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Singular Perturbation Problems Arising from the Anisotropy of Crystalline Grain Boundaries

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Mathematically, the problem considered here is that of heteroclinic connections for a system of two second-order differential equations of gradient type, in which a small parameter ϵ conveys a singular perturbation. The physical motivation comes from a multi-order-parameter phase field model developed by Braun et al. *Trans. R. Soc. Lond. A,* **355**, 1997 and Tanoglu, Ph.D. Thesis, University of Delawere, (2000) for the description of crystalline interphase boundaries. In this, the smallness of ϵ is related to large anisotropy. The geometric theory of singular perturbations is employed.

KEY WORDS: Crystalline interphase boundaries; travelling wave solutions; singular perturbations.

1. INTRODUCTION

In this note, we introduce a class of singular perturbation problems that are mathematically challenging and then settle a special case. In [4] a continuum model was derived for studying interfaces in the context of crystals. It is based on the free energy functional

$$J(X,Y,Z)=\int_{\Omega}[Q(\nabla X,\nabla Y,\nabla Z)+F(X,Y,Z)]\,d\xi_1 d\xi_2 d\xi_3, \qquad (1)$$

where X,Y,Z are composition variables and (ξ_1,ξ_2,ξ_3) space coordinates and Ω the volume occupied by the sample. Here Q is a positive definite

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quadratic form and F is positive except at its several global minima. The bulk free energy F must conform to certain crystalline symmetries, for instance it must be invariant under permutation of X, Y, Z. If it is restricted to be a fourth degree polynomial its general form is that given below in (2).

The function Q represents the influence on the free energy of the difference between the order parameters at a crystalline vertex and those at nearest neighbors. It is generally the case that this contribution depends on the orientation of the line between those nearby points, and this dependence is a source of anisotropy. The simplest type of quadratic form Q which accounts for anisotropy and which satisfies other symmetry conditions is of the form $Q = AQ_1 + BQ_2$ where Q_i are the simple sums of squares of derivatives given below in (3). The ratio $B/A \equiv \epsilon^2$ then will be taken as a measure of the degree of anisotropy of the free energy. Isotropy corresponds to the case $B = A$ as we show below ($\epsilon = 1$); our focus will be on the anisotropic case $\epsilon \ll 1$. The simplest example for F and Q is

$$F(X,Y,Z) = a_2(X^2+Y^2+Z^2) + a_3XYZ + a_{41}(X^4+Y^4+Z^4) + a_{42}(X^2Y^2 + X^2Z^2 + Y^2Z^2), \tag{2}$$

$$\begin{aligned} Q_1 &= \frac{1}{2}\left[\left(\frac{\partial X}{\partial \xi_1}\right)^2 + \left(\frac{\partial Y}{\partial \xi_2}\right)^2 + \left(\frac{\partial Z}{\partial \xi_3}\right)^2\right], \\ Q_2 &= \frac{1}{2}\left[\left(\frac{\partial X}{\partial \xi_2}\right)^2 + \left(\frac{\partial X}{\partial \xi_3}\right)^2 + \left(\frac{\partial Y}{\partial \xi_1}\right)^2 + \left(\frac{\partial Y}{\partial \xi_3}\right)^2 + \left(\frac{\partial Z}{\partial \xi_1}\right)^2 + \left(\frac{\partial Z}{\partial \xi_2}\right)^2\right]. \end{aligned} \tag{3}$$

The approach here will be to assume dynamics governed by a gradient flow with respect to J, and examine the nature of the interface between grains of ordered and disordered material. In general, these two states will enjoy different bulk free energies, and the interface will migrate. However, the motion depends on the values of the coefficients in (2), which in turn depend on the temperature. The simplest situation is when the two bulk values of F are the same. In this case, we are led as we will see below in (6) to a Hamiltonian system. In the specific example (2) if the temperature is chosen appropriately then this is the case, with the two equilibria $(0,0,0)$ and $(1,1,1)$ representing the disordered and ordered state, respectively. A possible choice of the coefficients in (2) such that $F(0,0,0) = F(1,1,1) = 0$ is $a_2 = 2,\ a_3 = -12,\ a_{41} = a_{42} = 1$.

1.1. The Phase Field Equations

The governing evolution PDE's are given by the L^2 gradient flow of the functional J. We obtain

$$\tau \frac{\partial}{\partial t}\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = L\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} - \nabla F(X, Y, Z), \tag{4}$$

where L is a diagonal matrix of second degree elliptic operators in the space variables, ∇ denotes the gradient with respect to the variables (X, Y, Z), and τ is a dimensionless relaxation time.

1.2. Grain Boundaries as Planar Solutions

Plane waves in the direction $\overline{n}$ and velocity V are solutions of (4) of the form

$$X = x(\overline{n}\cdot(\xi_1, \xi_2, \xi_3) - Vt) = x(s), \quad Y = y(s), \quad Z = z(s), \tag{5}$$

with boundary conditions $x(-\infty) = y(-\infty) = z(-\infty) = 0$, $x(\infty) = y(\infty) = z(\infty) = 1$. They represent planar interfaces with normal $\overline{n}$ separating an ordered state from a disordered state. The functions $\overline{x} = (x, y, z)$ satisfy (derivatives are with respect to s):

$$-V\overline{x}' = \Lambda\overline{x}'' - \nabla F(x, y, z), \tag{6}$$

where Λ is a diagonal matrix whose elements are linear functions of A and B and quadratic functions of $\overline{n}$. However recall that the coefficients of F are such that F has equal depth wells at the equilibria at the order disorder transition, i.e., $F(0, 0, 0) = F(1, 1, 1)$. We see, by taking the scalar product of (6) with $\overline{x}'$ and integrating, that $V = 0$. The resulting system is Hamiltonian.

1.3. Symmetries

Simplifications to system (6) can be made by seeking only those profiles which satisfy certain symmetry constraints. Doing so reduces the dimensionality to two. Of course the direction $\overline{n}$ must be chosen so that the resulting profile satisfies those constraints, and the function F and the matrix Λ have to be compatible with them as well.

One such possible constraint is the restriction of the order parameters to the plane $Y = Z$ (hence $y = z$). In the crystal, this is tied to the symmetry between certain sites [2,4]. It turns out that the two symmetric sites share the same ξ_1 coordinate. Therefore if we take $\overline{n}$ so that $n_2 = n_3$, the symmetry $Y = Z$ should be preserved through the transition. This is indeed true. To exhibit the resulting system, we define our anisotropy parameter $\epsilon = \sqrt{B/A}$; the reduced free energy

$$g(x, r) = F\left(x, \frac{1}{\sqrt{2}}r, \frac{1}{\sqrt{2}}r\right) \tag{7}$$

(r is a modified order parameter); and the angle α by $\overline{n} = (\cos\alpha, \frac{1}{\sqrt{2}}\sin\alpha, \frac{1}{\sqrt{2}}\sin\alpha)$, $0 \le \alpha \le \pi$. Then (6) is reduced to

$$\begin{aligned} &(\cos^2\alpha + \epsilon^2 \sin^2\alpha)x'' - g_x(x, r) = 0, \quad x(-\infty) = r(-\infty) = 0, \\ &(\epsilon^2\cos^2\alpha + \tfrac{1+\epsilon^2}{2}\sin^2\alpha)r'' - g_r(x, r) = 0, \quad x(\infty) = 1, \quad r(\infty) = \sqrt{2}. \end{aligned} \tag{8}$$

Isotropy means that the coefficients here are independent of the orientation $\overline{n}$, i.e., of α. This happens when $\epsilon = 1$; our main interest is the extreme anisotropic case $\epsilon \ll 1$.

As can be easily verified, the gradient flow (4) that determines the full dynamics of the phase field model leaves invariant the subspace of functions

$$S = \{(X(\xi_1, \xi_2, \xi_3), Y(\xi_1, \xi_2, \xi_3), Z(\xi_1, \xi_2, \xi_3)) : Y = Z\}. \tag{9}$$

We remark that each α corresponds to a certain cut of the crystal and the solution of (8) gives the corresponding interface profile. The plot of the energy J for each such profile as a function of the orientation α corresponds to the Frank diagram. The Wulff shape can be identified with the dual set of the convexified Frank diagram.

Remark 1. For notational convenience we will often not write the obvious dependence of functions on $\epsilon > 0$.

2. THE SINGULAR PERTURBATION SYSTEMS

The cases $\alpha = 0$ and $\alpha = \pi/2$ correspond to the distinguished cuts $(1, 0, 0)$ and $(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$. When $\epsilon \ll 1$, the problem for the profile at $\alpha = 0$ or $\alpha = \pi/2$ is a singular perturbation problem from a limit profile at $\epsilon = 0$, "singular" because passing to the limit $\epsilon = 0$ reduces the order of the system (8) from 4 to 2. We now focus on these two cases, which modulo a simple rescaling take the form

$$\begin{aligned} \epsilon^2 x'' &= g_x(x, r), \\ r'' &= g_r(x, r). \end{aligned} \tag{10}$$

$$\begin{aligned} x'' &= g_x(x, r), \\ \epsilon^2 r'' &= g_r(x, r). \end{aligned} \tag{11}$$

We introduce structure assumptions on g that abstract the essential features of (7) discussed above.

2.1. The Structure Hypotheses on g

Let g be a function of two variables with the following features:

(i) Minima. g has three minima on the same level. Thus $(0,0)$, (x_1,r_1), (x_2,r_2) are nondegenerate minima (so $g_{xx}g_{rr}-g_{xr}^2>0$ at each one of them).
(ii) Symmetry. We assume that $g(x,r)=g(x,-r)$. Hence we take $r_2=-r_1$, $x_1>0$, $r_1>0$.
(iii) Level sets. The set $g_x=0$ is connected and smooth and the set $g_r=0$ has a pitchfork structure at $x=x_c$, hence it is not smooth.

In case g has more than three minima we demand $(0,0)$, (x_1,r_1) to be consecutive in the connected level set $g_x=0$. In the figures below we sketch such a surface and the level sets $g_x=0$, $g_r=0$.

The simplest such g should be a fourth order polynomial and by (ii) $g(x,r)=Ax^2+r^2+Bx^3+Cxr^2+Dx^4+Ex^2r^2+Fr^4$.

If further one wants g to be coercive and satisfy $g_{xx}\geqq C_1$ for $x\geqq 0$, $r\in\mathbb{R}$, for some $C_1>0$ then necessary conditions are:

$$A>0,\ \ C<0,\ \ F>0,\ \ C^2>4E,\ \ D>0,\ \ B\geqslant 0.$$

An example of g with the desired behavior is:

$$g(x,r)=x^2+r^2-3xr^2+\frac{1}{2}x^4+\frac{1}{2}x^2r^2+\frac{3}{8}r^4 \tag{12}$$

see [1,2,4]. In this case, we have $(x_1,r_1)=(1,\sqrt{2})$.

2.2. Relationships with Mechanics

Consider systems (10) and (11) above. Then if s stands for time and $(x(s),r(s))$ for position, each system corresponds to Newton's second law for a material point under the potential $-g$ and with very different inertias in the x and r direction, with corresponding Hamiltonians

$$\begin{aligned} H_I(x,r) &= \frac{1}{2}\left(\epsilon^2 x'^2+r'^2\right)-g(x,r),\\ H_{II}(x,r) &= \frac{1}{2}\left(x'^2+\epsilon^2 r'^2\right)-g(x,r) \end{aligned}$$

for (10), and (11), respectevely (Fig. 1).

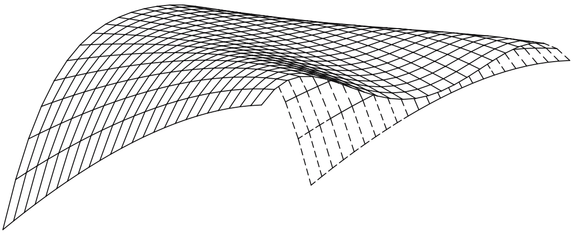

Figure 1. The graph of -g.

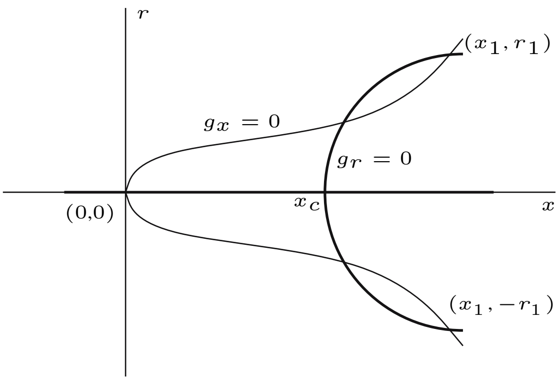

Figure 2. The sets $g_x(x,r)=0$, $g_r(x,r)=0$.

The specific solution we seek to construct, satisfying

$$\lim_{s\to-\infty}(x(s),r(s))=(0,0), \quad \lim_{s\to\infty}(x(s),r(s))=(x_1,r_1) \tag{13}$$

corresponds to a motion which for $s\to\pm\infty$ is asymptotic to the two equal maxima at $(0,0)$ and (x_1,r_1) of the potential energy $-g$. This special solution usually is called a *heteroclinic connection*. The *trajectory*, that is the trace of the solution in the $x-r$ plane, to the first approximation ($\epsilon\ll 1$) should be given by the appropriate pieces of level sets

$$\begin{aligned} g_x &= 0 \quad \text{for (10)},\\ g_r &= 0 \quad \text{for (11)} \end{aligned}$$

shown in Fig. 2.

The question under investigation here is whether such a heteroclinic connection exists for $0<\epsilon\ll 1$.

2.3. The Reduced Systems for $\epsilon = 0$

We begin with system (10). The corresponding system for $\epsilon = 0$ is

$$\begin{aligned} 0 &= g_x(x,r), \\ r'' &= g_r(x,r). \end{aligned} \tag{14}$$

By the implicit function theorem and the structure hypotheses (iii) above $g_x(x,r) = 0$ defines $x = \chi(r)$ with $\chi(0) = 0$ and $\chi(r_1) = x_1$. Hence (14) is reduced to the study of

$$r'' - g_r(\chi(r), r) = 0. \tag{15}$$

We look for a solution to this equation such that $r(-\infty) = 0$, $r(\infty) = r_1$. Setting $G(r) = g(\chi(r), r)$, $r \in \mathbb{R}$ we have

$$G'(r) = g_x(\chi(r), r)\chi'(r) + g_r(\chi(r), r) = g_r(\chi(r), r).$$

Thus (15) can be written as

$$r'' - G'(r) = 0. \tag{16}$$

It can be checked from (i) that $G''(0) > 0$ and $G''(r_1) > 0$ (using also that $\chi'(r) = -\frac{g_{xr}}{g_{xx}}(\chi(r), r)$. Since also $G(0) = G(r_1)$, $G'(0) = G'(r_1) = 0$, and $G(r) - G(0) \neq 0$, $r \in (0, r_1)$, we get [3,7] that in the phase plane (r, r') there is a heteroclinic orbit (r_0, r_0') connecting $(0,0)$ and $(r_1, 0)$. Furthermore this solution is unique up to translation and satisfies $r_0'(s) > 0$, $s \in \mathbb{R}$. Let $x_0 := \chi(r_0)$, then $(x_0, r_0) \in C^2(\mathbb{R}) \times C^2(\mathbb{R})$ solves (14), (13) with $\epsilon = 0$.

***Theorem* 1.** [2]. *If $\epsilon > 0$ is sufficiently small and g is given by* (12)*, then there exists a solution $(x_\epsilon, r_\epsilon) \in C^2(\mathbb{R}) \times C^2(\mathbb{R})$ of* (10)*, and* (13) *such that*

$$\epsilon ||x_\epsilon' - x_0'||_{L^2(\mathbb{R})} + ||x_\epsilon - x_0||_{L^2(\mathbb{R})} + ||r_\epsilon - r_0||_{H^1(\mathbb{R})} \leqslant C\epsilon^2$$

and the linear operator

$$L_\epsilon \begin{pmatrix} x \\ r \end{pmatrix} = \begin{pmatrix} -\epsilon^2 x'' + g_{xx}(x_\epsilon, r_\epsilon)x + g_{xr}(x_\epsilon, r_\epsilon)r \\ -r'' + g_{xr}(x_\epsilon, r_\epsilon)x + g_{rr}(x_\epsilon, r_\epsilon)r \end{pmatrix}$$

satisfies $\sigma(L_\epsilon) \subset \{0\} \cup [c, \infty)$ with 0 a simple eigenvalue. ($C, c > 0$ *are constants independent of* $\epsilon > 0$).

Remark 2. As it can be verified from the proof which is based on the contraction mapping principle, the above theorem also holds for a function g satisfying (H1), (H2), (H3), (H4) below.

Next we turn to system (11). The corresponding system for $\epsilon = 0$ is

$$\begin{aligned} x'' &= g_x(x, r), \\ 0 &= g_r(x, r). \end{aligned} \tag{17}$$

By the structure hypothesis (iii) the second equation renders $r = R(x) \geqslant 0$ that is only Hölder continuous. For the example (12)

$$R(x) = \begin{cases} 0, & x \leqslant x_c, \\ \sqrt{\dfrac{-(x-x_c)^2 + b(x-x_c)}{a}}, & x_c < x < x_1 + \delta, \end{cases}$$

for some $a, b > 0$.

Setting $\hat{G}(x) = g(x, R(x))$ we can check that $\hat{G}''$ exists also at $x = x_c^-, x_c^+$, although $\hat{G}$ is not C^2 there.We have that

$$\hat{G}'(x) = \begin{cases} g_x(x, R(x)) + g_r(x, R(x))R'(x) = g_x(x, R(x)), & x \neq x_c, \\ g_x(x_c, 0), & x = x_c. \end{cases}$$

Hence (17) is reduced to the study of

$$x'' - \hat{G}'(x) = 0. \tag{18}$$

Note that $\hat{G}(0) = g(0,0)$, $\hat{G}(x_1) = g(x_1, r_1)$ and G is a double well potential with equal global minima at $x = 0$ and $x = x_1$ and smooth at 0 and x_1. As before (18) has a unique heteroclinic solution $x_0(s)$ with $x_0(-\infty) = 0$, $x_0(\infty) = x_1$, $x_0(0) = x_c$ and it is monotonically increasing. Let $r_0 := R(x_0)$, then $(x_0, r_0) \in C^2(\mathbb{R}) \times C(\mathbb{R})$ solves (17) and (13).

***Theorem* 2.** [10]. *If $\epsilon > 0$ is sufficiently small and g is given by* (12)*, then there exists a solution $(x_\epsilon, r_\epsilon) \in C^2(\mathbb{R}) \times C^2(\mathbb{R})$ of* (11)*, and* (13) *such that*

$$||x_\epsilon - x_0||_{H^2(\mathbb{R})} + \epsilon^{1/3}||r_\epsilon - r_0||_{L^2(\mathbb{R})} + \epsilon^{2/3}||r_\epsilon - r_0||_{L^\infty(\mathbb{R})} \leqslant C\epsilon$$

($C > 0$ independent of $\epsilon > 0$).

Remark 3. As it can be verified from the proof which is based on the contraction mapping principle, the above theorem also holds for a more general class of functions g.

Remark 4. A similar result appears in [6]. There a shooting type-argument is used. This produces a solution (x_ϵ, r_ϵ) of (11) and (13) (with g given by (12)) that converges to (x_0, r_0) as $\epsilon \to 0$, although less information about this convergence was obtained.

Problem (11) is significantly harder than (10) because of the limited smoothness of the level set $g_r = 0$ and it will not be considered here. Problem (10) fits the framework of the geometric singular perturbation theory and is the object of the following section. See [8, 11] for other applications of the geometric method.

3. THE EXISTENCE PROOF

We study system (19)

$$\begin{aligned} \epsilon^2 x'' &= g_x(x,r), \\ r'' &= g_r(x,r) \end{aligned} \tag{19}$$

under the following hypotheses on g:

(H1): $g \in C^m(\mathbb{R} \times \mathbb{R})$ (for simplicity), $m \geqslant 2$, $(0,0)$ and (x_1, r_1) ($x_1, r_1 > 0$ for simplicity) are nondegenerate minima of g (so $g_{xx} g_{rr} - g_{xr}^2 > 0$ at $(0,0)$ and (x_1, r_1)) and $g(0,0) = g(x_1, r_1)$.
(H2): There exists a C^m function $\chi : I \to \mathbb{R}$ with $[0, r_1] \subset I$, such that:

$$g_x(\chi(r), r) = 0, \quad r \in I, \quad \chi(0) = 0, \quad \chi(r_1) = x_1.$$

(H3): $g_{xx}(\chi(r), r) \geqslant C_1 > 0, \; r \in I$.
(H4): $g(\chi(r), r) - g(0,0) \neq 0, \quad r \in (0, r_1)$.

This can be viewed as a singular perturbation of the $\epsilon = 0$ system

$$\begin{aligned} 0 &= g_x(x,r), \\ r'' &= g_r(x,r) \end{aligned} \tag{20}$$

which may be called the reduced problem.

In the following we will be using well known work of Fenichel [5] to obtain an invariant manifold M_ϵ for (19), $\epsilon > 0$, which depends in a smooth way on ϵ, the smoothness extended all the way to $\epsilon = 0$. In particular, the $\lim_{\epsilon \to 0} M_\epsilon = M_0$ is meaningful and the set M_0 is given by (a compact piece of)

$$M_0 = \{(x,r) : g_x(x,r) = 0\}. \tag{21}$$

For applying this theory, there are two hypotheses that have to be verified:

(1) The set M_0 should have a degree of smoothness.
(2) The set M_0 should be normally hyperbolic.

After verifying these hypotheses and thus obtaining the invariant manifold M_ϵ, we proceed to examine the problem of the existence of the heteroclinic connection stated in Theorem 4: There exists $(x(s), r(s))$ solution of (19), satisfying

$$\lim_{s\to-\infty}(x(s), r(s)) = (0,0), \qquad \lim_{s\to\infty}(x(s), r(s)) = (x_1, r_1). \tag{22}$$

The benefit of this kind of result is twofold. First, we achieve the reduction of problem (19) on the manifold M_ϵ, a lower dimensional object. Second, the regular dependence on ϵ all the way to $\epsilon = 0$ allows, for a regular perturbation argument that takes advantage of the existence of such heteroclinic connections for system (20).

The perturbation of a heteroclinic connection in general does not render a heteroclinic connection. However for the problem at hand, the Hamiltonian structure of (19) plays a crucial role and provides a heteroclinic connection, thus a solution satisfying (22).

We now present the details. For Fenichel's work, we refer to [5,9,11, 13] and the article by Jones [8]. For studying (19) in regions where x varies rapidly, we shall sometimes use the (fast) independent variable

$$\zeta = \frac{s}{\epsilon}, \qquad {}^{\cdot} = \frac{d}{d\zeta}.$$

In this variable we obtain the system equivalent (when $\epsilon > 0$) to (19)

$$\begin{aligned} \ddot{x} &= g_x(x, r), \\ \ddot{r} &= \epsilon^2 g_r(x, r). \end{aligned} \tag{23}$$

The corresponding systems of equations are obtained by setting $u_1 = x$, $u_2 = \epsilon x'$, $u_3 = r$, $u_4 = r'$. Thus (19), (20), (23) become

$$\begin{aligned} \epsilon u_1' &= u_2, \\ \epsilon u_2' &= g_x(u_1, u_3), \\ u_3' &= u_4, \\ u_4' &= g_r(u_1, u_3), \end{aligned} \tag{24}$$

$$\begin{aligned} 0 &= u_2, \\ 0 &= g_x(u_1, u_3), \\ u_3' &= u_4, \\ u_4' &= g_r(u_1, u_3), \end{aligned} \tag{25}$$

$$\begin{aligned} \dot{u}_1 &= u_2, \\ \dot{u}_2 &= g_x(u_1, u_3), \\ \dot{u}_3 &= \epsilon u_4, \\ \dot{u}_4 &= \epsilon g_r(u_1, u_3) \end{aligned} \tag{26}$$

and

$$\begin{aligned}\dot{u}_1 &= u_2,\\ \dot{u}_2 &= g_x(u_1, u_3),\\ \dot{u}_3 &= 0,\\ \dot{u}_4 &= 0,\end{aligned} \qquad \text{corresponds to} \qquad \begin{aligned}\ddot{x} &= g_x(x, r),\\ \ddot{r} &= 0.\end{aligned} \tag{27}$$

Now M_0 is defined as the set of equilibria of (27):

$$M_0 = \{(u_1, u_2, u_3, u_4)\,|u_2 = 0,\ u_1 = \chi(u_3),\ u_3 \in I\}.$$

We can represent M_0 as the graph of a C^m function $(u_1, u_2) = h^0(u_3, u_4)$, where $h^0(u_3, u_4) = (\chi(u_3), 0)$.

We now check the normal hyperbolicity of M_0 in the context of (27). Thus we consider the linearized operator about a point on M_0, namely

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ g_{xx} & 0 & g_{xr} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

where $g_{xx},\ g_{xr}$ are evaluated at $(\chi(u_3), u_3)$. Its eigenvalues are determined by

$$\lambda^2(\lambda^2 - g_{xx}) = 0$$

from which we find that $\lambda = 0$ (double) and $\lambda = \pm\sqrt{g_{xx}}$. Recall that $g_{xx}(\chi(u_3), u_3) \geq C_1 > 0$ by (H3). Thus M_0 is normally hyperbolic, i.e. there are only the two zero eigenvalues on the imaginary axis. We remark that the matrix A is simplectic, a reflection of the Hamiltonian character of (19) (to be exploited later), and so its spectrum should not come as a surprise. The following theorem (see [11]) can therefore be applied:

***Theorem* 3.** (Fenichel). *Under the hypotheses of C^m smoothness and normal hyperbolicity of M_0, for a given compact subset K of the (u_3, u_4) plane, there is a function $h(u_3, u_4, \epsilon)$, and an $\epsilon_0 = \epsilon_0(m, K)$ so that for $0 < \epsilon < \epsilon_0$ the graph*

$$M_\epsilon = \{(u_1, u_2, u_3, u_4)|\,(u_1, u_2) = h(u_3, u_4, \epsilon),\ (u_3, u_4) \in K\} \tag{28}$$

is locally invariant under (26). *Furthermore*

$$h : K \times [0, \epsilon_0) \longrightarrow \mathbb{R}^2 \text{ is } C^{m-1},\ \textit{jointly in } (u_3, u_4, \epsilon), \tag{29}$$

and

$$h(u_3, u_4, 0) = h^0(u_3, u_4), \quad (u_3, u_4) \in K. \tag{30}$$

Here $\epsilon_0 > 0$ is a generally small number, and h^0 was defined previously in relation to M_0.

The manifold M_ϵ is center-like for (26) and (24) and generally not unique. The compact set K will be chosen later. Note that $(0,0,0,0)$ and $(x_1,0,r_1,0)$ are still equilibria of (26) for small $\epsilon>0$, and thus they lie on M_ϵ. This is because every invariant set of (26) in a sufficiently small ϵ-independent neighborhood of M_0 must be on M_ϵ, see [5]. Linearizing (26) and evaluating at $(0,0,0,0)$, we find

$$A_\epsilon(0,0,0,0)=\begin{bmatrix} 0 & 1 & 0 & 0 \\ g_{xx} & 0 & g_{xr} & 0 \\ 0 & 0 & 0 & \epsilon \\ \epsilon g_{xr} & 0 & \epsilon g_{rr} & 0 \end{bmatrix}$$

with g_{xx}, g_{xr}, g_{rr}, evaluated at $(0,0)$. The eigenvalues of $A_\epsilon(0,0,0,0)$ are determined by $\lambda^4-(\epsilon^2 g_{rr}+g_{xx})\lambda^2+\epsilon^2(g_{xx}g_{rr}-g_{xr}^2)=0$. Hence, using (H1), if ϵ sufficiently small, we get four real eigenvalues $\lambda_1=O(1)>0$, $\lambda_2=-\lambda_1$, $\lambda_3=O(\epsilon)>0$, $\lambda_4=-\lambda_3$. The first two eigenvalues correspond to motion normal to M_ϵ, and the latter two correspond to motion on M_ϵ. The dynamics within M_ϵ therefore has a saddle point at the origin with one dimensional stable and unstable manifolds $W_\epsilon^s(0,0,0,0)$, $W_\epsilon^u(0,0,0,0)$ (*on* M_ϵ). Note that these manifolds are the intersection of the two-dimensional stable/unstable manifolds of $(0,0,0,0)$ with M_ϵ.

These same calculations also hold at the other critical point $(x_1,0,r_1,0)$, and thus it is a saddle with respect to the dynamics on M_ϵ with one-dimensional stable/unstable manifolds $W_\epsilon^s(x_1,0,r_1,0)$, $W_\epsilon^u(x_1,0,r_1,0)$ (*on* M_ϵ).

Our strategy for proving the existence of a heteroclinic orbit connecting $(0,0,0,0)$ and $(x_1,0,r_1,0)$ is based on showing that *on* M_ϵ the unstable manifold of one of the equilibria meets the stable manifold of the other, and thus, since they are one-dimensional, they have to coincide.

We will be establishing the following

***Theorem* 4.** *For each ϵ sufficiently small, there is a heteroclinic orbit of (24) connecting the critical points* $(0,0,0,0)$, $(x_1,0,r_1,0)$ *which lies on* M_ϵ, *and hence is* $O(\epsilon)$ *away from* M_0. *Moreover along the orbit we have the relations*

$$\begin{aligned} u_1&=\chi(u_3)+O(\epsilon),\\ u_2&=\epsilon\chi'(u_3)u_4+O(\epsilon^2). \end{aligned} \tag{31}$$

Proof. We begin by deriving the equations on M_ϵ. By (28), (29), (30) we have

$$\begin{aligned} u_1&=\chi(u_3)+\epsilon h_1(u_3,u_4,\epsilon),\\ u_2&=\epsilon h_2(u_3,u_4,\epsilon). \end{aligned}$$

□

From the invariance of M_ϵ we obtain

$$\epsilon h_2(u_3,u_4,\epsilon)=u_2=\epsilon u_1'=\epsilon\left[\chi'(u_3)u_3'+\epsilon\frac{\partial h_1}{\partial u_3}u_3'+\epsilon\frac{\partial h_1}{\partial u_4}u_4'\right].$$

Thus (31) follows.

The flow on M_ϵ is given by

$$\begin{aligned} u_3' &= u_4,\\ u_4' &= g_r(\chi(u_3)+O(\epsilon),u_3). \end{aligned} \tag{32}$$

There exists $u_3^0\in(0,r_1)$ such that

$$\chi'(u_3^0)>0.$$

In the (u_3,u_4) plane, let

$$C_\epsilon=\left\{(u_3,u_4):\chi(u_3)+O(\epsilon)=\chi(u_3^0)\right\},$$

where $O(\epsilon)$ refers to the corresponding term in (32). When $\epsilon=0$, there is a heteroclinic orbit (r_0,r_0') of (32) connecting $(0,0)$ to $(r_1,0)$ with $r_0'>0$, intersecting transversally C_0 at a point (u_3^0,u_4^0) (this follows from (H1),(H2),(H3),(H4) as in (16)) (see Fig. 3).

We shall choose K to be a large compact connected set in the (u_3,u_4) plane with the above mentioned heteroclinic orbit in its interior. When $\epsilon>0$ is sufficiently small, then $(0,0)$ and $(r_1,0)$ remain saddles of (32) (since equilibria of (32) give equilibria of (24)). Also their unstable/stable manifolds $W_\epsilon^u(0,0)/W_\epsilon^s(r_1,0)$ depend smoothly on $\epsilon\geq 0$ and intersect C_ϵ at $(u_{3,\epsilon}^-,u_{4,\epsilon}^-)/(u_{3,\epsilon}^+,u_{4,\epsilon}^+)$ with $u_{i,\epsilon}^j\to u_i^0$ as $\epsilon\to 0$, $i=3,4$, $j=-,+$. This

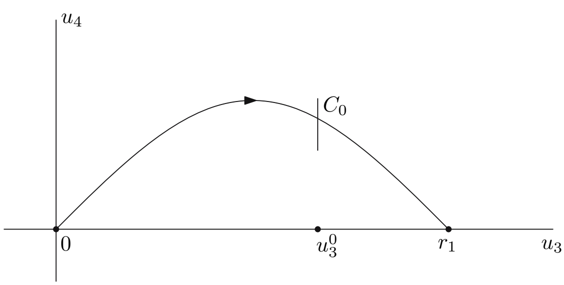

Figure 3. The heteroclinic orbit (r_0,r_0').

is a consequence of the implicit function theorem and $\chi'(u_3^0) > 0$. Indeed, $(u_{3,\epsilon}^-, u_{4,\epsilon}^-)$ is a solution of

$$\begin{aligned} &\chi(u_3) + O(\epsilon) = \chi(u_3^0), \\ &u_4 = h^u(u_3, \epsilon), \end{aligned} \tag{33}$$

where $(u_3, h^u(u_3, \epsilon))$, $u_3 \in (u_3^0 - \delta, u_3^0 + \delta)$ ($\delta > 0$ a small number independent of $\epsilon \geq 0$) is a parametrization of $W_\epsilon^u(0,0)$, $\epsilon \geq 0$. The same holds for $(u_{3,\epsilon}^+, u_{4,\epsilon}^+)$.

To conclude, we will be utilizing the Hamiltonian structure of (24). Notice that (24) can be written in the form

$$\begin{aligned} \epsilon u_1' &= \frac{\partial H}{\partial u_2}, \\ u_3' &= \frac{\partial H}{\partial u_4}, \\ \epsilon u_2' &= -\frac{\partial H}{\partial u_1}, \\ u_4' &= -\frac{\partial H}{\partial u_3}, \end{aligned} \tag{34}$$

where

$$H(u_1, u_3, u_2, u_4) = \frac{1}{2}(u_2^2 + u_4^2) - g(u_1, u_3).$$

Thus the solutions of (34) lie on level sets of H. Let now $U_\epsilon^-(s), U_\epsilon^+(s)$ be solutions of (24) parameterizing $W_\epsilon^u(0,0,0,0)$ and $W_\epsilon^s(x_1, 0, r_1, 0)$ with $U_\epsilon^\pm(0) = (\chi(u_3^0), u_{2,\epsilon}^\pm, u_{3,\epsilon}^\pm, u_{4,\epsilon}^\pm) \in M_\epsilon$, i.e., $U_\epsilon^\pm(s) = (u_1^\pm(s), u_2^\pm(s), u_3^\pm(s), u_4^\pm(s))$. Recall that $W_\epsilon^u(0,0,0,0) \setminus W_\epsilon^s(x_1, 0, r_1, 0)$ is the image of $W_\epsilon^u(0,0) \setminus W_\epsilon^s(r_1, 0)$ on M_ϵ.

We claim that $u_{i,\epsilon}^- = u_{i,\epsilon}^+$, $i = 2, 3, 4$, from which it will follow that $U_\epsilon^- \equiv U_\epsilon^+$. Notice that we want to determine three variables, although (31) with (33) furnishes only two equations. The third equation is provided by the Hamiltonian, via the fact that $(0,0)$ and (x_1, r_1) are minima of equal energy for g by (H1). Thus $H(0,0,0,0) = H(x_1, r_1, 0, 0) = -g(0,0)$, and consequently

$$H(\chi(u_3^0), u_{3,\epsilon}^-, u_{2,\epsilon}^-, u_{4,\epsilon}^-) = H(\chi(u_3^0), u_{3,\epsilon}^+, u_{2,\epsilon}^+, u_{4,\epsilon}^+) = -g(0,0).$$

Collecting all the equations together, we have that $(u_{2,\epsilon}^\pm, u_{3,\epsilon}^\pm, u_{4,\epsilon}^\pm)$ both solve

$$\begin{aligned} \chi(u_3^0) - (\chi(u_3) + \epsilon h_1(u_3, u_4, \epsilon)) &= 0, \\ u_2 - (\epsilon \chi'(u_3) u_4 + O(\epsilon^2)) &= 0, \\ g(\chi(u_3^0), u_3) - \tfrac{1}{2}(u_2^2 + u_4^2) &= g(0,0). \end{aligned} \tag{35}$$

But via the implicit function theorem, for $\epsilon > 0$ sufficiently small (35) has a unique solution in a neighborhood of $(0, u_3^0, u_4^0)$ (since $\chi'(u_3^0)u_4^0 > 0$), i.e., $U_\epsilon^-(0) = U_\epsilon^+(0)$. Thus

$$U_\epsilon(s) = \begin{cases} U_\epsilon^-(s), & s \leq 0, \\ U_\epsilon^+(s), & s \geq 0, \end{cases}$$

is the required heteroclinic orbit of (24). This completes the proof of Theorem 4. □

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