Q_{k,l}} = - \int_{\Omega_\epsilon} \phi_{\epsilon, \mathbf{Q}} \frac{\partial Z_{i,j}}{\partial Q_{k,l}} = O(\epsilon^{1-\eta}).$$

Note that

$$\int_{\Omega_\epsilon} Z_{i,j} \frac{\partial w_{\epsilon, \mathbf{Q}}}{\partial Q_{k,l}} = \epsilon_{ik} \epsilon_{jl} A_0 (1 + o(1)),$$

where

$$A_0 = \int_{R^N} g'(w) \left( \frac{\partial w}{\partial y_1} \right)^2 = \int_{R^N} [|\nabla \left( \frac{\partial w}{\partial y_1} \right)|^2 + a \left( \frac{\partial w}{\partial y_1} \right)^2] > 0.$$

Thus (5.5) becomes a system of homogeneous equations for  $\beta_{ij}$  and the matrix of the system is nonsingular since it is dominated by its diagonal. So  $\beta_{ij} \equiv 0, i = 1, \dots, K, j = 1, \dots, N$ .

Hence  $u_\epsilon = w_{\epsilon, \mathbf{Q}^\epsilon} + \phi_{\epsilon, \mathbf{Q}^\epsilon}$  is a solution of (1.2). ■

## 6 The Reduced Problem: Proof of Theorem 1.1

In this section, we study a maximization problem.

Fix  $\mathbf{Q} \in \bar{\Gamma}$ . Let  $\Phi_{\delta, \mathbf{Q}}$  be the solution given by Lemma 4.3.

We shall prove

**Proposition 6.1** *For  $\epsilon$  small, the following maximization problem*

$$\max\{M_\epsilon(\mathbf{Q}) : \mathbf{Q} \in \bar{\Gamma}\} \quad (6.1)$$

*has a solution  $\mathbf{Q}^\epsilon$  which belongs to  $\Gamma$ .*

Before we prove the above proposition, we present two lemmas on a finite dimensional problem.

**Lemma 6.2** *Consider the function*

$$h(\rho) = c_3 \delta \epsilon^2 K(\rho) - \frac{1}{2} \alpha(\rho), \quad \rho \geq \frac{1-\eta}{\sqrt{a}} \log \frac{1}{\delta \epsilon^2}. \quad (6.2)$$

*Then, for  $\delta \epsilon^2$  small enough,  $h(\rho)$  has a unique maximum point  $\rho_{\max}$ . Moreover we have*

$$\rho_{\max} = \frac{1}{\sqrt{a}} \log \frac{1}{\delta \epsilon^2} + O(\log \log \frac{1}{\delta \epsilon^2}) \quad (6.3)$$

and

$$h(\rho_{\max}) = \frac{c_3}{2\pi} \delta \epsilon^2 \log \frac{1}{\rho_{\max}} + o(\delta \epsilon^2). \quad (6.4)$$

**Proof:** This is a calculus problem since for  $\rho$  large we have  $w(\rho) = c_9 \rho^{-\frac{1}{2}} e^{-\sqrt{a}\rho} (1 + O(\frac{1}{\rho}))$  and  $K(\rho) = \frac{1}{2\pi} \log \frac{1}{\rho}$ . Differentiating  $h$  with respect to  $\rho$  gives an equation for the critical point of  $h(\rho)$ :

$$\left( c_3 \delta \epsilon^2 \frac{1}{\rho_{\max}} - \sqrt{a} \rho_{\max}^{-1/2} e^{-\sqrt{a}\rho_{\max}} \right) \left( 1 + O\left(\frac{1}{\rho_{\max}}\right) \right) = 0.$$

After taking the logarithm, (6.3) and (6.4) follow. The proof of the uniqueness of the maximum is elementary by considering the sign of the second derivative.  $\blacksquare$

**Proof of Proposition 6.1:**

Since the set  $\Gamma$  is compact, the function  $M_\epsilon(\mathbf{Q})$  has a maximum point  $\mathbf{Q}^\epsilon \in \bar{\Gamma}$ . We need to show that  $\mathbf{Q}^\epsilon$  must lie in the interior of  $\Gamma$ .

We first obtain an upper bound for  $M_\epsilon(\mathbf{Q}^\epsilon)$ . Let  $Q_0$  be a point such that  $H(Q_0) = \min_{Q \in \Omega} H(Q)$ . Let  $\mathbf{Q}^0 = (Q_1^0, \dots, Q_K^0)$  be an optimal configuration given in Lemma 2.1. We choose  $\mathbf{Q} = Q_0 + \rho_{\max} \mathbf{Q}^0$ , where  $\rho_{\max}$  is given by Lemma 6.2. It is easy to see that this choice of  $\mathbf{Q}$  belongs to  $\Gamma$ . Then we have

$$\begin{aligned} M_\epsilon(\mathbf{Q}^\epsilon) &\geq \sum_{i \neq j} h(\rho_{\max} |Q_i^0 - Q_j^0|) - c_4 \delta \epsilon^2 H(Q_0) + o(\delta \epsilon^2) \\ &\geq K(K-1)h(\rho_{\max}) - \frac{1}{2\pi} \delta \epsilon^2 R[Q_1^0, \dots, Q_K^0] - \delta \epsilon^2 c_4 H_0 + o(\delta \epsilon^2) \end{aligned} \quad (6.5)$$

by Lemma 6.2.

Let  $l^\epsilon = \min_{i \neq j} |Q_i^\epsilon - Q_j^\epsilon|$ . (Without loss of generality, we may assume that  $l^\epsilon = |Q_1^\epsilon - Q_2^\epsilon|$ .) Then  $l^\epsilon > (1 - \eta) \frac{1}{\sqrt{a}} \epsilon \log \frac{1}{\delta}$ . In fact, suppose not. Then we have

$$M_\epsilon(\mathbf{Q}^\epsilon) \leq h\left(\frac{l^\epsilon}{\epsilon}\right) + \left( \sum_{i \neq j, (i,j) \neq (1,2)} [h(\rho_{\max})] \right) - \delta \epsilon^2 c_4 H_0 + o(\delta \epsilon^2) \leq -C(\delta \epsilon^2)^{(1-\frac{\eta}{2})} < 0 \quad (6.6)$$

which contradicts with (6.5).

Consider the rescaled vertex  $\hat{Q}_i^\epsilon = \frac{1}{l^\epsilon} Q_i^\epsilon$ . Then we have

$$\begin{aligned} M_\epsilon(\mathbf{Q}^\epsilon) &\leq c_3 \delta \epsilon^2 \sum_{i \neq j} K \left( \frac{l^\epsilon |\hat{Q}_i^\epsilon - \hat{Q}_j^\epsilon|}{\epsilon} \right) - \frac{1}{2} \sum_{i \neq j} \alpha \left( \frac{l^\epsilon |\hat{Q}_i^\epsilon - \hat{Q}_j^\epsilon|}{\epsilon} \right) - c_4 \delta \epsilon^2 h(\bar{Q}^\epsilon) + o(\delta \epsilon^2) \\ &\leq K(K-1) c_3 \delta \epsilon^2 \frac{1}{2\pi} \log \frac{\epsilon}{l^\epsilon} - c_3 \delta \epsilon^2 \frac{1}{2\pi} R[Q_1^\epsilon, \dots, Q_K^\epsilon] - \delta \epsilon^2 c_4 h(\bar{Q}^\epsilon) + o(\delta \epsilon^2). \end{aligned} \quad (6.7)$$

From (6.5) and (6.7), we deduce that

$$K(K-1) c_3 \delta \epsilon^2 \frac{1}{2\pi} \log \frac{\epsilon \rho_{\max}}{l^\epsilon} - c_3 \delta \epsilon^2 \frac{1}{2\pi} (R[\hat{Q}_1^\epsilon, \dots, \hat{Q}_K^\epsilon] - m(K)) - \delta \epsilon^2 c_4 (H(\bar{Q}^\epsilon) - H_0) + o(\delta \epsilon^2) \geq 0, \quad (6.8)$$

where  $m(K)$  was defined in (2.3). If either  $H(\bar{Q}^\epsilon) \geq H_0 + c_0$  or  $R[\hat{Q}_1^\epsilon, \dots, \hat{Q}_K^\epsilon] \geq m(K) + c_0$  for some  $c_0 > 0$ , then we have

$$\log \frac{\epsilon}{l^\epsilon \rho_{\max}} \geq c_5$$



which implies that

$$\frac{l^\epsilon}{\epsilon} \leq e^{-c_5} \rho_{\max},$$

and

$$h\left(\frac{l^\epsilon}{\epsilon}\right) \leq -C(\delta\epsilon^2)^{1-c_6} \quad (6.9)$$

for some  $c_5, c_6 > 0$ . Now arguments similar to those leading to (6.6) give a contradiction.

So we have  $h(\bar{Q}^\epsilon) \rightarrow H_0$  and  $R[\hat{Q}_1^\epsilon, \dots, \hat{Q}_K^\epsilon] \rightarrow m(K)$  as  $\epsilon \rightarrow 0$ . This implies that  $|Q_i^\epsilon - Q_j^\epsilon| \leq C l^\epsilon$ .

Finally, we claim that  $l^\epsilon \leq C\epsilon \log \frac{1}{\delta\epsilon^2}$ . In fact, from (6.8) we deduce that  $\limsup_{\epsilon \rightarrow 0} \frac{l^\epsilon}{\epsilon\rho_{\max}} \leq 1$ . It then follows that  $\lim_{\epsilon \rightarrow 0} \frac{l^\epsilon}{\epsilon\rho_{\max}} = 1$  as otherwise  $\liminf_{\epsilon \rightarrow 0} \frac{l^\epsilon}{\epsilon\rho_{\max}} < 1$ , which is impossible by (6.6) again.

In conclusion, we have proved that  $\lim_{\epsilon \rightarrow 0} \frac{l^\epsilon}{\epsilon\rho_{\max}} = 1$ ,  $R[\frac{Q_1^\epsilon}{l^\epsilon}, \dots, \frac{Q_K^\epsilon}{\epsilon}] \rightarrow m(K)$ ,  $H(\bar{Q}^\epsilon) \rightarrow H_0$ , as  $\epsilon \rightarrow 0$ . This implies that  $\mathbf{Q}^\epsilon$  is in the interior of  $\Gamma$ .

Proposition 6.1 follows from the proof. ■

### Completion of the Proof of Theorem 1.1:

Theorem 1.1 is proved by combining Proposition 6.1 and Lemma 5.2. ■

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