A phase plane analysis of a corner layer problem arising in the study of crystalline grain boundaries

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1 Preliminaries

We study the heteroclinic connections described in [1], which are based on the multiparameter phase field model in [6, 2, 3]. Such heteroclinics represent, in that model, interfacial profiles in a highly anisotropic FCC crystal. They are governed by the singularly perturbed equations:

$$\begin{aligned} \ddot{x} &= g_x(x,r) \\ \epsilon^2 \ddot{r} &= g_r(x,r). \end{aligned} \tag{1}$$

The right sides are given by (5), (6). Here derivatives are with respect to the space variable z measuring distance normal to the grain boundary, but we shall generally prefer to use the fast independent variable $\zeta = \frac{z}{\epsilon}$. Denoting derivatives with respect to ζ by primes, we obtain the system

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

The corresponding system of first order equations is obtained by setting $x_1 = x, \quad x_2 = x'$, etc.

$$\begin{aligned} x_1' &= \epsilon x_2 \\ x_2' &= \epsilon g_x(x_1, r_1) \\ r_1' &= r_2 \\ r_2' &= g_r(x_1, r_1). \end{aligned} \tag{3}$$

We shall use the vector notation

$$U = \begin{bmatrix} x_1 \\ x_2 \\ r_1 \\ r_2 \end{bmatrix}.$$

We look for a heteroclinic solution, satisfying

$$U(-\infty) = 0, \quad U(\infty) = U_c \equiv \begin{bmatrix} 1 \\ 0 \\ \sqrt{2} \\ 0 \end{bmatrix} \tag{4}$$

For reference, note

$$g_x = 4x - 6r^2 + 2xr^2 + 4x^3, \quad g_{xx} = 4 + 2r^2 + 12x^2 \geq 4, \tag{5}$$

$$g_r = r(4 - 12x + 2x^2 + 3r^2) = 3r(r^2 - p(x)), \quad p(x) = -\frac{4}{3} + 4x - \frac{2}{3}x^2, \tag{6}$$

$$g_{rr} = 4 - 12x + 2x^2 + 9r^2 = 3(3r^2 - p(x)), \quad g_{xr} = -4r(3 - x) \leq 0. \tag{7}$$

Note that $p(x) < 0$ for $x \in [0, x_c)$ and > 0 for $x \in (x_c, 3)$. Here $x_c = 3 - \sqrt{7} \approx .35$.

We have the manifold M_0 of critical points

$$M_0 = \{r = 0,\ 0 \leq x \leq x_c\} \cup \{r = \sqrt{p(x)},\ x_c \leq x \leq 1\}.$$

Our object is to prove

Theorem 1 *For each small enough $\epsilon > 0$, there exists a heteroclinic solution of (3), (4). The projection of its trajectory in the (x, r) plane can be expressed as $r = R(x, \epsilon) \geq 0$ where, for every fixed $\delta > 0$, and some constants c and C depending on δ,*

(a) $R(x, \epsilon) \geq 0$ is exponentially small as a function of ϵ, uniformly for $x \in [0, x_c - \delta]$.

(b) $c\epsilon^{1/3} < R(x_c, \epsilon) < C\epsilon^{1/3}$,

(c) $|R(x, \epsilon) - \sqrt{p(x)}| < C\epsilon$, uniformly for $x \in [x_c + \delta, 1]$.

Note More accurate estimates for the discrepancy $|R(x, \epsilon) - R(x, 0)|$, where $R(x, 0) = \max{[0, \sqrt{p(x)}]}$, can be obtained from the proofs.

The trajectory of any solution is a curve in 4D space; however when the context is appropriate, we shall also use the word "trajectory" to mean the projection of a 4D trajectory onto the (x, r) plane.

We consider the linearization of (3) about a critical point U^0. The Jacobian matrix is

$$A_\epsilon(U^0) = \begin{bmatrix} 0 & \epsilon & 0 & 0 \\ \epsilon g_{xx}(x_1^0, r_1^0) & 0 & \epsilon g_{xr}(x_1^0, r_1^0) & 0 \\ 0 & 0 & 0 & 1 \\ g_{rx}(x_1^0, r_1^0) & 0 & g_{rr}(x_1^0, r_1^0) & 0 \end{bmatrix}. \tag{8}$$

Its eigenvalues satisfy

$$D_\epsilon(\lambda) \equiv (\lambda^2 - \epsilon^2 g_{xx})(\lambda^2 - g_{rr}) + \epsilon^2 g_{xr}^2 = 0. \tag{9}$$

Throughout the paper, we shall usually simply use the symbols x and r in place of x_1 and r_1. We consider only values of x in the interval $[0, 3)$.

Let

$$\psi(x) = \frac{2x(1 + x^2)}{3 - x}. \tag{10}$$

Then $g_x \geq 0$ for $r^2 \leq \psi(x)$; $g_x < 0$ otherwise.

We use the following notation in our estimates. The symbols c and C will denote positive constants which are independent of ϵ, k, x, r and whose values change from line to line. The relation

$$a \approx b$$

means that there are constants c and C, as described above, such that

$$c \leq \frac{a}{b} \leq C.$$

Here a and b may depend on ϵ, in which case the inequality is assumed to hold when ϵ is small enough.

2 Solutions linking the origin with $\{x = x_c\}$

2.1 Solutions near the origin

At the origin $U^0 = 0$, we have

$$A_\epsilon(0) = \begin{bmatrix} 0 & \epsilon & 0 & 0 \\ 4\epsilon & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 4 & 0 \end{bmatrix}, \tag{11}$$

with eigenvalues

$$\lambda = \pm 2\epsilon, \quad \pm 2. \tag{12}$$

We look at the unstable (positive) eigenvalues. We call the eigenvectors corresponding to $\lambda = 2\epsilon$ slow, and the ones with $\lambda = 2$ fast. Convenient choices are

$$\text{fast:} \quad \phi_f = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 2 \end{bmatrix} \tag{13}$$

$$\text{slow:} \quad \phi_s = \begin{bmatrix} 1 \\ 2 \\ 0 \\ 0 \end{bmatrix}. \tag{14}$$

The unstable manifold $W^u(0)$ is 2-dimensional, tangent at 0 to span$\{\phi_f, \phi_s\}$.

The one-parameter family of trajectories leaving the origin in a direction such that x is increasing can be realized, using μ as a real parameter, by the solutions whose behavior as $\zeta \to -\infty$ is given by

$$U(\zeta, \mu) \approx \phi_s e^{2\epsilon\zeta} + \mu \phi_f e^{2\zeta}. \tag{15}$$

We denote the components of these solutions by $x_1(\zeta, \mu)$, etc.

The particular solution $U(\zeta, 0)$ can be identified, since $r_1 \equiv r_2 \equiv 0$ satisfies the last two equations of (3). Namely, we have that when $\mu = 0$,

$$\begin{aligned} x_1' &= \epsilon x_2 \\ x_2' &= \epsilon g_x(x_1, 0) = 4\epsilon x_1(1 + x_1^2) \\ r_1 &\equiv r_2 \equiv 0 \end{aligned} \tag{16}$$

We will mainly focus attention on values $\mu \geq 0$.

2.2 Linking to $\{x = x_c\}$

Theorem 2 *There exists a continuous family $U^-(\zeta, r^*)$ of solutions of (3) defined for $0 \leq r^* \leq .3$, $\zeta \leq 0$, satisfying*

$$\begin{gathered} U^-(-\infty, r^*) = 0, \quad x^-(0, r^*) = x_c, \quad r^-(0, r^*) = r^*, \\ (x^-)'(\zeta, r^*) \geq 0, \quad (r^-)'(\zeta, r^*) \geq 0, \quad (r^-)''(\zeta, r^*) \geq 0. \end{gathered} \tag{17}$$

Also

$$x_c \exp(\sqrt{2}\,\epsilon\,\zeta) \geq x^-(\zeta, r^*) \geq x_c \exp(\sqrt{5}\,\epsilon\,\zeta), \quad \zeta \leq 0. \tag{18}$$

and

$$\sqrt{2}\,\epsilon x_c \leq (x^-)'(0, r^*) \leq \sqrt{5}\,\epsilon x_c. \tag{19}$$

Proof We consider trajectories lying in the region

$$Q_0 \equiv \{0 \le x \le x_c, \quad x \ge 3r^2\}. \tag{20}$$

We assume this inequality in making the estimates, and then verify that indeed our functions lie in Q_0.

Our solutions will belong to the family $U(\zeta, \mu)$ (15), with the variable ζ translated so that $x = x_c$ when $\zeta = 0$.

It may be checked that $r^2 \le \psi(x)$ for points in Q_0 (10), so that $g_x > 0$ and (3) $x_2' > 0$ there. From (15), (13), (14), $x_1(\zeta, \mu)$ and $x_2(\zeta, \mu) > 0$ for large negative ζ, so continue positive and bounded away from 0 as long as the solution's (projected) trajectory remains in Q_0. In particular, this is the case, by continuity, for small $\mu \ge 0$, since $r = 0$ when $\mu = 0$.

Therefore the trajectory intersects the line $\{x = x_c\}$, unless it first leaves Q_0.

Again, since $r'' = g_r \ge 0$ in Q_0 and r and r' begin positive when ζ is large negative, r and r' are increasing in ζ. Therefore $r(\zeta, \mu) > 0$ for $\mu > 0$ and r attains its maximum at $\zeta = 0$. It can be shown that $r^*(\mu) = r|_{x=x_c}$ is strictly monotone in μ, so that $r^*(\mu)$ may be used as alternate parameter in place of μ. This monotonicity relies on the facts that g_r is an increasing function of r and a decreasing function of x, while g_x is just the opposite. We write $U^-(\zeta, r^*)$, $x^-(\zeta, r^*)$, etc. Also, (x, r) remains in Q_0 for $\zeta \le 0$ as long as (x_c, r^*) does, and that is the case when $r^* \le .3$. Therefore the set of values of r on trajectories when $x = x_c$ fills out an interval as described. The estimates (18) and (19) will be established below.

2.3 Estimates for $x(\zeta)$

Recall that $x^-(0, r^*) = x_c$.

From (5) and (20), $g_x(x, r) = x(4 + 2r^2 + 4x^2) - 6r^2 \ge 4x - 6r^2 \ge 2x$. Also $g_x(x, r) \le 5x$, so that in all,

$$2x \le g_x(x, r) \le 5x. \tag{21}$$

From (2), $x(\zeta) = x^-(\zeta, r^*)$ satisfies

$$x'' = \epsilon^2 g_x, \quad x(-\infty) = 0, \quad x(0) = x_c. \tag{22}$$

Denote by $\overline{x}(\zeta)$ the solution of (22) with g_x replaced by $2x$, and the same boundary conditions:

$$\overline{x}(\zeta) = x_c \exp(\sqrt{2}\, \epsilon\zeta). \tag{23}$$

Then by (21), it will be a supersolution lying above the exact solution. The opposite happens when we replace g_x by $5x$. Thus (18) holds.

Since equality in (18) holds at $\zeta = 0$, (19) follows. This completes the proof of Theorem 2.

3 Trajectories linking $\{x = x_c\}$ to U_c.

We are interested in trajectories connecting to the critical point $U = U_c$ from the hyperplane $\{x_1 = x_c\}$.

3.1 Solutions approaching U_c

The linearization of (3) about $U = U_c$ yields

$$\tilde{U}' = A_\epsilon(U_c)\tilde{U}, \tag{24}$$

where (8)

$$A_\epsilon(U_c) = \begin{bmatrix} 0 & \epsilon & 0 & 0 \\ 20\,\epsilon & 0 & -8\sqrt{2}\,\epsilon & 0 \\ 0 & 0 & 0 & 1 \\ -8\sqrt{2} & 0 & 12 & 0 \end{bmatrix} \tag{25}$$

The eigenvalues of this linearization are

$$\lambda = \pm\sqrt{12} + O(\epsilon), \quad \pm\sqrt{28/3}\,\epsilon + O(\epsilon^2). \tag{26}$$

We are interested in the stable manifold of U_c, which by (26) is two-dimensional. There are two stable eigenvectors, a fast one ψ_f corresponding to $\lambda = -\sqrt{12} + O(\epsilon)$ and a slow one ψ_s corresponding to $\lambda = -\sqrt{28/3}\,\epsilon + O(\epsilon^2)$:

$$\text{fast:} \;\; \psi_f = \begin{bmatrix} 0 \\ 0 \\ -1 \\ \sqrt{12} \end{bmatrix} + O(\epsilon) \tag{27}$$

$$\text{slow:} \;\; \psi_s = \begin{bmatrix} -1 \\ \sqrt{28/3} \\ -\frac{2\sqrt{2}}{3} \\ 0 \end{bmatrix} + O(\epsilon). \tag{28}$$

The trajectories on the stable manifold may be parameterized by a single real parameter ν and realized by the solutions which have the following behavior for large ζ:

$$U(\zeta,\nu) \approx U_c + \psi_s \exp\left(\left(-\sqrt{28/3} + O(\epsilon)\right)\,\epsilon\zeta\right) + \nu\psi_f \exp\left(\left(-\sqrt{12} + O(\epsilon)\right)\zeta\right). \tag{29}$$

3.2 Linking solutions

Our object here is to prove the existence of trajectories on the stable manifold $W^s(U_c)$ whose projections onto the (x,r) plane intersect arbitrary points with $0 \le r \le O(\epsilon^{1/3})$ and $x = x_c$.

We shall also show that these (projected) trajectories lie close to the curve $\{r = \sqrt{p(x)} \equiv R_0(x)\}$, the distance from that curve being $O(\epsilon)$ except for $r \le O(\epsilon^{1/3})$.

To prove this, we use an ϵ-dependent closed set Ω in the (x,r) plane, in which all trajectories on $W^s(U_c)$ are guaranteed to lie for large ζ, and into which every trajectory on that manifold enters transversally for some finite ζ. Every point on a section of the boundary $\partial\Omega$ is therefore an entry point for some trajectory. This includes all points on $\{x = x_c,\; 0 < r < O(\epsilon^{1/3})\}$.

Lemma 1 *For some $\delta > 0$ and some x_0, let $R(x)$ be a smooth function of x, defined for $x \in (x_0 - \delta, x_0 + \delta)$ with $R'(x) > 0$. Let $\Gamma = \{(x,r) : r = R(x),\; x \in (x_0 - \delta, x_0 + \delta)\}$, and S_r be the right neighborhood of Γ with width δ: $S_r = \Gamma + ([0,\delta], 0)$. Let S_l be the similarly defined left neighborhood.*

Let T be (the projection onto the (x, r) plane of) a trajectory of (3), which intersects Γ at the point (x_0, r_0) when $\zeta = \zeta_0$. Also, $x'(\zeta_0) \neq 0$.

(a) Assume, at the point $\zeta = \zeta_0$ $(x = x_0,\ r = r_0)$, that

$$g_r - \epsilon^2 R' g_x > (x')^2 R''. \tag{30}$$

If, for some $\delta_1 > 0$, T lies in S_r either for $\zeta \in [\zeta_0, \zeta_0 + \delta_1]$ or for $\zeta \in [\zeta_0 - \delta_1, \zeta_0]$, then T crosses Γ transversally at (x_0, r_0).

(b) Assume, at the point $\zeta = \zeta_0$, that

$$g_r - \epsilon^2 R' g_x < (x')^2 R''. \tag{31}$$

If, for some $\delta_1 > 0$, T lies in S_l either for $\zeta \in [\zeta_0, \zeta_0 + \delta_1]$ or for $\zeta \in [\zeta_0 - \delta_1, \zeta_0]$, then T crosses Γ transversally at (x_0, r_0).

Proof Consider case (a), so that (30) holds. Let $m(\zeta) = \frac{r'(\zeta)}{x'(\zeta)}$ be the slope of T. We calculate

$$m'(\zeta) = \frac{d}{d\zeta}\left(\frac{r'}{x'}\right) = \frac{r''x' - x''r'}{(x')^2}$$

and from this and (2),

$$\frac{dm}{dx} = \frac{m'(\zeta)}{x'(\zeta)} = \frac{r''x' - x''r'}{(x')^3} = \frac{g_r - \epsilon^2 g_x m}{(x')^2}. \tag{32}$$

Assume the assertion of transversality is not true. Then T is tangent to Γ at (x_0, r_0), so that at that point, $m = R'$. Hence from (32) and (30), we obtain, again at (x_0, r_0),

$$\frac{dm}{dx} = \frac{g_r - \epsilon^2 g_x R'}{(x')^2} > R''. \tag{33}$$

This inequality implies that T lies in the interior of S_l for all $\zeta \neq \zeta_0$ close to ζ_0 on either side of ζ_0, which contradicts the assumption following (30) and proves part (a) with (30). Part (b) is proved in the analogous manner.

We proceed by defining a closed region Ω in the (x, r) plane, whose boundary consists of several pieces Γ_i. In the following, $R_0(x) = \sqrt{p(x)}$ (6) and the number m_1 and points $(\tilde{x}, \tilde{r})$ and $(\bar{x}, \bar{r})$ will be defined below. The number k will be chosen large enough, as explained later, independently of ϵ.

$$\begin{aligned}
&\Gamma^* = \{(x, r) : r = R_0(x),\ x_c \le x \le 1\}\\
&\Gamma_0 = \{(x, r) : r = R_0(x - k\epsilon),\ \tilde{x} \le x \le 1\}\\
&\Gamma_1 = \{(x, r) : r = R_0(x + \epsilon),\ \bar{x} \le x \le 1\}\\
&\Gamma_2 = \{(x, r) : r = k\epsilon^{1/3} + m_1(x - x_c),\ x_c \le x \le \bar{x}\}\\
&\Gamma_3 = \{(x, r) : 0 \le r \le k\epsilon^{1/3},\ x = x_c\}\\
&\Gamma_4 = \{(x, r) : r = \epsilon^{-1/4}(x - x_c),\ 0 \le x \le \tilde{x}\}\\
&\Gamma = \cup_{i=0}^{4} \Gamma_i.
\end{aligned} \tag{34}$$

Here $m_1,\ \bar{x},\ \bar{r}$ are chosen so that Γ_2 is tangent to Γ_1 at $(\bar{x}, \bar{r})$:

$$\bar{r} \equiv k\epsilon^{1/3} + m_1(\bar{x} - x_c) = R_0(\bar{x} + \epsilon), \quad m_1 = R_0'(\bar{x} + \epsilon); \tag{35}$$

and $\tilde{x}$, $\tilde{r}$ so that Γ_4 and Γ_0 intersect at $(\tilde{x}, \tilde{r})$, it being the intersection point with the least positive value of $\tilde{x}$:

$$\tilde{r} \equiv \epsilon^{-1/4}(\tilde{x} - x_c) = R_0(\tilde{x} - k\epsilon), \quad R_0'(\tilde{x} - k\epsilon) > \epsilon^{-1/4}. \tag{36}$$

Note that the mere existence of $(\tilde{x}, \tilde{r})$ automatically implies the inequality on the right of (36).

The region Ω is the closed region bounded by the curve Γ as well as on the right by the vertical segment of $\{x = 1\}$ connecting Γ_0 with Γ_1.

Lemma 2 *We have*

$$m_1 \approx \epsilon^{-1/3}, \ (\bar{x} - x_c) \approx k^2\epsilon^{2/3}, \ \bar{r} \approx \epsilon^{1/3}, \ (\tilde{x} - x_c) \approx \epsilon^{1/2}, \ \tilde{r} \approx \epsilon^{1/4}. \tag{37}$$

For x small,

$$R_0'(x) \approx (x - x^c)^{-1/2}, \ R_0''(x) \approx \ -(x - x^c)^{-3/2}. \tag{38}$$

Proof The estimates (38) follow since $p'(x_c) > 0$ (6). Then (37) are derived from (35), (36) by first assuming $\tilde{x} - x_c \gg \epsilon$, deriving estimates, and then verifying that the assumption is correct.

Lemma 3 *(a) On all trajectories in $W^s(U_c)$ or $W^u(0)$, there is a constant $C > 0$ such that*

$$|x'| < C\epsilon; \quad |r'| < C. \tag{39}$$

(b) For $a > 0$, let S_a be the rectangle $\{x \in [0, 2], \ r \in [0, 2]\}$ with disks of radii a about 0 and U_c excluded. There exist constants $\alpha(a) > 0$ and $\beta(a) > 0$ such that in S_a if $|x'| < \alpha\epsilon$, then $|r'| > \beta$.

Proof

From (3) we obtain that for any solution,

$$x_2 x_2' + r_2 r_2' = \frac{1}{\epsilon} x_1' \epsilon g_x + r_1' g_r = \frac{d}{d\zeta} g(x_1(\zeta), r_1(\zeta)). \tag{40}$$

Consider solutions on $W^s(U_c)$. Integrating and using the boundary condition at $\zeta = \infty$ as well as the fact that $g = 0$ at U_c, we obtain

$$\frac{1}{2}\left(x_2^2(\zeta) + r_2^2(\zeta)\right) = g\left(x(\zeta), r(\zeta)\right). \tag{41}$$

This is also true for solutions on $W_u(0)$. By (3), we may write (41) as

$$\left(\frac{x'}{\epsilon}\right)^2 + (r')^2 = 2g(x, r), \tag{42}$$

valid for trajectories on either $W_u(0)$ or $W^s(U_c)$. This, together with the boundedness of g in the region of interest and the positive lower bound of g in S_a, establishes both parts of the lemma.

Lemma 4 *Every trajectory on $W^s(U_c)$ which lies in the closed set Ω for $\zeta \geq \zeta_1$, and is not identically U_c, satisfies $x'(\zeta) > 0$ for all $\zeta \geq \zeta_1$.*

Proof Let $(\hat{x},\hat{r}) = (x(\zeta_1), r(\zeta_1))$. Our first task is to show that near this point, $g_x > c > 0$ with c independent of ϵ. From (29), (27), (28) we know that $x'(\zeta) > 0$ for large ζ, i.e. at points near U_c. Suppose, contrary to the lemma's assertion, that there exists a solution $U(\zeta,\nu)$ with trajectory T_ν on $W^s(U_c)$ with $U(\zeta) \in \Omega$ and $x' > 0$ for $\zeta > \zeta_1$, and $x'(\zeta_1) = 0$. . For large ζ, U can be approximated by the asymptotic representation (29) for some fixed ν. From now on, we suppress dependence on ν. Since the second component in ψ_s (28) is positive and $x_2 = \frac{x'}{\epsilon}$, it follows that there exists a value ζ_2 (large) and c independent of ϵ such that $x'(\zeta_2) > \epsilon c > 0$.

Let us follow T backwards in "time", i.e. with ζ decreasing from ζ_2. By assumption, T stays in Ω as long as $x' > 0$. Since $r^2 > \psi(x)$ (10) for x near (but not equal) to 1, we have $x'' < 0$ $(2)_1$, so that x' increases as ζ decreases, until it reaches a maximum value $x'_m > 0$ at the point where T crosses $\{r^2 = \psi(x)\}$. In fact, that curve crosses the thin region Ω transversally, so there is such a point, which can with a minor effort be shown to be unique (if we exclude the trivial intersection at U_c.) Let the corresponding value of ζ be denoted by ζ_3. Since $x'_m > x'(\zeta_2)$, we have $x'_m > c\epsilon$.

Finally, let ζ_4 be the value of ζ where $x'(\zeta_4) = \frac{1}{2}x'_m$. It exists, because x' by assumption decreases from x'_m to 0 on T. By (39), we also have $x' < C\epsilon$ for all points on T. Therefore

$$x' \approx \epsilon \text{ for } \zeta \in [\zeta_4, \zeta_3]. \tag{43}$$

We now have

$$\epsilon \approx \frac{1}{2}x'_m = x'_m - \frac{1}{2}x'_m = \epsilon^2 \int_{\zeta_4}^{\zeta_3} g_x(x(\zeta), r(\zeta))d\zeta = \epsilon^2 \int_{x_4}^{x_3} \frac{g_x(x, r(x))}{x'}dx, \tag{44}$$

where $r(x)$ denotes the dependence of r on x induced by T. Now $g_x = 0$ at $x = x_3$, and for trajectories in the region Ω, $g_x(x, r(x))$ rises roughly linearly in x as x decreases from x_3, at least in a neighborhood of x_3. So on T, $g_x \approx (x_3 - x)$ for $x_3 - x$ small. From this observation, (44), and (43), we have

$$\epsilon \approx \epsilon(x_4 - x_3)^2,$$

which implies $x_3 - x_4 \approx 1$, i.e. x_4 is bounded away from x_3 (where $x' = x'_m$). Therefore the same is true at the point $(\hat{x},\hat{r})$ ($\zeta = \zeta_1$), where $x' = 0$. This implies that $g_x(\hat{x},\hat{r})$, is also bounded away from 0, and the same is true at nearby points: there is a number $\delta > 0$ independent of ϵ such that:

$$g_x(x,r) > c > 0 \text{ for } (x,r) \text{ in a } \delta - \text{neighborhood of } (\hat{x},\hat{r}). \tag{45}$$

We now proceed by recalling (32): $\frac{dm}{dx} = \frac{g_r - \epsilon^2 g_x m}{(x')^2}$. The postulated trajectory satisfies this, with $m \to \infty$ or $m \to -\infty$ as $x \downarrow \hat{x}$. We first suppose the former. When x is near $\hat{x}$, the inequality $g_r > -\epsilon^2 g_x m$ is certainly satisfied, because of (45) and the fact that m is indefinitely large. Therefore there is an x-interval $I = (\hat{x}, x_5)$ on which (46) holds. Secondly, we require that $x' < \alpha\epsilon$ on I, where α is the constant in Lemma 3. In short, since (45) holds and $g_r > -ck\epsilon$ in Ω, our two requirements on I are

$$m > \frac{ck}{\epsilon}; \quad x' < \alpha\epsilon. \tag{46}$$

From Lemma 3 we have $r' \geq \beta$ and $x' = \frac{r'}{m} \geq \frac{\beta}{m}$ on I. Therefore from (32), (46),

$$\frac{dm}{dx} > -\frac{2\epsilon^2 m}{(x')^2} \geq -\frac{2\epsilon^2 m^3}{\beta^2}, \tag{47}$$

so that

$$m^{-3}\frac{dm}{dx} > -\frac{2\epsilon^2}{\beta^2}. \tag{48}$$

For numbers $x_i \in I$ with $\hat{x} < x_6 < x_7$, by integrating (48), we get

$$-\frac{1}{2}(m^{-2}(x_6) - m^{-2}(x_5)) \geq -\frac{2\epsilon^2}{\beta^2}(x_6 - x_5).$$

Let $x_5 \downarrow \hat{x}$ and set $x_6 = x$ to get

$$\frac{dr}{dx} = m(x) > \left(\frac{\beta}{2\epsilon}\right)(x - \hat{x})^{-1/2}. \tag{49}$$

Integrating again, we find the following for r, considered as a function of x:

$$r(x) \geq \hat{r} + \frac{\beta}{\epsilon}(x - \hat{x})^{1/2}. \tag{50}$$

Any trajectory satisfying (50) would leave Ω as x increases before $x - \hat{x} = \epsilon^{1/2}$. But it can be seen from (49), the relation $x' = r'/m$, and $(39)_2$, that (46) remains valid as long as $x - \hat{x} \leq \epsilon^{1/2}$ and (x, r) remains in Ω. Therefore our trajectory takes us out of Ω, no matter where in Ω the starting point $(\hat{x}, \hat{r})$ is located. This contradicts our assumption.

The other case, $m \to -\infty$, is handled in a similar way. Lemma 3 now implies $r' < -\beta$. On T, we require $-m > C/\epsilon$, and $x' < \alpha\epsilon$. We use $x' = r'/m \geq -\beta/m$, which leads to an equation like (49): $\frac{dr}{dx} = m(x) < -\frac{\beta}{\epsilon}(x - \hat{x})^{-1/2}$, which leads to a trajectory which must depart from Ω. This completes the proof.

Lemma 5 *Let T be the projection, onto the (x, r) plane, of a trajectory in $W^s(U_c)$. There exists a minimal value ζ_0 such that T lies in the interior of Ω for all $\zeta > \zeta_0$. For large enough k independent of ϵ and for small enough ϵ, T enters Ω transversally through Γ at $\zeta = \zeta_0$.*

Proof By Lemma 4, the inequality $x' > 0$ holds true as long as T is in Ω, including its boundary. Therefore there exists a minimal ζ_0 with property that T lies in the interior of Ω for all $\zeta > \zeta_0$. We show that T must have entered Ω transversally at (x_0, r_0), the point on T corresponding to $\zeta = \zeta_0$. By Lemma 4, $x_0 < 1$, so $(x_0, r_0) \in \Gamma$. There are five cases.

Case $(x_0, r_0) \in \Gamma_0$ By Lemma 1(b), we need only verify that at (x_0, r_0),

$$g_r - \epsilon^2 R' g_x < (x')^2 R'', \tag{51}$$

where $R(x) = R_0(x - k\epsilon)$.

Since $g_r = 3r(r^2 - p(x))$, we have that on Γ_0 for ϵ small, by Lemma 2,

$$g_r = 3r(p(x - k\epsilon) - p(x)) \approx -rk\epsilon \leq -\tilde{r}k\epsilon \approx -k\epsilon^{5/4}.$$

Also from Lemma 2, when $x - x_c \gg \epsilon$, $R''(x) \approx -(x - x_c)^{-3/2} \geq -(\tilde{x} - x_c)^{-3/2} \geq -C\epsilon^{-3/4}$. And since from Lemma 3 $(x')^2 \leq C\epsilon^2$, we have $(x')^2 R''(x) \geq -C\epsilon^{5/4}$.

Therefore (51) holds if k is chosen large enough, which we do.

Case $(x_0, r_0) \in \Gamma_1$ Lemma 1(a) applies, and we must verify (30). Since $R'' < 0$, (30) will hold provided that at (x_0, r_0),

$$g_r - \epsilon^2 R' g_x \geq 0. \tag{52}$$

On Γ_1, by Lemma 2, $g_r \geq c\bar{r}\epsilon \approx \epsilon^{4/3}$ and $R' \leq C\bar{x}^{-1/2} \approx \epsilon^{-1/3}$, so that $g_r - \epsilon^2 R' g_x \geq c\epsilon^{4/3} - C\epsilon^{5/3}$, which (for small ϵ) verifies (52) and proves the transversality in this case.

Case $(x_0, r_0) \in \Gamma_2$ Again, we verify (52), which by Lemma 2 will be true if $g_r > \epsilon^2 R' g_x = \epsilon^2 m_1 g_x \approx \epsilon^{5/3}$. But as before, on Γ_2 $g_r > c\epsilon^{4/3}$, which establishes (52) for small ϵ.

Case $(x_0, r_0) \in \Gamma_3$ The transversality in this case follows directly from Lemma 4.

Case $(x_0, r_0) \in \Gamma_4$ On this piece, $R'' = 0$, so we must verify (by Lemma 1(b)) that $g_r - \epsilon^2 R' g_x < 0$ with $R' = \epsilon^{-1/4}$. But this is true, since Γ_4 lies where $g_r \leq 0$.

This completes the proof of the lemma.

We denote by $U^+(\zeta, \nu)$ the solution (29), with ζ translated so that $x^+(0, \nu) = 0$.

Theorem 3 *Given any point (x_c, r^*) on Γ_3, i.e. with $0 \leq r^* \leq k\epsilon^{1/3}$, there exists a trajectory T^+ connecting (x_c, r^*) to the critical point $(1, \sqrt{2})$, lying entirely in Ω between those two points. There exists a continuous function $r^*(\nu)$, defined in an interval $\nu \in N = [\nu_1, \nu_2]$, whose range is $[0, k\epsilon^{1/3}]$, such that $r^+(0, \nu) = r^*(\nu)$.*

Proof For fixed ν, consider the solution $U^+(\zeta, \nu)$, with projected trajectory T_ν. Follow it "backwards", i.e. for decreasing ζ. Since the r-component of ψ_f in (29) is -1, for large positive ν, say $\nu > \nu^+$, T exits Ω (in the backward direction) through Γ_0 near U_c, and for large negative ν, say $\nu < \nu^- < 0$, it exits Ω through Γ_1, again near U_c.

We consider the family of solutions $U^+(\zeta, \nu)$ with $\nu^- \leq \nu \leq \nu^+$.

By Lemma 5, each T_ν must intersect Γ for some $\zeta = \zeta_0$. The point of intersection P, which we take to be the first one as ζ decreases, depends on ν, and that dependence must be continuous, since (Lemma 5) T always crosses Γ transversally. Thus for each point P on the part of Γ covered as we proceed counterclockwise on Γ from $P(\nu^-)$ to $P(\nu^+)$ to Γ, there must be a value ν for which the corresponding trajectory exits Ω (for the first time, relative to backwards ζ) at P.

In particular, this is true for points on Γ_3, which proves the first assertion.

Since $P = P(\nu)$ depends continuously on ν, there must be an interval $N = [\nu_1, \nu_2]$ with $P(\nu_1) = (x_c, k\epsilon^{1/3})$, $P(\nu_2) = (x_c, 0)$, and $P(\nu) \in \Gamma_3$ for all $\nu \in N$. We set $P(\nu) = (x_c, r^*(\nu))$. This completes the proof.

4 Derivative estimates on $\{x = x_c\}$

4.1 Transforming to corner coordinates

We change variables as follows:

$$x = x_c + \epsilon^{2/3}\xi, \quad r = \epsilon^{1/3}\eta, \tag{53}$$

$$\zeta = \frac{z}{\epsilon} = \epsilon^{-1/3}\tau, \quad \frac{d}{d\zeta} = \epsilon^{1/3}\frac{d}{d\tau}, \tag{54}$$

$$\tilde{p}(\xi) = \epsilon^{-2/3} p(x_c + \epsilon^{2/3}\xi). \tag{55}$$

As we know from Theorem 2, given any $0 \leq r^* \leq .3$, there exists a solution connecting 0 with (x_c, r^*), Set $r^* = \epsilon^{1/3}\eta^*$. Let $\xi(\tau), \eta(\tau)$ be that solution, written in terms of the new coordinates. Note that ξ, as well as η, depends on η^*; however we shall find estimates for it which are independent of η^* when the latter is not too large.

The equation $(2)_2$, which we write in the form $r'' = 3r(r^2 - p(x))$, for r becomes

$$L\eta \equiv \eta_{\tau\tau} - 3\eta(\eta^2 - \tilde{p}(\xi)) = 0. \tag{56}$$

In this operator L, we treat the function $\xi(t)$ as known, so it is an operator applied to η alone.

4.2 A supersolution for $\tau < 0$.

From (6) we have

$$3 < p'(x) < 4, \tag{57}$$

so that from this and (53),

$$4\xi \le \tilde{p}(\xi) \le 3\xi, \quad \text{for } \xi \le 0. \tag{58}$$

From (18) and (53), we have the bound, valid for $\tau \le 0$,

$$\xi \le \epsilon^{-2/3} x_c \left(\exp(\sqrt{2}\epsilon^{2/3}\tau) - 1\right) \equiv \overline{\xi}(\tau). \tag{59}$$

and

$$4\xi \le \tilde{p}(\xi) \le 3\overline{\xi}(\tau). \tag{60}$$

Let $\xi(\tau), \eta(\tau)$ be the solution for $\tau \le 0$, satisfying $\eta(0) = \eta^*$, where $\eta^* \in (1, k]$. The existence follows from Theorem 2. Let

$$\overline{\eta}(\tau) = \eta^* e^{\alpha\tau}, \tag{61}$$

where the positive number α will be chosen later. Recalling the operator L given in (56), we calculate

$$\begin{aligned} L\overline{\eta} &= \eta^* e^{\alpha\tau}\left[\alpha^2 - 3\left((\eta^*)^2 e^{2\alpha\tau} - \tilde{p}(\xi(\tau))\right)\right] \\ &\le \eta^* e^{\alpha\tau}\left[\alpha^2 - 3\left((\eta^*)^2 e^{2\alpha\tau} - 3\overline{\xi}(\tau)\right)\right]. \end{aligned} \tag{62}$$

This function will be a supersolution, provided that

$$\alpha^2 - A(\tau) \equiv \alpha^2 - 3\left((\eta^*)^2 e^{2\alpha\tau} - 3\overline{\xi}(\tau)\right) \le 0, \quad \tau < 0. \tag{63}$$

We examine this requirement for two ranges of τ, recalling $\eta^* > 1$, so that $\ln\eta^* > 0$.

The range $-\frac{\ln\eta^*}{2\alpha} < \tau < 0$. In this case, $A(\tau) \ge 3(\eta^*)^2 \exp(-\ln\eta^*) = 3\eta^*$.

The range $-\infty < \tau < -\frac{\ln\eta^*}{2\alpha}$. In this case, $-\overline{\xi}(\tau) \ge \frac{1}{2}\epsilon^{-2/3} x_c \left(\sqrt{2}\epsilon^{2/3}\frac{\ln\eta^*}{2\alpha}\right) = \frac{\sqrt{2}}{4\alpha} x_c \ln\eta^*$, so that $A(\tau) \ge \frac{3\sqrt{2}}{4\alpha} x_c \ln\eta^*$.

The requirement (63) will be satisfied if $\alpha^2 \le 3\eta^*$ and also $\alpha^2 \le \frac{3\sqrt{2}}{4\alpha} x_c \ln\eta^*$. Thus we may set

$$\alpha = \min\left[(3\eta^*)^{1/2}, \left(\frac{3\sqrt{2}x_c}{4}\ln\eta^*\right)^{1/3}\right]. \tag{64}$$

For large enough η^*, α may be set equal to the second member.

Lemma 6 *When η^* is large enough, the solution $\eta(\tau)$ satisfies*

$$\eta_\tau(0) \ge \overline{\eta}_\tau(0) = \eta^*\alpha = \eta^*\left(\frac{3\sqrt{2}x_c}{4}\ln\eta^*\right)^{1/3}. \tag{65}$$

The proof follows since $\eta(\tau) \le \overline{\eta}(\tau)$ for $\tau \le 0$, with equality holding at $\tau = 0$; and $\overline{\eta}_\tau(0) = \eta^*\alpha$.

4.3 A supersolution for $\tau > 0$.

Let $\xi(\tau), \eta(\tau)$ be the solution, shown to exist in Theorem 3, of (56) for $\tau > 0$ satisfying $\eta(0) = \eta^*$, $\epsilon^{1/3}\eta(\infty) = r(\infty) = \sqrt{2}$. Here η^*, the value at $\tau = 0$, i.e. when $x = x_c$ ($\xi = 0$), is the same as that satisfied by the function η in the previous subsection 4.2.

Our supersolution this time will be

$$\overline{\eta}(\tau) = \eta^*\sqrt{\tau + 1}. \tag{66}$$

We calculate

$$L\overline{\eta} = \overline{\eta}_{\tau\tau} - 3\overline{\eta}(\overline{\eta}^2 - \tilde{p}(\xi(\tau))) = -\frac{1}{4}\eta^*(\tau+1)^{-3/2} - 3\eta^*(\tau+1)^{1/2}B(\tau), \quad \tau \geq 0, \tag{67}$$

where

$$B(\tau) = (\eta^*)^2(\tau + 1) - \tilde{p}(\xi(\tau)). \tag{68}$$

We employ the maximum principle on the interval $0 \leq \tau \leq \tau_0$, where τ_0 will be chosen later.

The desired inequality

$$L\overline{\eta} \leq 0 \tag{69}$$

will be satisfied provided that

$$B(\tau) \geq 0 \quad \text{for } 0 < \tau < \tau_0. \tag{70}$$

The inequality $x' < C\epsilon$ from (39) implies $x(\zeta) - x_c \leq C\epsilon\zeta$. Also $p(x) \leq C(x - x_c),\ x > x_c$, so that

$$\tilde{p}(\xi) \leq C\xi = C\epsilon^{-2/3}(x - x_c) \leq C\epsilon^{1/3}\zeta = C\tau.$$

Therefore

$$B(\tau) \geq (\eta^*)^2(\tau + 1) - C\tau > 0 \tag{71}$$

for η^* large enough.

The two functions $\eta(\tau)$ and $\overline{\eta}(\tau)$ are equal at $\tau = 0$. We now choose $\tau_0 = 4(\eta^*)^{-2}\epsilon^{-2/3} - 1$, so that $\overline{\eta}(\tau_0) = 2\epsilon^{-1/3}$. Since $r(\zeta)\uparrow\sqrt{2}$, we have $\eta\uparrow\sqrt{2}\epsilon^{-1/3}$, so that $\eta(\tau_0) < \sqrt{2}\epsilon^{-1/3} < 2\epsilon^{-1/3} = \overline{\eta}(\tau_0)$. By the maximum principle, we therefore have

$$\overline{\eta}(\tau) \geq \eta(\tau) \tag{72}$$

for $0 \leq \tau \leq \tau_0$.

The inequality (72), together with the equality of the two functions at $\tau = 0$, implies

$$\eta_\tau(0+) \leq \overline{\eta}_\tau(0+) = \eta^*. \tag{73}$$

4.4 The discontinuity in $\eta_\tau(\tau)$ at $\tau = 0$.

We patch together the two solutions $\eta(\tau)$, which were defined for negative and positive τ, respectively. By design, the patched function is continuous at $\tau = 0$. We show now

Lemma 7

$$\eta_\tau(0-) > \eta_\tau(0+) \tag{74}$$

for large enough η^*.

This follows from the fact that for large η^*, the left hand derivative grows at least as fast as $O\left(\eta^*(\ln\eta^*)^{1/3}\right)$ (65) whereas the right hand one grows at most like $O(\eta^*)$ (73).

At this point we further increase the parameter k (recall the upper bound in Γ_3 was $k\epsilon^{1/3}$ and k is the upper bound of η^*) so that (74) holds for $\eta^* = k$.

We have a complementary result with $\eta^* = 0$:

Lemma 8 *When $\eta^* = 0$,*

$$\eta_\tau(0-) = 0 < \eta_\tau(0+). \tag{75}$$

Proof It was noted in (16) that $r \equiv 0$ is the r-component of the solution (15) corresponding to $\mu = 0$. It, of course, satisfies $r = 0$ when $x \le x_c$, so that in the terminology of Section 4.1, it corresponds to $r^* = 0$. Transforming in accordance with (53), (54), we see that $\eta = 0$ is the solution of (56) for $\tau \le 0$ corresponding to $\eta^* = 0$. The left part of (75) follows.

For the right part, we merely observe that the trajectory connecting $(x = x_c,\ r = 0)$ with U_c in Theorem 3 lies in Ω, so that $r' > 0$ when $x = x_c$. This completes the proof of Lemma 8.

5 The heteroclinic

5.1 Existence

Theorem 4 *There exists a $\nu_0 \in N$ such that the solutions $U^-(\zeta, r^*(\nu_0))$ (Theorem 2) and $U^+(\zeta,\nu_0)$ (Theorem 3) match at $\zeta = 0$, forming a heteroclinic.*

Proof Both $U^-(\zeta, r^*(\nu))$ and $U^+(\zeta,\nu)$ are continuous in ν. Let $q(\nu) = (r^-)'(0, r^*(\nu)) - (r^+)'(0,\nu)$. According to Lemma 8, $q(\nu_2) < 0$ and to Lemma 7, $q(\nu_1) > 0$. There must be an intermediate value ν_0 where

$$q(\nu_0) = 0. \tag{76}$$

For the combined function

$$U(\zeta) = \begin{cases} U^-(\zeta, r^*(\nu_0)), & \zeta \le 0, \\ U^+(\zeta,\nu_0), & \zeta \ge 0, \end{cases} \tag{77}$$

to be a heteroclinic, it merely needs to be continuous at $\zeta = 0$. The continuity of x_1 and r_1 follows by construction, and that of r_2 by (76). Finally, the continuity of x_2 follows from these, together with (42). This completes the proof.

5.2 Magnitude of r when $x < x_c$.

Lemma 9 *There are positive constants c_3 and α, bounded above and below independently of ϵ, such that when $x \le x_c$,*

$$r \le c_3\epsilon^{1/3}\left(\frac{x}{x_c}\right)^{\alpha\epsilon^{-2/3}}.$$

Proof From Section 4.2 we know that when $\tau \le 0$,

$$\eta(\tau) \le \overline{\eta}(\tau) = \eta_0^* e^{\alpha_1\tau},$$

where η_0^* and α_1 are bounded above and below by positive constants independent of ϵ. Hence

$$r(\zeta) = \epsilon^{1/3}\eta\left(e^{1/3}\zeta\right) \le \epsilon^{1/3}\eta_0^*\exp\left(\alpha_1\epsilon^{1/3}\zeta\right). \tag{78}$$

We also have, by (18), $\exp(\sqrt{5}\,\epsilon\zeta) \leq \frac{x(\zeta)}{x_c}$, or $e^{\zeta} \leq \left(\frac{x}{x_c}\right)^{1/\sqrt{5}\,\epsilon}$. Combining this with (78), we get

$$r \leq \epsilon^{1/3}\eta_0^* \left(\frac{x}{x_c}\right)^{(1/\sqrt{5}\,\epsilon\alpha_1)\epsilon^{1/3}} \leq c_3\epsilon^{1/3} \left(\frac{x}{x_c}\right)^{\alpha\epsilon^{-2/3}}, \tag{79}$$

for appropriate c_3 and α.

5.3 Proof of the main theorem

This lemma refers to the heteroclinic constructed in the previous theorem 4.

Lemma 10 *(a) For each fixed small $\delta > 0$, uniformly for x in the interval $[0, x_c - \delta$, r is exponentially small as a function of ϵ.*

(b) There exist constants $c_i > 0$, independent of ϵ, such that

$$c_1\epsilon^{1/3} < r < c_2\epsilon^{1/3} \tag{80}$$

when $x = x_c$.

(c) The trajectory T is ϵ-close to the set Γ^* uniformly for $x \geq x_c + O(\epsilon^{2/3})$.

Proof Part (a) follows from (79). Part (b) follows from the fact that our solution passes through Γ_3. Finally Part (c) follows from the fact that our trajectory lies in Ω for $x > x_c$, and that set lies close to Γ^* in the sense indicated.

Proof of Theorem 1 The existence comes from Theorem 4. The possibility of the representation $r = R(x, \epsilon)$ comes from the fact (Lemma 4 and (17)) that x is a monotone increasing function of ζ. The estimates (a) and (b) follow from Lemmas 9 and 10. Estimate (c) follows because the trajectory lies in Ω, as does $\Gamma^* = \{r = \sqrt{p(x)}\}$. For each $x \geq x_c + \delta$, all values of r in Ω for that x lie at least as close as $O(\epsilon)$ from Γ^*. This completes the proof.

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