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Close-to-equilibrium behaviour of quadratic reaction–diffusion systems with detailed balance

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ABSTRACT

We study general quadratic reaction–diffusion systems with detailed balance, in space dimension $d \leq 4$. We show that close-to-equilibrium solutions (in an L^2 sense) are regular for all times, and that they relax to equilibrium exponentially in a strong sense. That is: all detailed balance equilibria are exponentially asymptotically stable in all L^p norms, at least in dimension $d \leq 4$. The results are given in detail for the four-species reaction–diffusion system, where the involved constants can be estimated explicitly. The main novelty is the regularity result and exponential relaxation in L^p norms for $p > 1$, which up to our knowledge is new in dimensions 3 and 4.

1. Introduction

Systems of reaction–diffusion equations model a wide variety of phenomena, and prominent among them is the behaviour of reacting chemical mixtures. The mathematical theory of these systems is far from complete, and in particular the existence of global regular solutions is unknown in many important cases. If we consider $I \geq 2$ species, denoted $A_1, \dots, A_I$, undergoing a number $R \geq 1$ of different reactions

$$\alpha_1^r A_1 + \cdots + \alpha_N^r A_I \underset{k_b^r}{\overset{k_f^r}{\rightleftharpoons}} \beta_1^r A_1 + \cdots + \beta_N^r A_I, \quad r = 1, \dots, R,$$

then the equation satisfied by the concentrations $a_i = a_i(t,x)$ of the A_i is

$$\partial_t a_i = d_i \Delta a_i - R_i(a), \quad i = 1, \dots, I, \tag{1}$$

$$\nabla_x a_i(t,x) \cdot \nu(x) = 0, \quad t > 0,\ x \in \partial\Omega,\ i = 1, \dots, I. \tag{2}$$

The positive numbers k_f^r and k_b^r, for $r = 1 \dots, R$, denote the forward and backward reaction rates, respectively, for each of the R reactions. The vectors $\alpha^r = (\alpha_1^r, \dots, \alpha_I^r)$ and $\beta^r = (\beta_1^r, \dots, \beta_I^r)$ are the

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stoichiometric coefficients which specify the number of particles of each species that take part in each reaction, and the *reaction term* $R_i(a)$ depends on $a = (a_i)_{i=1,\dots,I}$ and is obtained from the law of mass action. Complete details on this setting are given in Section 6, and for the moment we omit them for brevity. A very interesting basic model that presents the main difficulties is the following, sometimes called the *four species model*: consider a set of four chemical substances A_1, A_2, A_3, A_4 which undergo the reactions

$$A_1 + A_3 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2 + A_4 \tag{3}$$

at positive rates k_1, k_2 as marked. We assume these substances are confined to a domain $\Omega \subseteq \mathbb{R}^d$ (a connected, bounded, open region with smooth boundary — at least $\mathcal{C}^{2+\alpha}$ with $\alpha > 0$), and we denote the concentration of A_i by $a_i = a_i(t,x)$, depending on time $t \geq 0$ and space $x \in \Omega$. Except in Section 6, it is understood that the index i always ranges from 1 to 4. If these substances also diffuse in a domain with diffusion constant d_i corresponding to A_i then the following system models the time evolution of the concentrations a_i:

$$\left.\begin{aligned} \partial_t a_1 &= d_1 \Delta a_1 - k_1 a_1 a_3 + k_2 a_2 a_4, \\ \partial_t a_2 &= d_2 \Delta a_2 + k_1 a_1 a_3 - k_2 a_2 a_4, \\ \partial_t a_3 &= d_3 \Delta a_3 - k_1 a_1 a_3 + k_2 a_2 a_4, \\ \partial_t a_4 &= d_4 \Delta a_4 + k_1 a_1 a_3 - k_2 a_2 a_4, \end{aligned}\right\} \quad t > 0, x \in \Omega. \tag{4}$$

We always assume that all d_i are strictly positive. We also assume no-flux boundary conditions which ensure that the total mass is conserved:

$$\nabla_x a_i(t,x) \cdot \nu(x) = 0, \quad t > 0,\ x \in \partial\Omega,\ i = 1, \dots, 4, \tag{5}$$

where $\nu(x)$ denotes the outer normal to the boundary of Ω at point x. The system (4) is quadratic in the nonlinearities and satisfies the *detailed balance condition*: there is a space-homogeneous equilibrium $(a_{i,\infty})_{i=1,\dots,4}$ which makes each of the reactions balanced, that is, it satisfies

$$k_1 a_{1,\infty} a_{3,\infty} = k_2 a_{2,\infty} a_{4,\infty}.$$

Since in this case there is only one reaction, it is obvious that all space-homogeneous equilibria must satisfy this. In general, when detailed balance holds one can show that all equilibria must be space-homogeneous and satisfy the same condition.

The existence of solutions and asymptotic behaviour of the system (4)–(5) and in general (1)–(2) have been studied in a number of works, and several previous results in reaction–diffusion systems apply to it. In general, difficulties increase with the strength of the nonlinearities and the space dimension. It is known that weak solutions to (4)–(5) in $L^2([0,T) \times \Omega)$ exist in all dimensions and for all $T > 0$, and in general weak L^2 solutions to (1)–(2) exist as long as the system is at most quadratic and satisfies the detailed balance condition [8]. In this paper we always work with this concept of solution. A general theory of renormalised solutions for entropy-dissipating systems that does not have the restriction of the system being quadratic has recently been developed in Fischer [15]. Classical solutions are more elusive: they exist for a short time thanks to general theory of parabolic equations [1], and global-in-time classical solutions are relatively well understood in a few cases. For the system (4)–(5) the current situation is the following:

1. Global regular solutions are known to exist in space dimension $d \leq 2$ [5,7,19,3].
2. Global regular solutions also exist in any space dimension whenever the nonlinearities are of degree <2 [4]. Notice that this does not apply to system (4), which has quadratic nonlinearities.
3. Regular solutions are also understood in any space dimension when diffusion coefficients are not too far from each other [3,12,11]. They are also understood if the diffusion coefficients satisfy $d_1 = d_2$ and $d_3 = d_4$ [18,16].