

TRANSPORT IN A MOLECULAR MOTOR SYSTEM<sup>\*,\*\*</sup>MICHEL CHIPOT<sup>1</sup>, STUART HASTINGS<sup>2</sup> AND DAVID KINDERLEHRER<sup>3</sup>

**Abstract.** Intracellular transport in eukarya is attributed to motor proteins that transduce chemical energy into directed mechanical energy. This suggests that, in nonequilibrium systems, fluctuations may be oriented or organized to do work. Here we seek to understand how this is manifested by quantitative mathematical portrayals of these systems.

**Mathematics Subject Classification.** 34D23, 35K50, 35K57, 92C37, 92C45.

Received: July 6, 2004. Revised: September 13, 2004.

## 1. INTRODUCTION

Intracellular transport in eukarya is attributed to motor proteins that transduce chemical energy into directed mechanical motion. Muscle myosin has been known since the mid-nineteenth century and its role as a motor in muscle contraction first explained by Huxley, [10], *cf.* [9]. Kinesins and the role of motor proteins in intracellular transport were discovered around 1985. There is an extremely large active cellular biology literature in this subject and much work in biophysics. Nanoscale motors like kinesins tow organelles and other cargo on microtubules or filaments. They function in a highly viscous setting with overdamped dynamics; Reynolds' numbers about  $5 \times 10^{-2}$ . Taken as an ensemble, they are in configurations far from conventional notions of equilibrium even though they are in an isothermal environment. Because of the presence of significant diffusion, they are sometimes referred to as Brownian motors. Since a specific type tends to move in a single direction, for example, anterograde or retrograde to the cell periphery, these proteins are sometimes referred to as molecular ratchets. Many models have been proposed to describe the functions of these proteins, or aspects of their thermodynamical behavior, beginning with Ajdari and Prost [1], Astumian and Bier, *cf. e.g.* [2], and Doering, Ermentrout, and Oster [5], Peskin, Ermentrout, and Oster [21]. They consist either in discussions of distribution functions directly or of stochastic differential equations, which give rise to the distribution functions *via* the Chapman-Kolmogorov Equation. We have also suggested an approach for motor proteins like conventional kinesin where a dissipation principle is derived based on viewing an ensemble of motors as independent conformational changing nonlinear spring mass dashpots, [4], as suggested in Howard [9]. The dissipation principle,

---

*Keywords and phrases.* Fokker-Planck, weakly coupled system, molecular motor, Brownian ratchet, transport.

\* Partially supported by Swiss National Science contract NF 20-67618.02 and the National Science Foundation through a grant to the Center for Nonlinear Analysis.

\*\* Partially supported by the National Science Foundation Grants DMS 0072194 and DMS 0305794.

<sup>1</sup> Angewandte Mathematik, University of Zurich, 8057 Zurich, Switzerland. e-mail: chipot@amath.unizh.ch

<sup>2</sup> Department of Mathematics, University of Pittsburgh, Pittsburgh, PA 15260, USA. e-mail: sph+pitt.edu

<sup>3</sup> Center for Nonlinear Analysis and Department of Mathematical Sciences, Carnegie Mellon University, Pittsburgh, PA 15213, USA. e-mail: davidk@andrew.cmu.edu

which involves a Kantorovich-Wasserstein metric, identifies the environment of the system and gives rise to an implicit scheme from which evolution equations follow [3, 11, 13, 17, 18, 28]. All of these descriptions consist, in the end, of Fokker-Planck type equations coupled *via* conformational change factors, typically known as weakly coupled parabolic systems. Our own is also distinguished because it has natural boundary conditions. Transport is not *a priori* conferred by the formulation and, indeed, does not have any particular relationship to our thermodynamic view of the system. Identical thermodynamical considerations may be used to derive equations for non moving motors. Establishing the predictive authority of the equations, and the model, is a separate task and must depend on features of the equations particular to motors which move along microtubules or filaments. Our approach is to supply appropriate features and to analyze the stationary solution of the evolution equations. We also show that the time dependent solution of the evolution equation tends to the stationary solution as time becomes large.

For a brief and much oversimplified view of the motion of conventional kinesin, we note that the motor apparatus consists primarily of two heads, heavy chains, which walk in a hand over hand fashion along a microtubule. As a motor head moves it responds to a potential and, on binding to its new site, it may change conformation, and consequently its other head can move. Our dissipation principle then allows us to write a system of evolution equations for the partial probabilities  $\rho = (\rho_1, \rho_2)$  of active heads in terms of nonnegative potentials  $\psi_1$  and  $\psi_2$  and nonnegative conformational change coefficients  $\nu_1$  and  $\nu_2$ ,

$$\frac{\partial \rho_1}{\partial t} = \frac{\partial}{\partial x} \left( \sigma \frac{\partial \rho_1}{\partial x} + \psi'_1 \rho_1 \right) - \nu_1 \rho_1 + \nu_2 \rho_2 \quad \text{in } \Omega, t > 0 \tag{1.1}$$

$$\frac{\partial \rho_2}{\partial t} = \frac{\partial}{\partial x} \left( \sigma \frac{\partial \rho_2}{\partial x} + \psi'_2 \rho_2 \right) + \nu_1 \rho_1 - \nu_2 \rho_2$$

$$\sigma \frac{\partial \rho_1}{\partial x} + \psi'_1 \rho_1 = 0 \quad \text{on } \partial\Omega, t > 0 \tag{1.2}$$

$$\sigma \frac{\partial \rho_2}{\partial x} + \psi'_2 \rho_2 = 0$$

$$\rho_i(x, 0) = \rho_i^0 \geq 0, \quad \text{in } \Omega, \quad i = 1, 2 \tag{1.3}$$

$$\int_{\Omega} (\rho_1 + \rho_2) dx = 1$$

where  $\Omega = (0, 1)$ . For (1.1), (1.2), (1.3) there is the stationary system of ordinary differential equations

$$\frac{d}{dx} \left( \sigma \frac{d\rho_1^\sharp}{dx} + \psi'_1 \rho_1^\sharp \right) - \nu_1 \rho_1^\sharp + \nu_2 \rho_2^\sharp = 0 \quad \text{in } \Omega \tag{1.4}$$

$$\frac{d}{dx} \left( \sigma \frac{d\rho_2^\sharp}{dx} + \psi'_2 \rho_2^\sharp \right) + \nu_1 \rho_1^\sharp - \nu_2 \rho_2^\sharp = 0$$

$$\sigma \frac{d\rho_1^\sharp}{dx} + \psi'_1 \rho_1^\sharp = 0 \quad \text{on } \partial\Omega \tag{1.5}$$

$$\sigma \frac{d\rho_2^\sharp}{dx} + \psi'_2 \rho_2^\sharp = 0$$

$$\int_{\Omega} (\rho_1^\sharp + \rho_2^\sharp) dx = 1. \tag{1.6}$$

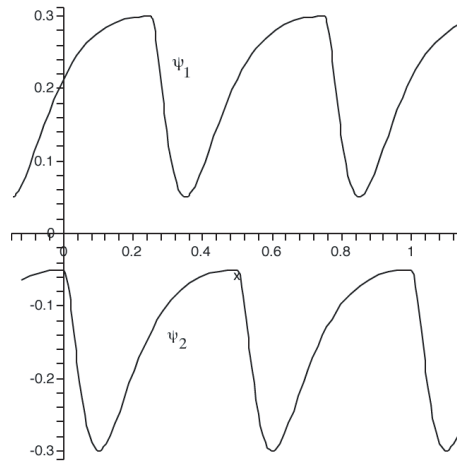


FIGURE 1. Caricature of the role of asymmetry of the potentials  $\psi_1$  and  $\psi_2$ .

Above we think of the potentials and conformational change coefficients as periodic in  $\Omega$ . Although there is no evident hint in the system itself as to why mass should be unevenly distributed, an important consideration has long been asymmetry of the potentials within their potential wells. Motor directionality is discussed in Chapter 9 of [24]. As a caricature, referring to Figure 1, suppose that type  $i$  heads are subject to the potential  $\psi_i, i = 1, 2$ , where one of the  $\psi_i$ 's is just a half period translate of the other. A molecule of type 1 distributed near  $x = 0.85$ , say, may change conformation and become type 2. Then, owing to the asymmetry of  $\psi_2$ , it is likely to move to the left to the next well bottom at  $x = 0.6$  with large probability  $p$ , say,  $p > 1/2$  and to the right to the well bottom at  $x = 1.2$  with probability  $1 - p$ . It may then change conformation again and become type 1. If it is at  $x = 0.6$ , it now moves to  $x = 0.35$  with probability  $p$  or back to  $x = 0.85$  with probability  $1 - p$ , and so forth. This corresponds to Bernoulli trials with a biased coin and, with some attention to the conditions at the first and last wells, the stationary distribution of its Markov chain decays exponentially away from the first well. Consequently, the asymmetry of the potentials in their well basins suggests exponential decay of the distribution. Unfortunately, this intuitive picture is not possible to convert into a proof. The conclusion, on the other hand, is true: the stationary distribution, referred to as  $\rho^\#$  above, decays exponentially and thus corresponds to Bernoulli trials with a biased coin, Theorem 4.1. This is our principal result.

The situation is, nonetheless, subtle, and involves delicate interplay between the potentials and the conformational change coefficients. At the beginning of Section 4 we give a synopsis of the analysis. The potentials represent all the interactions involved with the motion, including the substrate microtubule. The conformational change is a result of ATP-hydrolysis. For transport, the hydrolysis step should take place at the binding site of the protein, cf. Hackney [7]. To promote this we ask the  $\psi_i$  and the  $\nu_i$  to be synchronized so that

$$\nu_i > 0 \quad \text{where} \quad \psi_i = \min.$$

A statistical interpretation of this is that the  $\nu_i$  are active where we expect the distribution to be highly populated. We may choose  $\nu_i$  so that (1.4) decouple, for example, with

$$\frac{\nu_1}{\nu_2} = ae^{\frac{1}{\sigma}(\psi_1 - \psi_2)},$$

for which

$$\rho^\# \propto \left( ae^{-\frac{1}{\sigma}\psi_1}, e^{-\frac{1}{\sigma}\psi_2} \right).$$

Here the mass in each period interval is about the same and the system lacks transport. The decoupling situation has an interpretation in terms of detailed balance.

There are rich and diverse expressions of Brownian motors, or the orientation of fluctuations in nonequilibrium systems, available for study [8, 20, 23, 27]. The flashing ratchet [2] consists in alternation of diffusion and transport in an asymmetric potential [6, 12, 15, 16]. The Janossy effect in a dichroic dye/nematic liquid crystal system consists in destabilizing an equilibrium state in an asymmetric fashion [19]. The mathematical examples are only shadows of the complexity found in nature.

The methods we employ come from partial differential equations, ordinary differential equations, and functional analysis. In the presentation, we have striven for accessibility; our intention is not to write a sequence of puzzles for the reader. The expert in any given field will no doubt find some familiar arguments.

## 2. STATIONARY SOLUTION: SCHAUDER METHOD

In this section we discuss a proof of existence of a solution to (1.4), (1.5) based on the Schauder fixed point theorem.

**Theorem 2.1.** *Suppose that  $\psi_i \geq 0$  and  $\nu_i \geq 0$  are smooth,  $\sigma > 0$ , and  $\nu_i \neq 0$ ,  $i = 1, 2$ . There is a unique solution  $\rho^\sharp \in H^{1,1}(\Omega)$  of (1.4), (1.5) with*

$$\rho_i^\sharp > 0 \text{ in } \Omega$$

and

$$\int_{\Omega} (\rho_1^\sharp + \rho_2^\sharp) dx = 1.$$

We show this in several steps with the Schauder Fixed Point Theorem. In the sequel we shall generally suppress the symbol  $\sharp$ . First we recall some versions of a maximum principle [22].

**Proposition 2.2** (elementary maximum principle). *Let  $\alpha, \lambda$  be smooth in  $\bar{\Omega}$  with  $\alpha \geq \alpha_0 > 0$  and  $\lambda \geq 0$ . Suppose  $w \in C^2(\bar{\Omega})$  satisfies*

$$-\frac{d}{dx} \left( \alpha \frac{dw}{dx} \right) + \lambda w \geq 0 \text{ in } \Omega. \tag{2.7}$$

Then

- (i)  $w$  does not attain a negative minimum in the open interval  $\Omega$ ;
- (ii)  $w \geq 0$  and  $w \not\equiv 0 \implies w > 0$  in  $\Omega$ ;
- (iii)  $w \geq 0$ ,  $w \not\equiv 0$ , and  $\inf_{\Omega} w = 0 \implies \inf_{\Omega} w$  is attained at  $a = 0$  or  $1$  and  $w_x(a) \neq 0$ .

*Proof.* We give a proof for the convenience of the reader. If strict inequality holds, i.e.,

$$-\frac{d}{dx} \left( \alpha \frac{dw}{dx} \right) + \lambda w > 0 \text{ in } \Omega \tag{2.8}$$

then, obviously,  $w$  does not have a negative minimum in  $\Omega$ . If  $w \geq 0$  then  $w > 0$  in  $\Omega$ . Suppose then that (2.7) holds and that for some  $a \in \bar{\Omega}$ ,

$$w(a) = \min w = 0.$$

Assume that  $a \in \Omega$ . Suppose, without loss of generality that  $w(a + \delta) > 0$  and set

$$\zeta(x) = 1 - e^{\kappa(x-a)}$$

with  $\kappa$  chosen large enough that

$$-\frac{d}{dx}(\alpha \zeta_x) + \lambda \zeta > 0.$$

Let  $\varphi(x) = w(x) + \epsilon\zeta(x)$ . Then  $\varphi(a) = 0$ , so  $\min \varphi \leq 0$ , and for  $\epsilon$  sufficiently small

$$\begin{aligned} &-\frac{d}{dx}(\alpha\varphi_x) + \lambda\varphi > 0 \\ &\varphi(a - \delta) > 0 \quad \text{and} \quad \varphi(a + \delta) > 0 \\ &\text{and} \quad \min_{|x-a|<\delta} \varphi(x) \leq \varphi(a) \leq 0. \end{aligned}$$

This is a contradiction to (2.8). The boundary point condition is proven similarly. □

**Proposition 2.3** (elementary maximum principle redux). *Let  $\sigma > 0$  and  $\psi$  and  $\mu \geq 0$  be smooth in  $\bar{\Omega}$ . Suppose that  $u \in C^2(\bar{\Omega})$  satisfies*

$$-\frac{d}{dx} \left( \sigma \frac{du}{dx} + \psi' u \right) + \mu u \geq 0 \quad \text{in } \Omega. \tag{2.9}$$

Then

- (i)  $u$  does not attain a negative minimum in the open interval  $\Omega$ ;
- (ii)  $u \geq 0$  and  $u \not\equiv 0 \implies u > 0$  in  $\Omega$ ;
- (iii)  $u \geq 0$ ,  $u \not\equiv 0$ , and  $\inf_{\Omega} u = 0 \implies \inf_{\Omega} u$  is attained at  $a = 0$  or  $1$  and

$$\sigma \frac{du}{dx} + \psi' u|_{x=a} \neq 0. \tag{2.10}$$

*Proof.* Define  $w$  by  $w(x) = e^{\frac{1}{\sigma}\psi(x)}$  and apply Proposition 2.2.

The point here is that we shall be able to apply Proposition 2.3, for example, component wise to solutions of the stationary system when all components are non-negative.

**Step 1.** Existence. Look at the scalar equation

$$-\frac{d}{dx} \left( \sigma \frac{du}{dx} + \psi' u \right) + \mu u = \hat{\mu} f \quad \text{in } \Omega \tag{2.11}$$

$$\sigma \frac{du}{dx} + \psi' u = 0 \quad \text{on } \partial\Omega \tag{2.12}$$

where  $\mu, \hat{\mu} \geq 0$  and  $\mu$  not identically 0. Assume  $f \in L^1(\Omega)$ .

The mapping

$$\begin{aligned} T_0 : L^1(\Omega) &\rightarrow L^1(\Omega) \\ f &\rightarrow u \end{aligned}$$

is compact. The reader may employ his favorite technique at this point. For example, (2.11), (2.12) has a bounded Green's Function. So,

$$|u(x)| \leq \frac{C_0}{\sigma} \|\hat{\mu} f\|_{L^1(\Omega)} \tag{2.13}$$

then integrating (2.11) gives the estimate

$$|u_x(x)| \leq \frac{C}{\sigma} \|\hat{\mu} f\|_{L^1(\Omega)}$$

from which the compactness of  $T_0$  follows by the Ascoli-Arzelà' theorem. In particular note that when  $f \geq 0$  from (2.11),

$$\|u\|_{L^1(\Omega)} = \int_{\Omega} u \, dx \leq \frac{C_0}{\sigma} \int_{\Omega} \hat{\mu} f \, dx. \tag{2.14}$$

□

Returning now to (1.4), (1.5), given  $f_1, f_2 \in L^1(\Omega)$ , let

$$T : L^1(\Omega) \times L^1(\Omega) \rightarrow L^1(\Omega) \times L^1(\Omega)$$

$$\eta = Tf$$

denote the solution of

$$\begin{aligned} -\frac{d}{dx} \left( \sigma \frac{d\eta_1}{dx} + \psi'_1 \eta_1 \right) + \nu_1 \eta_1 &= \nu_2 f_2 \quad \text{in } \Omega \\ -\frac{d}{dx} \left( \sigma \frac{d\eta_2}{dx} + \psi'_2 \eta_2 \right) + \nu_2 \eta_2 &= \nu_1 f_1 \quad \text{in } \Omega \\ \sigma \frac{d\eta_1}{dx} + \psi'_1 \eta_1 &= 0 \quad \text{on } \partial\Omega \\ \sigma \frac{d\eta_2}{dx} + \psi'_2 \eta_2 &= 0 \quad \text{on } \partial\Omega \end{aligned}$$

$T$  is compact. Let  $K \subset L^1(\Omega) \times L^1(\Omega)$  denote the  $f = (f_1, f_2)$  which satisfy

$$f_i \geq 0, \quad i = 1, 2 \tag{2.15}$$

$$\int_{\Omega} (\nu_1 f_1 + \nu_2 f_2) \, dx = 1 \tag{2.16}$$

$$\int_{\Omega} (\nu_1 f_1 - \nu_2 f_2) \, dx = 0 \tag{2.17}$$

$$0 \leq \int_{\Omega} f_i \, dx \leq \frac{C_0}{\sigma}, \quad i = 1, 2. \tag{2.18}$$

$K$  is a bounded convex subset in  $L^1(\Omega) \times L^1(\Omega)$ . For  $\eta = Tf$ , with  $f \in K$ , we have  $\eta_i \geq 0$  from the maximum principle already cited. Adding and subtracting the equations for  $\eta_i$ , we check that (2.16), (2.17) are satisfied. Now (2.16) implies in particular that

$$0 \leq \int_{\Omega} \nu_i f_i \, dx \leq 1.$$

Hence from (2.14),

$$0 \leq \int_{\Omega} \eta_i \, dx \leq \frac{C_0}{\sigma}, \quad i = 1, 2.$$

Thus  $\eta \in K$ . Hence  $T(K) \subset K$ . Now we apply the Schauder Fixed Point Theorem to  $T$  and  $K$  to conclude that  $T$  has a fixed point

$$f = Tf.$$

Let  $\rho$  denote the normalized fixed point with total mass 1.

**Step 2.** Uniqueness. From the existence, we know that  $\rho_i \geq 0$  in  $\Omega$ . Rewrite the system, considering it to be independent equations for the components as

$$\begin{aligned} -\frac{d}{dx} \left( \sigma \frac{d\rho_1}{dx} + \psi'_1 \rho_1 \right) + \nu_1 \rho_1 &= \nu_2 \rho_2 \geq 0 \quad \text{in } \Omega \\ \sigma \frac{d\rho_1}{dx} + \psi'_1 \rho_1 &= 0 \quad \text{on } \partial\Omega \end{aligned}$$

and

$$-\frac{d}{dx} \left( \sigma \frac{d\rho_2}{dx} + \psi'_2 \rho_2 \right) + \nu_2 \rho_2 = \nu_1 \rho_1 \geq 0 \text{ in } \Omega$$

$$\sigma \frac{d\rho_2}{dx} + \psi'_2 \rho_2 = 0 \text{ on } \partial\Omega.$$

By the elementary maximum principle redux, Proposition 2.3, quoted prior to the proof, we know that  $\rho_i > 0$  in  $\overline{\Omega}$ .

Suppose we have two solutions,  $\rho$  and  $\hat{\rho}$  with non-negative components. Hence for  $\epsilon > 0$  small enough,

$$\rho_i - \epsilon \hat{\rho}_i > 0 \text{ in } \Omega.$$

Choose  $\epsilon$  as large as possible:

$$\rho_i - \epsilon \hat{\rho}_i > 0 \text{ in } \Omega, \quad i = 1, 2$$

$$\rho_j(x_0) - \epsilon \hat{\rho}_j(x_0) = 0, \quad \text{for some } j = 1, 2, \text{ and } x_0 \in \overline{\Omega}.$$

So  $\rho - \epsilon \hat{\rho}$  is a solution with non-negative components and with minimum zero. Just as above, each component satisfies a differential inequality with a homogeneous boundary condition. Again according to Proposition 2.3,  $\rho_i = \epsilon \hat{\rho}_i$  and, by the mass requirement,  $\epsilon = 1$ . This verifies the uniqueness.

We shall use variations of this argument many times.

### 3. STATIONARY SOLUTION: SHOOTING METHOD

In this section, we give an alternate proof of existence and uniqueness while setting up the apparatus for discussion of the behavior of the solution. Let  $\rho = (\rho_1, \rho_2)$  be the solution of (1.4), (1.5) and set

$$\phi_i = \sigma \frac{d\rho_i}{dx} + \psi'_i \rho_i, \quad i = 1, 2$$

so (1.4), (1.5) may be written as the first order system

$$\sigma \frac{d\rho_1}{dx} = \phi_1 - \psi'_1 \rho_1$$

$$\sigma \frac{d\rho_2}{dx} = \phi_2 - \psi'_2 \rho_2$$

$$\frac{d\phi_1}{dx} = \nu_1 \rho_1 - \nu_2 \rho_2$$

$$\frac{d\phi_2}{dx} = -\nu_1 \rho_1 + \nu_2 \rho_2$$

with

$$\phi_1(0) = \phi_2(0) = \phi_1(1) = \phi_2(1) = 0.$$

Observe from the last two equations of the system that  $\phi_1 + \phi_2 = \text{const}$  and this  $\text{const} = 0$  by the boundary conditions, so we may write the first order system in terms of three functions, with  $\phi = \phi_1$  as

$$\sigma \frac{d\rho_1}{dx} = \phi - \psi'_1 \rho_1 \tag{3.19}$$

$$\sigma \frac{d\rho_2}{dx} = -\phi - \psi'_2 \rho_2 \quad \text{in } \Omega \tag{3.20}$$

$$\frac{d\phi}{dx} = \nu_1 \rho_1 - \nu_2 \rho_2 \tag{3.21}$$

$$\phi(0) = \phi(1) = 0. \tag{3.22}$$

Introduce

$$p = \begin{pmatrix} \rho_1 \\ \rho_2 \\ \phi \end{pmatrix} \quad \text{and} \quad A = \frac{1}{\sigma} \begin{pmatrix} -\psi'_1 & 0 & 1 \\ 0 & -\psi'_2 & -1 \\ \sigma\nu_1 & -\sigma\nu_2 & 0 \end{pmatrix}$$

so the system of ODE's assumes the form

$$\frac{d}{dx} p = Ap, \quad \phi(0) = \phi(1) = 0. \tag{3.23}$$

We shall now prove Theorem 1 again. Let  $p^{(1)}$  and  $p^{(2)}$  be the solutions of (3.23) with

$$p^{(1)}(0) = (1, 0, 0) \quad \text{and} \quad p^{(2)}(0) = (0, 1, 0).$$

**Lemma 3.1.** *For  $p^{(1)}$  we have that  $\rho_1 \geq 0, \rho_2 \leq 0$  and  $\phi \geq 0$  and for  $p^{(2)}$  we have that  $\rho_1 \leq 0, \rho_2 \geq 0$  and  $\phi \leq 0$ .*

*Proof.* Suppose first that  $\nu_1 > 0$  and  $\nu_2 > 0$  in  $\overline{\Omega}$  and consider  $p^{(1)}$ . Here

$$\begin{aligned} \rho_2(0) &= 0 \\ \rho'_2(0) &= 0 \\ \rho''_2(0) &= -\phi'(0) = -\nu_1(0) < 0. \end{aligned}$$

So there is an initial interval  $(0, \epsilon)$  in which

$$\rho_1 > 0, \quad \rho_2 < 0, \quad \phi > 0, \quad x \in [0, \epsilon).$$

Suppose there is a first  $x = \xi$  where one or more of these inequalities is violated. Since  $\phi' > 0$  whenever  $\rho_1 > 0$  and  $\rho_2 < 0$ , we must have  $\rho_1(\xi) = 0$  or  $\rho_2(\xi) = 0$ . If  $\rho_1(\xi) = 0$ , then  $\sigma\rho'_1(\xi) = \phi(\xi) > 0$ . Thus  $p^{(1)} \equiv 0$ , which is not the case. A similar contradiction results if  $\rho_2(\xi) = 0$ . This proves the lemma in the case where the  $\nu_i > 0$ .

Now suppose that there are  $\psi_i$  and  $\nu_i$  such that the lemma is false. This means that there is an  $x^* \in \Omega$  where either  $\rho_1 < 0, \rho_2 > 0$  or  $\phi < 0$ . Consider the problem with functions  $\nu_i + \delta$  in place of the  $\nu_i$ , for small  $\delta > 0$ . The solution  $p^{(1)}$  is a continuous function of  $\delta$ , so for small enough  $\delta$  one of the inequalities is violated at  $x^*$ . This contradicts what was already shown when  $\nu_i > 0$ .

Similar remarks hold for  $p^{(2)}$ . This proves the lemma. □

**Lemma 3.2.** *For  $p^{(1)}$  we have that  $\rho_1 > 0$  on  $\Omega$  and for  $p^{(2)}$  we have that  $\rho_2 > 0$  on  $\Omega$ .*

*Proof.* For  $p^{(1)}$ , if  $\rho_1(\xi) = 0$  for some  $\xi \in (0, 1]$ , then  $\rho'_1(\xi) = 0$  since we know already that  $\rho_1 \geq 0$  on  $\overline{\Omega}$ . But  $\phi' \geq 0$  and hence, since  $\phi(0) = 0, \phi \equiv 0$  on  $[0, \xi]$ , a contradiction, since this would imply  $\rho_1 > 0$  on  $[0, \xi]$ . Similar remarks apply to  $p^{(2)}$ . □



*Proof of theorem.* Since each of the  $\nu_i$  is positive somewhere in  $\Omega$ , for  $p^{(1)}$ ,  $\phi(1) > 0$  and for  $p^{(2)}$ ,  $\phi(1) < 0$ . Therefore there is a unique  $c > 0$  such that

$$p = cp^{(1)} + p^{(2)}$$

satisfies

$$\begin{aligned} \phi(0) &= \phi(1) = 0 \\ \rho_2(0) &= 1 \quad \text{and} \\ \rho_1(0) &= c > 0. \end{aligned}$$

We claim that for this  $p$ ,  $\rho_1 > 0$  and  $\rho_2 > 0$ . We argue by inspection of (3.23), although we could simply invoke the existence portion of the previous theorem at this point. Let  $\xi$  be the first point such that  $\rho_1(\xi) = 0$ . Then

$$\frac{d\rho_1}{dx}(\xi) \leq 0.$$

If  $\rho_2(\xi) = 0$  as well, then

$$\frac{d\rho_2}{dx}(\xi) \leq 0$$

and hence  $\pm\phi(\xi) \leq 0$ , so  $\phi(\xi) = 0$ . Thus we have that  $\rho_1 = \rho_2 = \phi = 0$  at  $\xi$ , so  $\rho_1 \equiv \rho_2 \equiv \phi \equiv 0$ , a contradiction (to the ODE existence and uniqueness theorem). Hence  $\rho_2(\xi) > 0$ .

We now apply the boundary point version of Proposition 2.3 to  $\rho_1$ , which is a positive solution of (2.9) on the interval  $[0, \xi]$ . Thus  $\phi(\xi) = \sigma\rho_1' + \psi_1'\rho_1 < 0$ , from the equation, while  $d\phi(\xi)/dx \leq 0$ , also from the equation. So  $\rho_1 < 0$ ,  $\rho_2 > 0$  and  $\phi < 0$  in an interval  $(\xi, \xi + \delta)$  while also  $d\phi/dx \leq 0$ . As long as  $\rho_1 < 0$ ,  $\rho_2 > 0$ , we have that  $\phi < 0$  and  $d\phi/dx \leq 0$ . Suppose that  $\rho_1(\xi') = 0$ ,  $\xi < \xi'$ . We still have that  $\phi(\xi') < 0$ , since otherwise the decreasing function  $\phi$  is identically zero on the interval (and thus  $\rho_1$  cannot vanish from the equation). But

$$0 \leq \frac{d\rho_1}{dx}(\xi') = \phi(\xi')$$

which is a contradiction. The same conclusion holds if  $\rho_2(\xi') = 0$ . Therefore, these inequalities are maintained until  $x = 1$ , whence  $\phi(1) < 0$ , which is a contradiction. If  $\rho_1(1) = 0$ , then by the boundary point lemma, we have again that  $\phi(1) < 0$ , but  $\phi(1) = 0$ . So  $\rho_1 > 0$  in  $\bar{\Omega}$ . Similarly,  $\rho_2 > 0$  in  $\bar{\Omega}$ . □

#### 4. TRANSPORT: ASYMPTOTIC BEHAVIOR OF THE SOLUTION FOR SMALL $\sigma$

In this section we show that our system exhibits transport, more precisely, that the mass of the stationary solution found in Theorem 2.1 decays exponentially away from one endpoint of the interval  $\Omega$ . The demonstration has two parts. First we show that  $\rho_1 + \rho_2$  decreases exponentially between successive maxima of the potentials. This involves a detailed study of the fundamental solution matrix of the first order system (3.23). To give a brief oversimplified idea, the solution of (3.23) may, locally, decrease exponentially, remain bounded, or increase exponentially as  $x \rightarrow 1$  depending on the eigenvalues of the system. These depend on the  $\psi_i'$  and the support of the  $\nu_i$ . To impede exponential increase, the potentials cannot be simultaneously decreasing and to have exponential decrease, there must be intervals where both potentials are increasing. This gives rise to the conditions below. Indeed, if we think of  $\psi_1$  as the translate by half a period of  $\psi_2$ , the role of asymmetry is now obvious, since the interval in which a  $\psi_i$  is increasing must be longer than the one in which it is decreasing. The second part of the proof is to apply a scaling argument to obtain the conclusion at all points between the maxima. The main estimate here is based on our usual maximum principle applied in a different context to a specially chosen solution of (1.4), (1.5).

Let us impose these general conditions on the data:

- (1)  $\psi_i$  and  $\nu_i, i = 1, 2$ , are in  $C^2(\overline{\Omega})$  of period  $1/N$ ;
- (2)  $\psi_i \geq 0$  and  $\nu_i \geq 0, i = 1, 2$ .

**Theorem 4.1.** *Assume that*

- (1) *in each period  $\psi_i$  has exactly one maximum and one minimum with  $\psi_i'' < 0$  at the maximum and  $\psi_i' \neq 0$  between the maxima and minima of  $\psi_i, i = 1, 2$ ;*
- (2)  *$\psi_1' > 0$  on each interval where  $\psi_2' \leq 0$  and  $\psi_2' > 0$  on each interval where  $\psi_1' \leq 0$ ;*
- (3) *there are  $c_0 > 0$  and  $\delta > 0$  and a positive integer  $m$  such that for a minimum  $a_i$  of  $\psi_i, \nu_i(x) \geq c_0(x - a_i)^m$  on  $(a_i, a_i + \delta)$ .*

Let  $\xi_0$  denote the first maximum of  $\psi_2$  and let  $x_j = \xi_0 + \frac{j}{N}, 1 \leq j \leq N - 1$  and  $x_N = 1$ . Then there are  $c > 0$ , independent of  $\sigma$  sufficiently small, and  $K > 0$ , which may depend on  $\sigma$ , but not  $j$  or  $N$ , such that the solution of (1.4), (1.5) satisfies

$$\max_{x_j \leq x \leq x_{j+1}} (\rho_1(x) + \rho_2(x)) \leq Ke^{-\frac{jc}{\sigma}}, \quad 1 \leq j \leq N. \tag{4.24}$$

With some trivial manipulation, (4.24) may be expressed as: there are constants  $K_0, c$  such that

$$\rho_1(x) + \rho_2(x) \leq K_0 e^{-\frac{cN}{\sigma}(x - \xi_0)}, \quad x \geq \xi_0. \tag{4.25}$$

Note that 3 above implies the asymmetric location of the minima of the  $\psi_i$  in their potential wells.

We now discuss exponential decay between potential maxima, the first part described at the beginning of the section. For convenience, we assume that the coefficients  $\psi_i$  and  $\nu_i$  have period 1 and the problem is defined on the interval  $(0, N)$ , where  $N > 1$ . To review,

$$\begin{aligned} \sigma \frac{d\rho_1}{dx} &= \phi - \psi_1' \rho_1 \\ \sigma \frac{d\rho_2}{dx} &= -\phi - \psi_2' \rho_2 \quad \text{in } [0, N] \\ \frac{d\phi}{dx} &= \nu_1 \rho_1 - \nu_2 \rho_2 \\ \phi(0) &= \phi(N) = 0. \end{aligned} \tag{4.26}$$

**Theorem 4.2.** *With the assumptions of Theorem 4.1, scaled to  $[0, N]$ , let  $y_0$  denote the first maximum of  $\psi_2$  and let  $y_j = y_0 + j, 1 \leq j \leq N - 1$ . Then there are  $c > 0$  and  $K > 0$ , independent of  $\sigma$  sufficiently small, such that the solution of (4.26) satisfies*

$$\rho_1(y_j) + \rho_2(y_j) \leq Ke^{-\frac{c}{\sigma}(\rho_1(y_{j-1}) + \rho_2(y_{j-1}))}, \quad j = 1 \dots N - 1. \tag{4.27}$$

*Proof.* To start, consider  $R(\xi, x)$  a fundamental solution of (4.26),  $\xi \leq x$ , with  $R(\xi, \xi) = \mathbf{1}$ , the  $3 \times 3$  identity matrix. So

$$p(x) = R(\xi, x)p(\xi).$$

Write

$$R = \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} \\ \rho_{21} & \rho_{22} & \rho_{23} \\ \phi_1 & \phi_2 & \phi_3 \end{pmatrix}.$$

The same comparison technique used in the proof of the Lemma 3.1 shows that

$$\begin{aligned} \rho_{11} &> 0 & \rho_{12} &\leq 0 & \rho_{13} &> 0 \\ \rho_{21} &\leq 0 & \rho_{22} &> 0 & \rho_{23} &< 0 & \text{for } x \in (\xi_1, \xi_2] \\ \phi_1 &\geq 0 & \phi_2 &\leq 0 & \phi_3 &\geq 1. \end{aligned}$$

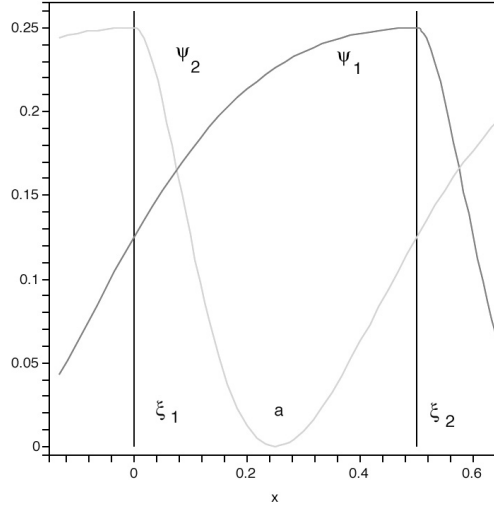


FIGURE 2. Setup for the proof of Theorem 4.2.

This gives us the convenient sign map

$$\text{sign}(R) = \begin{pmatrix} + & - & + \\ - & + & - \\ + & - & + \end{pmatrix}.$$

Let  $[\xi_1, \xi_1 + 1]$  be a period interval of  $\psi_2$  with  $\psi_2(\xi_1) = \psi_2(\xi_1 + 1) = \max \psi_2$  and let  $a$ ,  $\xi_1 < a < \xi_1 + 1$  be the minimum of  $\psi_2$  in  $[\xi_1, \xi_1 + 1]$ . Say  $\psi_2(a) = 0$ . According to the hypothesis, there is a  $\xi_2$  with  $\psi_1(\xi_2) = \max \psi_1$ , and

$$\xi_1 < a < \xi_2 < \xi_1 + 1.$$

We have, for example,

$$p(a) = R(\xi_1, a)p(\xi_1) \quad \text{and} \quad p(\xi_2) = R(\xi_1, \xi_2)p(\xi_1).$$

Since  $\rho_i > 0$ , the additional function  $\phi$  can be eliminated from the equation (4.26) in favor of an inequality. Indeed,

$$0 < \rho_1(x) = \rho_{11}\rho_1(\xi) + \rho_{12}\rho_2(\xi) + \rho_{13}\phi(\xi), \quad x > \xi \tag{4.28}$$

$$0 < \rho_2(x) = \rho_{21}\rho_1(\xi) + \rho_{22}\rho_2(\xi) + \rho_{23}\phi(\xi), \quad x > \xi \tag{4.29}$$

where the  $\rho_{ij}$  are evaluated at  $x$ . Hence, checking the sign map,

$$\phi(\xi) > -\frac{\rho_{11}}{\rho_{13}}\rho_1(\xi) - \frac{\rho_{12}}{\rho_{13}}\rho_2(\xi) \quad \text{and} \tag{4.30}$$

$$\phi(\xi) < -\frac{\rho_{21}}{\rho_{23}}\rho_1(\xi) - \frac{\rho_{22}}{\rho_{23}}\rho_2(\xi). \tag{4.31}$$

Combining this with (4.28), (4.29) and reconfiguring gives that

$$\begin{aligned} \rho_1(x) &< \frac{\rho_{13}\rho_{21} - \rho_{11}\rho_{23}}{-\rho_{23}}\rho_1(\xi) + \frac{\rho_{22}\rho_{13} - \rho_{12}\rho_{23}}{-\rho_{23}}\rho_2(\xi) \\ \rho_2(x) &< \frac{\rho_{13}\rho_{21} - \rho_{11}\rho_{23}}{\rho_{13}}\rho_1(\xi) + \frac{\rho_{22}\rho_{13} - \rho_{12}\rho_{23}}{\rho_{13}}\rho_2(\xi). \end{aligned}$$

A first thought here is that when a typical  $\rho_{ij}$  varies with  $\exp(c/\sigma)$ , the fraction varies like  $\exp(c/\sigma)^2 / \exp(c/\sigma) = \exp(c/\sigma)$ , that is, exponential in  $1/\sigma$ . Interesting here is that the numerators in the fractions are the terms  $(adj R)_{23}$  and  $(adj R)_{13}$  and the adjugate itself satisfies an equation (a variation of Abel's formula), cf. [14, 25],

$$\frac{d}{dx} adj R = adj R M, \quad M = (\text{trace } A)\mathbf{1} - A \tag{4.32}$$

where we are taking the adjugate to be

$$adj(R) = \det(R)R^{-1} :$$

which means that the numerator and the denominator are typically of the same order. This is the starting point of the proof.

Our objective is to show that

$$\lim_{\sigma \rightarrow 0^+} \frac{\rho_{13}\rho_{21} - \rho_{11}\rho_{23}}{-\rho_{23}} = 0, \quad \lim_{\sigma \rightarrow 0^+} \frac{\rho_{22}\rho_{13} - \rho_{12}\rho_{23}}{-\rho_{23}} = 0,$$

and

$$\lim_{\sigma \rightarrow 0^+} \frac{\rho_{13}\rho_{21} - \rho_{11}\rho_{23}}{\rho_{13}} = 0, \quad \lim_{\sigma \rightarrow 0^+} \frac{\rho_{22}\rho_{13} - \rho_{12}\rho_{23}}{\rho_{13}} = 0$$

with an exponential rate of decay in each case. Consider first

$$\frac{\rho_{13}\rho_{21} - \rho_{11}\rho_{23}}{-\rho_{23}}. \tag{4.33}$$

Let

$$W = adj(R) = (w_{ij}) = \begin{pmatrix} \rho_{22}\phi_3 - \rho_{23}\phi_2 & \rho_{13}\phi_2 - \rho_{12}\phi_3 & \rho_{12}\rho_{23} - \rho_{13}\rho_{22} \\ \rho_{23}\phi_1 - \rho_{21}\phi_3 & \rho_{11}\phi_3 - \rho_{13}\phi_1 & \rho_{13}\rho_{21} - \rho_{11}\rho_{23} \\ \rho_{21}\phi_2 - \rho_{22}\phi_1 & \rho_{12}\phi_1 - \rho_{11}\phi_2 & \rho_{11}\rho_{12} - \rho_{21}\rho_{22} \end{pmatrix}.$$

For this way of writing, the rows of  $W$  satisfy the system (4.32) determined by  $M$ .

Note that

$$M = \begin{pmatrix} -\frac{1}{\sigma}\psi'_2 & 0 & -\frac{1}{\sigma} \\ 0 & -\frac{1}{\sigma}\psi'_1 & \frac{1}{\sigma} \\ -\nu_1 & \nu_2 & -\frac{1}{\sigma}(\psi'_1 + \psi'_2) \end{pmatrix}.$$

Now the term in (4.33) that we are considering is  $w_{23}$  in the second row of  $W$ . Dropping the subscript 2, let

$$w = (w_1, w_2, w_3)$$

denote this second row. Then our usual comparison methods, and what we already know from the sign matrix, tell us that

$$w_1 \leq 0, \quad w_2 \geq 0, \quad w_3 > 0 \quad \text{and} \quad w(\xi_1) = (0, 1, 0).$$

**Lemma 4.3.** *There are  $K > 0$  and  $c > 0$  independent of  $\sigma$  so that*

$$|w(a)| \leq K e^{\frac{1}{\sigma}\psi_2(\xi_1)} \tag{4.34}$$

and

$$|w(\xi_2)| \leq K e^{\frac{1}{\sigma}(\psi_2(\xi_1) - c)} \tag{4.35}$$

as  $\sigma \rightarrow 0$ .

*Proof.* Let

$$v(x) = e^{\frac{1}{\sigma}\psi_2(x)}w(x), \quad x \geq \xi_1$$

so that

$$\frac{dv}{dx} = v(M + \frac{1}{\sigma}\psi_2' \mathbf{1}), \quad M + \frac{1}{\sigma}\psi_2' \mathbf{1} = \begin{pmatrix} 0 & 0 & -\frac{1}{\sigma} \\ 0 & \frac{1}{\sigma}(\psi_2' - \psi_1') & \frac{1}{\sigma} \\ -\nu_1 & \nu_2 & -\frac{1}{\sigma}\psi_1' \end{pmatrix}.$$

We prove the first part of the lemma by estimating  $v$ . Note that  $\psi_1' \geq \alpha$  and  $\psi_2' \leq 0$  on  $[\xi_1, a]$ . This means that we can compare  $v$  with  $q$ , where

$$\frac{dq}{dx} = qP, \quad \text{with } P = \begin{pmatrix} 0 & 0 & \frac{1}{\sigma} \\ 0 & -\frac{\alpha}{\sigma} & \frac{1}{\sigma} \\ \bar{\nu} & \bar{\nu} & -\frac{\alpha}{\sigma} \end{pmatrix} \tag{4.36}$$

$$q(\xi_1) = (0, e^{\frac{1}{\sigma}\psi_2(\xi_1)}, 0) \tag{4.37}$$

where  $\bar{\nu} = \max_i\{\nu_i(x)\}$ . Namely, simple comparison methods show that  $0 \leq -v_1 \leq q_1, 0 \leq v_2 \leq q_2$  and  $0 \leq v_3 \leq q_3$ . To see this, note that  $q(\xi_1) = v(\xi_1)$  and let  $q_\delta$  be the solution of

$$\frac{dq_\delta}{dx} = q_\delta P + \delta(1, 1, 1), \quad q_\delta(\xi_1) = q(\xi_1).$$

Now  $q'_i \delta(x) > v'_i(x)$  for  $x \in [\xi_1, a]$  and also  $q_i \delta(x) > v_i(x)$  for  $x \in [\xi_1, \xi_1 + \epsilon]$ . If there is an initial point  $x_1$  where  $q_i \delta(x_1) = v_i(x_1)$ , then  $q'_i \delta(x_1) \leq v'_i(x_1)$ , a contradiction. Now let  $\delta \rightarrow 0$ .

The eigenvalues of  $P$  are of the form

$$-\frac{\alpha}{\sigma} + O(1), -\frac{\alpha}{\sigma} + O(1), O(1) \quad \text{as } \sigma \rightarrow 0.$$

This implies that  $|q(a)| \leq K|q(\xi_1)| = Ke^{\frac{1}{\sigma}\psi_2(\xi_1)}$  for some  $K > 0$  independent of  $\sigma$ .

We now wish to extend the estimate to  $x = \xi_2$ , which is the maximum point of  $\psi_1$ . Note that

$$\psi_1' \geq 0, \quad \psi_2' \geq 0, \quad \text{and } \psi_1' + \psi_2' \geq \alpha > 0, \quad \text{in } [a, \xi_2] \text{ independent of } \sigma$$

for some  $\alpha$ . We must separate the interval  $[a, \xi_2]$  into three subintervals  $[a, a + \delta], [a + \delta, \xi_2 - \delta]$  and  $[\xi_2 - \delta, \xi_2]$ . On the first and last intervals  $w$  is bounded while in the middle  $|w|$  decreases with  $|w(\xi_2 - \delta)/w(a + \delta)|$  exponentially small.

Suppose that  $\psi_1' \geq \beta$  on  $[a, a + \delta]$ . We compare  $w$  with  $q$  where

$$\frac{dq}{dx} = qP, \quad \text{with } P = \begin{pmatrix} 0 & 0 & \frac{1}{\sigma} \\ 0 & -\frac{\beta}{\sigma} & \frac{1}{\sigma} \\ \bar{\nu}_1 & \bar{\nu}_2 & -\frac{\alpha}{\sigma} \end{pmatrix} \tag{4.38}$$

$$q(a) = (-w_1(a), w_2(a), w_3(a)) \tag{4.39}$$

where  $\bar{\nu}_i = \max_x \nu_i(x)$ . Then  $-w_1 \leq q_1, w_2 \leq q_2$  and  $w_3 \leq q_3$  on  $[a, a + \delta]$ . The eigenvalues of  $P$  are of the form

$$-\frac{\alpha}{\sigma} + O(1), -\frac{\beta}{\sigma} + O(1), O(1) \text{ as } \sigma \rightarrow 0,$$

from which it follows that  $|v| \leq K|w(a)|$  for some  $K$  independent of  $\sigma$  on  $[a, a + \delta]$ .

So far we have used that  $\psi_1$  is increasing to maintain the boundedness of  $w$ . Now we use that both are increasing on  $[a + \delta, \xi_2 - \delta]$  to show that  $w$  is exponentially decreasing. Say

$$\psi'_1 \geq \kappa \text{ and } \psi'_2 \geq \kappa, \text{ in } [a + \delta, \xi_2 - \delta] \text{ independent of } \sigma.$$

The relevant comparison system here is

$$\frac{dq}{dx} = qP, \text{ with } P = \begin{pmatrix} -\frac{\kappa}{\sigma} & 0 & \frac{1}{\sigma} \\ 0 & -\frac{\kappa}{\sigma} & \frac{1}{\sigma} \\ \bar{\nu}_1 & \bar{\nu}_2 & -\frac{2\kappa}{\sigma} \end{pmatrix} \tag{4.40}$$

$$q(a + \delta) = (-w_1(a + \delta), w_2(a + \delta), w_3(a + \delta)). \tag{4.41}$$

For this  $P$ , the eigenvalues are of the form

$$-\frac{\kappa}{\sigma} + O(1), -\frac{\kappa}{\sigma} + O(1), -\frac{2\kappa}{\sigma} + O(1) \text{ as } \sigma \rightarrow 0.$$

From this it follows that

$$|w(\xi_2 - \delta)| \leq Ke^{-\frac{c}{\sigma}}|w(a + \delta)|.$$

Finally, we may check that  $|w(\xi_2)|/|w(\xi_2 - \delta)|$  remains bounded using the same technique as for the interval  $[a, a + \delta]$ .

Putting together all these estimates shows that

$$|w(\xi_2)| \leq Ke^{\frac{1}{\sigma}(\psi_2(\xi_1) - c)} \text{ as } \sigma \rightarrow 0. \tag{4.42}$$

This proves the lemma. □

Maintaining our interest in the minimum point  $a$  and the maximum point  $\xi_1$ , we look for an upper bound on  $\rho_{23}$ .

**Lemma 4.4.** *There is are  $\epsilon > 0, K > 0$ , and  $k$ , all independent of  $\sigma$ , such that*

$$\rho_{23}(a) \leq -Ke^{\frac{1}{\sigma}\psi_2(\xi_1)} \tag{4.43}$$

and

$$\rho_{23}(\xi_2) \leq -K\sigma^k e^{\frac{1}{\sigma}\psi_2(\xi_1)}. \tag{4.44}$$

*Proof.* From the equation, we have that

$$\frac{d}{dx}\rho_{23} = -\frac{\phi_3}{\sigma} - \frac{\psi'_2}{\sigma}\rho_{23} \leq -\frac{1}{\sigma} - \frac{\psi'_2}{\sigma}\rho_{23}, \quad x \geq \xi_1$$

since  $\phi_3(\xi_1) = 1$  and  $\phi'_3 = \nu_1\rho_{13} - \nu_2\rho_{23} \geq 0$ . Therefore,

$$\frac{d}{dx} \left( \rho_{23}(x)e^{\frac{1}{\sigma}\psi_2(x)} \right) \leq -\frac{1}{\sigma}e^{\frac{1}{\sigma}\psi_2(x)}, \text{ with } \rho_{23}(\xi_1) = 0.$$

So we find that

$$\rho_{23}(a) \leq -\frac{1}{\sigma} e^{-\frac{1}{\sigma}\psi_2(a)} \int_{\xi_1}^a e^{\frac{1}{\sigma}\psi_2(x)} dx.$$

Now we have assumed that  $\psi_2(a) = 0$  and  $\psi_2'$  is bounded. There are  $\gamma_1 > 0, \delta > 0$  such that

$$\psi_2(x) \geq \psi_2(\xi_1) - \gamma_1(x - \xi_1) \quad \text{in } \xi_1 \leq x \leq \xi_1 + \delta.$$

Consequently

$$\rho_{23}(a) \leq -\frac{1}{\sigma} e^{\frac{1}{\sigma}\psi_2(\xi_1)} \int_{\xi_1}^{\xi_1+\delta} e^{-\frac{\gamma_1}{\sigma}(x-\xi_1)} dx.$$

Hence we obtain that for  $\sigma$  sufficiently small,

$$\rho_{23}(a) \leq -K e^{\frac{1}{\sigma}\psi_2(\xi_1)} \tag{4.45}$$

which is the statement of the first part of the lemma.

We now proceed to the lower bound for  $\rho_{23}(\xi_2)$ . Integrating the equation satisfied by  $\rho_{23}$  over  $[a, \xi_2]$ , we obtain, using (4.45),

$$\rho_{23}(x) = \rho_{23}(a) e^{\frac{1}{\sigma}(\psi_2(a) - \psi_2(x))} - \frac{1}{\sigma} \int_a^x \phi_3(s) e^{\frac{1}{\sigma}(\psi_2(s) - \psi_2(x))} ds. \tag{4.46}$$

We estimate  $\phi_3$  by noting that  $\phi_3' \geq -\nu_2 \rho_{23} \geq 0$ ; whence,

$$\phi_3(x) - \phi_3(a) \geq - \int_a^x \nu_2(t) \rho_{23}(t) dt \tag{4.47}$$

$$\geq - \int_a^x \nu_2(t) \rho_{23}(a) e^{\frac{1}{\sigma}(\psi_2(a) - \psi_2(x))} dt \tag{4.48}$$

by (4.46). Now  $\phi_3 \geq 0$ , so

$$-\phi_3(x) \leq \int_a^x \nu_2(t) \rho_{23}(a) e^{\frac{1}{\sigma}(\psi_2(a) - \psi_2(x))} dt. \tag{4.49}$$

This resubstituted into (4.46) gives that (note:  $\psi_2(a) = 0$ )

$$\rho_{23}(x) \leq e^{-\frac{1}{\sigma}\psi_2(x)} \frac{1}{\sigma} \int_a^x e^{\frac{1}{\sigma}\psi_2(s)} \int_a^s \nu_2(t) \rho_{23}(a) e^{\frac{1}{\sigma}(\psi_2(a) - \psi_2(t))} dt ds \tag{4.50}$$

$$= -K e^{\frac{1}{\sigma}(\psi_2(\xi_1) - \psi_2(x))} \int_a^x \frac{1}{\sigma} e^{\frac{1}{\sigma}\psi_2(s)} \int_a^s \nu_2(t) e^{-\frac{1}{\sigma}\psi_2(t)} dt ds \tag{4.51}$$

using (4.45). Therefore

$$\rho_{23}(\xi_2) \leq -K e^{\frac{1}{\sigma}(\psi_2(\xi_1) - \psi_2(\xi_2))} \int_{\xi_2 - \delta}^{\xi_2} \frac{1}{\sigma} e^{\frac{1}{\sigma}\psi_2(s)} \int_a^{a+\delta} \nu_2(t) e^{-\frac{1}{\sigma}\psi_2(t)} dt ds. \tag{4.52}$$

To show that this leads to a nondegenerate estimate, that is, that the right hand side is less than zero, we employ here our hypothesis that  $\nu_2(x) \geq c_0(x - a)^m$  for  $x \geq a$ . So

$$\int_a^{a+\delta} \nu_2(t) e^{-\frac{1}{\sigma}\psi_2(t)} dt \geq C_1 \sigma^k \tag{4.53}$$

for some  $k$  and  $C_1 > 0$ . Now let us do the accounting. (4.52) implies that for some  $\epsilon > 0, K > 0$ , and  $k$ , all independent of  $\sigma$ ,

$$\rho_{23}(\xi_2) \leq -K e^{\frac{1}{\sigma}(\psi_2(\xi_1) - \psi_2(\xi_2))} e^{\frac{1}{\sigma}\psi_2(\xi_2)} \sigma^k \tag{4.54}$$

$$\leq -K \sigma^k e^{\frac{1}{\sigma}\psi_2(\xi_1)}. \tag{4.55}$$

This proves the lemma. □

Combining (4.42) with this, (4.44), with shows that

$$\frac{\rho_{13}\rho_{21} - \rho_{11}\rho_{23}}{-\rho_{23}} = O\left(e^{-\frac{\epsilon}{\sigma}}\right) \text{ as } \sigma \rightarrow 0^+.$$

To estimate

$$\frac{\rho_{13}\rho_{21} - \rho_{11}\rho_{23}}{\rho_{13}} \tag{4.56}$$

we compute a lower bound for  $\rho_{13}$ , known to be nonnegative and to vanish at  $\xi_1$ . One difference between this estimate and the preceding one for  $\rho_{23}$  is that it involves both  $\psi_1$  and  $\psi_2$ . Since the estimate follows by direct integration, we do not isolate it as a separate lemma. The equation for  $\rho_{13}$  is

$$\frac{d}{dx}\rho_{13} = \frac{1}{\sigma} \left( -\frac{d}{dx}\psi_1\rho_{13} + \phi_3 \right)$$

so, since  $\phi_3 \geq 0$ ,

$$\rho_{13}(x) = \frac{1}{\sigma} e^{-\frac{1}{\sigma}\psi_1(x)} \int_{\xi_1}^x e^{\frac{1}{\sigma}\psi_1(s)} \phi_3(s) ds \tag{4.57}$$

$$\geq \frac{1}{\sigma} e^{-\frac{1}{\sigma}\psi_1(x)} \int_a^x e^{\frac{1}{\sigma}\psi_1(s)} \phi_3(s) ds \tag{4.58}$$

and using (4.49), (4.53), for some  $k, K$ , which are independent of  $\sigma$  but which may change from line to line,

$$\rho_{13}(\xi_2) \geq -\frac{1}{\sigma} e^{-\frac{1}{\sigma}\psi_1(\xi_2)} \int_a^{\xi_2} e^{\frac{1}{\sigma}\psi_1(s)} \int_a^s \nu_2(t) \rho_{23}(a) e^{\frac{1}{\sigma}(\psi_2(a) - \psi_2(t))} dt ds \tag{4.59}$$

$$\geq K \sigma^k e^{\frac{1}{\sigma}\psi_2(\xi_1)} \int_{\xi_2 - \delta}^{\xi_2} e^{\frac{1}{\sigma}(\psi_1(s) - \psi_1(\xi_2))} \int_a^{a+\delta} \nu_2(t) e^{-\frac{1}{\sigma}\psi_2(t)} dt ds \tag{4.60}$$

$$\geq K \sigma^k e^{\frac{1}{\sigma}\psi_2(\xi_1)} \tag{4.61}$$

for  $\sigma$  sufficiently small. Now combining this with (4.42) shows that

$$\frac{\rho_{13}\rho_{21} - \rho_{11}\rho_{23}}{\rho_{13}} = O\left(e^{-\frac{\epsilon}{\sigma}}\right) \text{ as } \sigma \rightarrow 0^+.$$

This establishes half of the estimates, but it is thankfully most of the work. To complete the proof, we must estimate terms involving

$$-w_{13} = \rho_{22}\rho_{13} - \rho_{12}\rho_{23}.$$

So we now let

$$w = (\rho_{22}\phi_3 - \rho_{23}\phi_2, \rho_{13}\phi_2 - \rho_{12}\phi_3, \rho_{12}\rho_{23} - \rho_{13}\rho_{22})$$

the first row of  $adj(R)$ , which satisfies

$$w(\xi_1) = (1, 0, 0).$$



The analysis is very similar to the previous case. Interchanging the roles of  $\psi_2$  and  $\psi_1$ , we extend the result to  $\xi_0 + 1$ . This concludes the proof of Theorem 4.2.  $\square$

We now address the second part of the enterprise, the extension of the estimates to the entire interval. Recall we are thinking of the problem as defined on  $(0, N)$  and, as usual,  $\Omega = (0, 1)$ .

**Theorem 4.5.** *Suppose that  $\varphi_i \geq 0$  and  $\lambda_i \geq 0$  are smooth,  $\sigma > 0$ , and  $\lambda_i \neq 0, i = 1, 2$ . Let  $\eta = (\eta_1, \eta_2)$  be a solution of*

$$L\eta = -\frac{d}{dx} \left( \sigma \frac{d\eta}{dx} + \eta \Phi' \right) - \eta \lambda = 0 \text{ in } \Omega$$

$$\eta|_{x=0} = \eta^{(0)}, \quad \eta|_{x=1} = \eta^{(1)}.$$

There is a constant  $M > 0$  (independent of  $\eta$ ) such that

$$\|\eta\|_{C(\bar{\Omega})} \leq M \left( |\eta^{(0)}| + |\eta^{(1)}| \right).$$

Above we have written the equation in the obvious vector form with

$$\Phi' = \begin{pmatrix} \varphi'_1 & 0 \\ 0 & \varphi'_2 \end{pmatrix} \quad \text{and} \quad \lambda = \begin{pmatrix} -\lambda_1 & \lambda_1 \\ \lambda_2 & -\lambda_2 \end{pmatrix}.$$

*Proof.* For the proof, let  $f$  denote the solution of

$$Lf = 0 \quad \text{in } \Omega \tag{4.62}$$

$$\frac{df}{dx} + f\Phi' = 0 \quad \text{on } \partial\Omega. \tag{4.63}$$

We know that this problem has a unique solution which may be also taken to satisfy

$$\int_{\Omega} (f_1 + f_2) dx = 1.$$

It enjoys the additional property that  $f_i > 0$  in  $\Omega$ . Hence for  $\epsilon > 0$  small enough,

$$f_i - \epsilon \eta_i > 0 \quad \text{in } \Omega.$$

Choose  $\epsilon$  as large as possible:

$$f_i - \epsilon \eta_i > 0 \quad \text{in } \Omega, \quad i = 1, 2$$

$$f_j(x_0) - \epsilon \eta_j(x_0) = 0, \quad \text{for some } j = 1, 2, \text{ and } x_0 \in \bar{\Omega}.$$

Say  $j = 1$ . Let  $v = f - \epsilon \eta$ . Then

$$-\frac{d}{dx} \left( \sigma \frac{dv_1}{dx} + \varphi'_1 v_1 \right) + \lambda_1 v_1 = \lambda_2 v_2 \geq 0 \quad \text{in } \Omega.$$

So if the minimum of  $v_1$  is attained in  $\Omega$ , it is positive. Thus, by our choice of  $\epsilon$ , it must be attained at  $x = 0$  or  $x = 1$  according to Proposition 2.3, the elementary maximum principle redux. Say  $v_1(0) = \min v_1$ . Then we compute that

$$\frac{1}{\epsilon} = \frac{\eta_1(0)}{f_1(0)} \quad \text{and} \quad \eta_1(x) \leq \frac{\eta_1(0)}{f_1(0)} f_1(x)$$

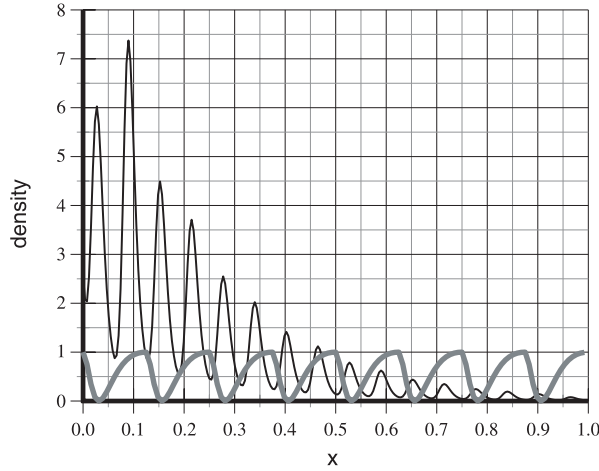


FIGURE 3. Transport realized in an eight well system. The upper curve is  $\rho_1(x) + \rho_2(x)$ . The lower gray curve is  $\psi_1(x)$  and  $\psi_2$  is  $\psi_1$  translated by half a period. The conformational change coefficients  $\nu_i$  have their maxima at the bottoms of the potential wells.

so in general,

$$\eta_i(x) \leq \frac{|\eta^{(0)}| + |\eta^{(1)}|}{\min(f_1(0), f_2(0), f_1(1), f_2(1))} f_i(x)$$

and the theorem is proved with

$$M = \frac{1}{\min(f_1(0), f_2(0), f_1(1), f_2(1))} \max_{i=1,2} \max_{\Omega} f_i(x).$$

To complete the proof of Theorem 4.1, still retaining the stretched coordinates  $(0, N)$ , we determine  $M$  by solving the problem (4.63) in a period interval, say  $\Omega = (\xi_0, \xi_0 + 1)$ . We take  $\eta = \rho$  in this interval and compare it with  $f$ . Then

$$\begin{aligned} \max_{y_j \leq x \leq y_{j+1}} (\rho_1 + \rho_2) &\leq M(\rho_1(y_j) + \rho_2(y_j) + \rho_1(y_{j+1}) + \rho_2(y_{j+1})) \\ &\leq MKe^{-\frac{\epsilon}{\sigma}}(\rho_1(y_{j-1}) + \rho_2(y_{j-1}) + \rho_1(y_j) + \rho_2(y_j)) \\ &= \hat{K}e^{-\frac{\epsilon j}{\sigma}}. \end{aligned}$$

The final detail is that there may be an unaccounted for interval  $(y_{N-1}, N)$  in this induction. For this interval, the  $\eta = \rho$  on  $(y_{N-1}, N)$  satisfies a mixed problem, Dirichlet on the left and natural boundary conditions on the right. This may be compared with a second choice of  $f$ , the solution of (4.62), (4.63) on  $(y_{N-1}, N)$ .

The result in Theorem 4.1 may be extended to piecewise continuous potentials. We observe that the scaling estimate argument of Theorem 4.5 may serve as the basis of an existence theory for the Dirichlet Problem for this system. □

### 5. LONG TIME BEHAVIOR: TREND TO STATIONARITY

The free energy associated to (1.1), (1.2) is

$$F(\rho) = \sum_i \int_{\Omega} (\psi_i \rho_i + \sigma \rho_i \log \rho_i) dx.$$

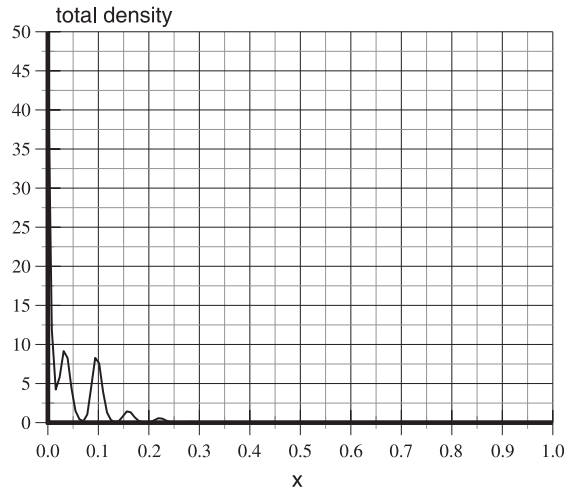


FIGURE 4. This simulation is identical to Figure 3 except that  $\psi_1$  and  $\psi_2$  have been replaced by  $2\psi_1$  and  $2\psi_2$ . This is approximately the same as halving the diffusion coefficient.

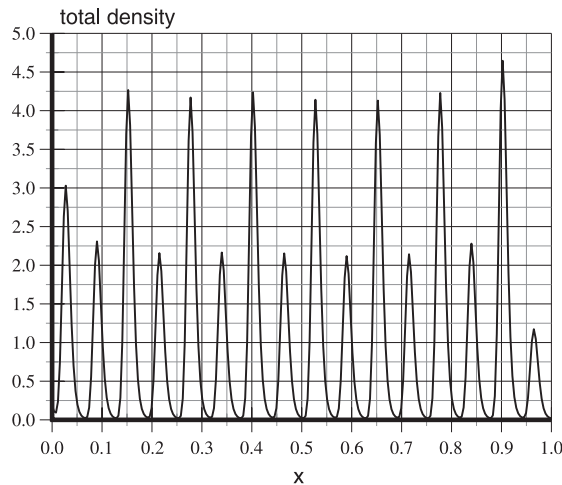


FIGURE 5. This simulation is identical to Figure 3 except that the conformational change coefficients  $\nu_i$  have been translated so their maxima occur at the maxima of the potential wells.

The solution  $\rho^\sharp$  of the stationary equations (1.4), (1.5) is not a minimum of  $F$  and, in fact, there does not seem to be a natural Lyapunov function or H-function for this system. Moreover,  $F(\rho)$  is not decreasing along a trajectory of (1.1), (1.2). This complicates the search for a proof of asymptotic behavior of the system. However, the analytical structure is simple enough that we may appeal to a variant of the Krein-Rutman Theorem to understand this issue, *cf.* for example [29] for an extensive discussion. The main tool is the standard maximum principle for weakly coupled parabolic systems, the version of Proposition 2.3, *the elementary maximum principle redux*, we introduced earlier for stationary systems, also found in Protter and Weinberger, [22], p. 188. Throughout we assume some simple properties of the data:

$$\begin{aligned} &\psi_i \in C^3(\overline{\Omega}), \psi_i \geq 0, i = 1, 2; \\ &\nu_i \in C^3(\overline{\Omega}), \nu_i \geq 0 \text{ and } \nu_i \neq 0 \text{ for each } i = 1, 2; \\ &\sigma > 0 \text{ constant.} \end{aligned}$$

It may be convenient to write the system in vector form, with

$$\Psi' = \begin{pmatrix} \psi'_1 & 0 \\ 0 & \psi'_2 \end{pmatrix} \quad \text{and} \quad \nu = \begin{pmatrix} -\nu_1 & \nu_1 \\ \nu_2 & -\nu_2 \end{pmatrix}$$

as

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} \left( \sigma \frac{\partial \rho}{\partial x} + \rho \Psi' \right) + \rho \nu \quad \text{in } \Omega, \quad t > 0 \tag{5.64}$$

$$\sigma \frac{\partial \rho}{\partial x} + \rho \Psi' = 0 \quad \text{on } \partial\Omega, \quad t > 0. \tag{5.65}$$

For

$$u_i = e^{\frac{1}{\sigma}\psi_i} \rho_i \quad \alpha_i = e^{-\frac{1}{\sigma}\psi_i}, \quad \mu_i = e^{-\frac{1}{\sigma}\psi_i} \nu_i, \quad i = 1, 2$$

we have a divergence form, actually the adjoint system, where to retain conventional notions, we express  $u$  as a column vector, and set

$$\alpha = \begin{pmatrix} \alpha_1 & 0 \\ 0 & \alpha_2 \end{pmatrix} \quad \text{and} \quad \mu = \begin{pmatrix} -\mu_1 & \mu_2 \\ \mu_1 & -\mu_2 \end{pmatrix}.$$

Then

$$\alpha \frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left( \sigma \alpha \frac{\partial u}{\partial x} \right) + \mu u \quad \text{in } \Omega, \quad t > 0 \tag{5.66}$$

$$\frac{\partial u}{\partial x} = 0 \quad \text{on } \partial\Omega, \quad t > 0. \tag{5.67}$$

We denote by  $\rho^\sharp$  the solution of the stationary equations (1.4), (1.5), whose components we know to be positive.

**Lemma 5.1.** *Let  $f \in C(\overline{\Omega}) \times C(\overline{\Omega})$ . There is a unique solution  $\rho$  of the evolution system (5.64), (5.65) with*

$$\rho|_{t=0} = f.$$

Moreover,

- (1)  $\rho \in L^\infty(\Omega \times (0, \infty)) \cap L^\infty(\epsilon, \infty; H^1(\Omega))$ , for  $\epsilon > 0$ , and there are  $M > 0, C_\tau > 0$  depending on the problem data such that

$$|\rho_i(x, t)| \leq M \|f\|_{C(\overline{\Omega})}, \quad i = 1, 2, \text{ and} \tag{5.68}$$

$$\|\rho(\cdot, \tau)\|_{H^1(\Omega)} \leq C_\tau \|f\|_{C(\overline{\Omega})} \quad \text{for } \tau > 0; \tag{5.69}$$

- (2) if  $f_i \geq 0$  in  $\Omega, i = 1, 2$  then  $\rho_i > 0$  in  $\Omega, i = 1, 2$ .

*Proof.*

**Step 1.** Let  $\rho_i^\sharp(x) \geq 1/C_0$  in  $\Omega$  and choose  $M$  so that  $C_0 \rho_i^\sharp(x) \leq M, x \in \Omega, i = 1, 2$ .

Assume initial data  $\eta^0$  smooth, not necessarily positive, for the parabolic system (5.64), (5.65). According to classical results, there is a solution  $\eta \in C^2(\overline{\Omega} \times (0, \infty))$  and  $u(x, 0) = u^0(x)$ . Now

$$-C_0 \|\eta^0\| \rho_i^\sharp \leq \eta_i^0 \leq C_0 \|\eta^0\| \rho_i^\sharp, \quad i = 1, 2$$

implies, by the maximum principle for weakly coupled systems, that

$$|\eta(x, t)| \leq C_0 \|\eta^0\| \rho_i^\sharp(x), \quad i = 1, 2,$$

and hence

$$\|\eta\|_{C(\bar{\Omega} \times (0, \infty))} \leq M \|\eta^0\|_{C(\bar{\Omega})}.$$

From this we conclude that we can extend the class of initial data to  $\rho^0 \in C(\bar{\Omega})$ , and second, that the solution of (5.64), (5.65) satisfies

$$|\rho_i(x, t)| \leq M \|f\|_{C(\bar{\Omega})}, \quad i = 1, 2.$$

and if  $f_i \geq 0$ ,

$$0 \leq \rho_i(x, t) \leq M \|f\|_{C(\bar{\Omega})}, \quad i = 1, 2.$$

**Step 2.** The integral estimates are routine. The main feature, as suggested in the conclusion above, is that the boundedness of  $\rho$  permits us uniform  $H^1$  estimates at each time. Note that it suffices to prove some estimate for  $u$  in view of the boundedness of  $\rho$  from Step 1. The argument has two parts, a and b.

Part a. Multiply the equation, for example, divergence form equation for  $u$  at a fixed time  $t$ , by  $u$  and integrate over  $\Omega$ . After integration by parts,

$$\frac{d}{dt} \int_{\Omega} \frac{1}{2} (\alpha_1 u_1^2 + \alpha_2 u_2^2) dx = -\sigma \int_{\Omega} (\alpha_1 (u_{1x})^2 + \alpha_2 (u_{2x})^2) dx + \int_{\Omega} u \cdot \mu u \, dx.$$

Since the  $\alpha_i$  are bounded away from 0, we obtain after rearranging that for a constants  $C, \delta > 0$ ,

$$\delta \int_{\Omega} |u_x|^2 dx \leq C \int_{\Omega} |u|^2 dx - \frac{d}{dt} \int_{\Omega} \frac{1}{2} (\alpha_1 u_1^2 + \alpha_2 u_2^2) dx.$$

Integrating this over  $T_1 \leq t \leq T_2$  and using the bound for  $u$  from step 1 and positiveness of the  $\alpha_i$  gives the estimate

$$\int_{T_1}^{T_2} \int_{\Omega} |u_x|^2 dx dt \leq C((T_2 - T_1) + 2) \max |u^0|^2, \tag{5.70}$$

for some constant  $C$ , where  $u^0$  denotes the initial values of  $u$ .

Part b. We repeat the previous argument for the differentiated equation. Here, by employing the divergence form system, the boundary integrals vanish when integrating by parts. Differentiating the equation, we obtain

$$\alpha u_{xt} + \alpha_x u_t = (\sigma \alpha u_x)_{xx} + (\mu u)_x \quad \text{in } \Omega, t > 0$$

and substituting the equation for  $\frac{\partial u}{\partial t}$  on the left gives

$$\alpha u_{xt} + \alpha_x \alpha^{-1} (\sigma (\alpha u_x)_x + \mu u) = (\sigma \alpha u_x)_{xx} + (\mu u)_x \quad \text{in } \Omega, t > 0.$$

Multiply this expression by  $\frac{\partial u}{\partial x}$  and integrate over  $\Omega$ . Integrate by parts in the first term on the right.

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \int_{\Omega} \left( \sum \alpha_i (u_{ix})^2 \right) dx \\ & + \int_{\Omega} (\alpha_x \alpha^{-1} (\sigma (\alpha u_x)_x + \mu u) \cdot u_x) dx = - \int_{\Omega} (\sigma \alpha u_x)_x \cdot u_{xx} dx + \int_{\Omega} (\mu u)_x \cdot u_x dx \\ & = - \int_{\Omega} \sigma \alpha u_{xx} \cdot u_{xx} dx - \int_{\Omega} \sigma \alpha_x u_x \cdot u_{xx} dx + \int_{\Omega} (\mu u)_x \cdot u_x dx \\ & \leq -c_0 \int_{\Omega} |u_{xx}|^2 dx - \int_{\Omega} \sigma \alpha_x u_x \cdot u_{xx} dx + \int_{\Omega} (\mu u)_x \cdot u_x dx. \end{aligned}$$

Employing “Young Inequality”  $ab \leq \epsilon a^2 + C_\epsilon b^2$  with  $\epsilon$  small in the usual fashion, we estimate the second integral on the right:

$$\left| \int_{\Omega} \sigma \alpha_x u_x \cdot u_{xx} dx \right| \leq \epsilon \int_{\Omega} |u_{xx}|^2 dx + C \int_{\Omega} |u_x|^2 dx.$$

All second derivative terms may be absorbed into the leading term on the right side of the equation, which is negative. These are then discarded. We then obtain the estimate

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega} \left( \sum \alpha_i (u_{ix})^2 \right) dx \leq C \int_{\Omega} (|u_x|^2 + |u|^2) dx.$$

Now integrating over  $t \leq s \leq \tau$

$$\frac{1}{2} \int_{\Omega} \left( \sum \alpha_i (u_{ix})^2 \right) dx|_{\tau} \leq C \int_t^{\tau} \int_{\Omega} (|u_x|^2 + |u|^2) dx ds + \frac{1}{2} \int_{\Omega} \left( \sum \alpha_i (u_{ix})^2 \right) dx|_t.$$

Integrate the above expression with respect to  $t$  over  $[\tau/2, 3\tau/4]$ . This gives

$$\frac{1}{2} \int_{\Omega} \left( \sum \alpha_i (u_{ix})^2 \right) dx|_{\tau} \leq C \int_{\tau/2}^{\tau} \int_{\Omega} (|u_x|^2 + |u|^2) dx ds + \frac{C'}{\tau} \int_{\tau/2}^{3\tau/4} \int_{\Omega} \left( \sum \alpha_i (u_{ix})^2 \right) dx dt.$$

Using now (5.70), and, as usual, that the  $\alpha_i > 0$ , and Part 1, we obtain the desired estimate that

$$\int_{\Omega} |u_x|^2 dx|_{\tau} \leq C \max |u^0|^2, \text{ for } \tau > 0.$$

This translates into an estimate of the same form for  $\rho$ . □

We now discuss the exponential decay of the time dependent solution  $\rho(x, t)$  to  $\rho^\sharp(x)$ . Let  $\tau > 0$  and define the linear mapping on initial data

$$T_{\tau} : C(\bar{\Omega}) \times C(\bar{\Omega}) \rightarrow C(\bar{\Omega}) \times C(\bar{\Omega}) \tag{5.71}$$

$$f(x) \rightarrow \rho(x, \tau) \tag{5.72}$$

where  $\rho(x, t)$  is the associated solution of (1.1), (1.2). So  $T_{\tau}^k f(x) = \rho(x, t), t = k\tau$ . We conclude from the Lemma, and the Ascoli-Arzela’ Theorem, that

$T_{\tau} : C(\bar{\Omega}) \times C(\bar{\Omega}) \rightarrow C(\bar{\Omega}) \times C(\bar{\Omega})$  is a (linear) compact positive operator.

So  $T_{\tau}$  has a discrete spectrum with eigenvalues  $\lambda_i \rightarrow 0$ . Let us adopt, for the purposes of brevity, the notation that for a vector  $\alpha, \alpha \geq 0$  means each  $\alpha_i \geq 0$  and  $\alpha > 0$  means each  $\alpha_j > 0$ . Then  $T_{\tau}$  is positive in the sense that

$$f \geq 0 \text{ in } \Omega \text{ and } f \not\equiv 0 \implies T_{\tau} f > 0 \text{ in } \Omega.$$

Since  $\rho^\sharp$  is a stationary solution of (1.1), (1.2), we have that

$$T_{\tau} \rho^\sharp = \rho^\sharp$$

for any  $\tau > 0$ . So  $T_{\tau}$  has a positive eigenvector with eigenvalue 1. Indeed, that  $\rho^\sharp > 0$  implies that  $\lambda = 1$  is the eigenvalue of maximum modulus and it has multiplicity one. We check this.

Suppose that  $\eta$  is an eigenfunction with real eigenvalue  $\lambda, |\lambda| \geq 1$  and  $\eta \neq \rho^\sharp$ ;

$$T_{\tau} \eta = \lambda \eta$$

say  $\lambda \geq 1$  for example. Then we can find an  $\epsilon > 0$  such that

$$\rho_i^\# - \frac{\epsilon}{\lambda} \eta_i \geq 0, \quad i = 1, 2, \quad \text{and} \quad \min_i \min_{\Omega} \left( \rho_i^\# - \frac{\epsilon}{\lambda} \eta_i \right) = 0.$$

Now

$$T_\tau \left( \rho^\# - \frac{\epsilon}{\lambda} \eta \right)_i > 0 \quad \text{in } \Omega$$

by positivity but

$$T_\tau \left( \rho^\# - \frac{\epsilon}{\lambda} \eta \right) = \rho^\# - \epsilon \eta$$

which is not strictly positive since  $\lambda \geq 1$  and  $\epsilon$  has been carefully chosen. Similarly if  $\lambda \leq -1$ . Thus  $\lambda = 1$  is the largest real eigenvalue of  $T_\tau$  and it has a unique (normalized) eigenfunction  $\rho^\#$ . An analogous argument prevails if  $\lambda$  is complex and  $|\lambda| \geq 1$ .

So we have verified that  $\lambda = 1$  is the eigenvalue of largest modulus of  $T_\tau$  and that it has multiplicity 1. Now consider the space  $X$  of functions  $f = (f_1, f_2) \in C(\bar{\Omega}) \times C(\bar{\Omega})$  with

$$\int_{\Omega} (f_1 + f_2) dx = 0.$$

From the boundary conditions (5.65),

$$f \in X \quad \text{implies} \quad T_\tau f \in X.$$

So

$$T_\tau : X \rightarrow X \quad \text{is compact, linear}$$

and 1 is not an eigenvalue; the largest eigenvalue is less than one. So there is a  $\lambda_0 < 1$  in the resolvent of  $T_\tau$  larger than any eigenvalue. Set  $r_0 = 1/\lambda_0$ . Then

$$(\lambda_0 \mathbf{1} - T_\tau)^{-1} f = \frac{1}{\lambda_0} \left( \mathbf{1} - \frac{1}{\lambda_0} T_\tau \right)^{-1} f \tag{5.73}$$

$$= \frac{1}{\lambda_0} \sum T_\tau^k f(x) \left( \frac{1}{\lambda_0} \right)^k \tag{5.74}$$

$$= r_0 \sum T_\tau^k f(x) r_0^k, \quad f \in X. \tag{5.75}$$

So the series  $\sum T_\tau^k f(x) z^k$  converges absolutely for  $|z| \leq r = r_0 - \epsilon, r > 1$ , so in particular the terms are bounded. Consequently, for each  $f \in X$  there is an  $M_\tau$  such that

$$|T_\tau^k f(x)| \leq M_\tau r^{-k} \rightarrow 0, \quad \text{as } k \rightarrow \infty.$$

Consequently, choosing  $f(x) = \rho(x, 0) - \rho^\#(x)$  for a solution  $\rho(x, t)$  of (1.1), (1.2), tells us that

$$|\rho(x, k\tau) - \rho^\#(x)| \leq M_\tau r^{-k} \rightarrow 0, \quad \text{as } k \rightarrow \infty$$

and using (5.68),

$$\sup_{t \geq k\tau} |\rho(x, t) - \rho^\#(x)| \leq M M_\tau r^{-k} \rightarrow 0, \quad \text{as } k \rightarrow \infty.$$

This proves the convergence of the solution of the evolution equations to the stationary solution, indeed, with an exponential rate of convergence determined by the second eigenvalue of  $T_\tau$  on  $C(\bar{\Omega}) \times C(\bar{\Omega})$ ; namely, with  $t = k\tau$ ,

$$r^{-k} = e^{-\frac{\log r}{\tau} t}, \quad \log r > 0.$$

To review,  $r$  above satisfies

$$\lambda_2 < \frac{1}{r} < 1$$

where  $\lambda_2$  is the second eigenvalue of  $T_\tau$ . We have shown

**Theorem 5.2.** *Under the hypotheses (5), let  $\rho(x, t)$  denote the solution of (1.1), (1.2), (1.3) and  $\rho^\sharp$  denote the solution of the stationary problem (1.4), (1.5), (1.6). Then there are  $M_0 > 0, \gamma > 0$  such that*

$$\sup_{\Omega} |\rho(x, t) - \rho^\sharp(x)| \leq M_0 e^{-\gamma t}. \quad (5.76)$$

*Acknowledgements.* We wish to thank Xinfu Chen, Irene Fonseca, Giovanni Leoni, Bryce McLeod, and Michal Kowalczyk for their extensive help. We also thank Dean Astumian for helpful comments.

## REFERENCES

- [1] A. Ajdari and J. Prost, Mouvement induit par un potentiel périodique de basse symétrie : diélectrophorèse pulse. *C. R. Acad. Sci. Paris II* **315** (1992) 1653.
- [2] R.D. Astumian, Thermodynamics and kinetics of a Brownian motor. *Science* **276** (1997) 917–922.
- [3] J.-D. Benamou and Y. Brenier, A computational fluid mechanics solution to the Monge-Kantorovich mass transfer problem. *Numer. Math.* **84** (2000) 375–393.
- [4] M. Chipot, D. Kinderlehrer and M. Kowalczyk, A variational principle for molecular motors. *Meccanica* **38** (2003) 505–518.
- [5] C. Doering, B. Ermentrout and G. Oster, Rotary DNA motors. *Biophys. J.* **69** (1995) 2256–2267.
- [6] J. Dolbeault, D. Kinderlehrer and M. Kowalczyk, *Remarks about the flashing ratchet*, in *Proc. PASI 2003* (to appear).
- [7] D.D. Hackney, The kinetic cycles of myosin, kinesin, and dynein. *Ann. Rev. Physiol.* **58** (1996) 731–750.
- [8] S. Hastings and D. Kinderlehrer, Remarks about diffusion mediated transport: thinking about motion in small systems. (to appear).
- [9] J. Howard, *Mechanics of Motor Proteins and the Cytoskeleton*. Sinauer Associates, Inc. (2001).
- [10] A.F. Huxley, Muscle structure and theories of contraction. *Prog. Biophys. Biophys. Chem.* **7** (1957) 255–318.
- [11] R. Jordan, D. Kinderlehrer and F. Otto, The variational formulation of the Fokker-Planck equation. *SIAM J. Math. Anal.* **29** (1998) 1–17.
- [12] D. Kinderlehrer and M. Kowalczyk, Diffusion-mediated transport and the flashing ratchet. *Arch. Rat. Mech. Anal.* **161** (2002) 149–179.
- [13] D. Kinderlehrer and N. Walkington, Approximation of parabolic equations based upon Wasserstein’s variational principle. *ESAIM: M2AN* **33** (1999) 837–852.
- [14] J.S. Muldowney, Compound matrices and ordinary differential equations. *Rocky Mountain J. Math.* **20** (1990) 857–872.
- [15] Y. Okada and N. Hirokawa, A processive single-headed motor: kinesin superfamily protein KIF1A. *Science* **283** (1999) 19.
- [16] Y. Okada and N. Hirokawa, Mechanism of the single headed processivity: diffusional anchoring between the K-loop of kinesin and the C terminus of tubulin, in *Proc. Nat. Acad. Sciences* **7** (2000) 640–645.
- [17] F. Otto, Dynamics of labyrinthine pattern formation: a mean field theory. *Arch. Rat. Mech. Anal.* **141** (1998) 63–103.
- [18] F. Otto, The geometry of dissipative evolution equations: the porous medium equation. *Comm. PDE* **26** (2001) 101–174.
- [19] P. Palfy-Muhoray, T. Kosa and E. Weinan, Dynamics of a light driven molecular motor. *Mol. Cryst. Liq. Cryst.* **375** (2002) 577–591.
- [20] A. Parmeggiani, F. Jülicher, A. Ajdari and J. Prost, Energy transduction of isothermal ratchets: generic aspects and specific examples close and far from equilibrium. *Phys. Rev. E* **60** (1999) 2127–2140.
- [21] C.S. Peskin, G.B. Ermentrout and G.F. Oster, *The correlation ratchet: a novel mechanism for generating directed motion by ATP hydrolysis*, in *Cell Mechanics and Cellular Engineering*, V.C Mow et al. Eds., Springer, New York (1995).
- [22] M. Protter and H. Weinberger, *Maximum principles in differential equations*, Prentice Hall, Englewood Cliffs, N.J. (1967).
- [23] P. Reimann, Brownian motors: noisy transport far from equilibrium. *Phys. Rep.* **361** (2002) 57–265.
- [24] M. Schliwa, *Molecular Motors*. Wiley-VCH Verlag, Weinheim (2003).
- [25] B. Schwarz, Totally positive differential systems. *Pacific J. Math.* **32** (1970) 203–230.
- [26] A. Tudorascu, *A one phase Stefan problem via Monge-Kantorovich theory*. CNA Report 03-CNA-007.
- [27] R.D. Vale and R.A. Milligan, The way things move: looking under the hood of motor proteins. *Science* **288** (2000) 88–95.
- [28] C. Villani, *Topics in optimal transportation*, Providence. *AMS Graduate Studies in Mathematics* **58** (2003).
- [29] E. Zeidler, *Nonlinear functional analysis and its applications*. I Springer, New York (1986).