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Heteroclinic connections for multiple-well potentials: the anisotropic case

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We investigate the existence of solutions to systems of N differential equations representing connections between minima of potentials with several equal depths in $\mathbb{R}^n$. Using variational techniques and in particular a method introduced by Alikakos and Fusco we first prove such existence for $N \geqslant 2$ and two minima. Dealing next with symmetric potentials corresponding to bulk free energies in crystals, we establish existence for $N \geqslant 2$ in various cases of more than two minima. Finally, we obtain a sufficient condition establishing existence of connections to potentials which are not necessarily symmetric for arbitrary N and three minima.

1. Introduction

In this article we study the existence of connections between global minima of a multiple-well potential in anisotropic media. We call such connections *heteroclinic connections* or simply *heteroclinics*.

The setting of our problem is as follows. Let $F : \mathbb{R}^n \to \mathbb{R}$ be a C^2 function satisfying the following.

(H1) $F(\xi_i) = 0$, $i = 1, \dots, n$, and $F(\xi) > 0$ for $\xi \notin \{\xi_1, \dots, \xi_n\}$.

(H2) $\underline{\lim}\, F(\xi) > 0$, as $|\xi| \to \infty$.

(H3) There exists a positive constant $\beta \ll 1$ such that $\langle \nabla F(\xi_i + \xi), \xi \rangle > 0$, whenever $0 < |\xi| < \beta$, for each $i = 1, \dots, n$.

Henceforth, by $\langle \cdot, \cdot \rangle$ we denote the Euclidean inner product in $\mathbb{R}^n$. For A^2 a constant, positive $N \times N$ matrix, we investigate the existence of solutions to the system $A^2 U'' - \nabla F(U) = 0$, with $U(x) = (u_1(x), \dots, u_N(x))^{\mathrm{T}}$, $x \in \mathbb{R}$, connecting global minima of F, that is, we consider the problem

$$A^2 U'' - \nabla F(U) = 0, \qquad \lim_{x \to -\infty} U(x) = \xi_p, \qquad \lim_{x \to \infty} U(x) = \xi_q, \tag{1.1}$$

where $\xi_p \neq \xi_q$ are zeros of F. The matrix A^2 in the physical applications is diagonal and represents anisotropy; thus, the isotropic case is the one where $A^2 = I$, the identity matrix.

Problem (1.1) is variational with associated functional

$$E(U) = \int_{\mathbb{R}} \{\tfrac{1}{2}|AU'|^2 + F(U)\}\, \mathrm{d}x. \tag{1.2}$$

We denote by A in (1.2) the positive square root of A^2, which makes sense by the definition of A^2. We note that (1.1) is a *Hamiltonian system* and the functional E, as defined in (1.2), represents the *action*.

The existence of solutions to (1.1) for arbitrary N, two minima and A^2 being the identity matrix is established in [2, 12]. While Sternberg's approach is based on the Jacobi functional, Alikakos and Fusco use the action. Although the change of variable $V = AU$ transforms (1.1) to the isotropic case $V'' - \nabla F_0(V) = 0$, where $F_0(V) = F(A^{-1}V)$ (see the end of this section), we apply the *unilateral constraint method*, introduced in [2], directly to the anisotropic case and we show that, for any N and for potentials with two global minima, there always exists a solution to (1.1). Our proof uses the Euler–Lagrange equation of (1.2) and in that respect is slightly different from that of [2], which is purely variational. Related issues, again for the isotropic case, arbitrary N and two minima, are discussed in [1, 7] for symmetric potentials and in [9], where the not necessarily symmetric potential satisfies more restrictive structural hypotheses.

One of the main goals of this paper is to show how the unilateral constraint method can be extended to establish existence of connections in the presence of several global minima. In this direction we first investigate such existence in the case of symmetric potentials having three or more global minima for some representative and quite general examples arising in the study of motion of interfaces in crystals. In particular, for $N = 2$ and three minima these examples have been studied in [4, 5, 10, 11]. The matrix A^2 there is diagonal, with diagonal $[1, \lambda^2]$, or $[\lambda^2, 1]$, where $\lambda > 0$ is the anisotropy parameter. Using functional analytic or geometric singular perturbation techniques, these authors establish existence and obtain detailed information for the solution, as λ approaches 0. For a class of this type of examples, we prove the existence of heteroclinic connections for general diagonal matrices in dimensions $N = 2, 3$.

Next, returning to general potentials with three global minima and $N \geqslant 2$, we obtain a sufficient condition for existence of connections of the type of a strict triangle inequality involving the action. For $N = 2$ this condition is also considered in [1], in the context of symmetric potentials, and in [2], where it is associated to geodesic distances defined by the Jacobi functional. In the latter paper it is shown that this condition is also necessary.

This paper consists of three parts. Sections 2–4 form the first part, which is actually an extension of the results of [2] to our non-isotropic setting and deals with existence of heteroclinic connections. Hence, for general N we define, in § 2, a constrained problem and we prove existence of a solution. We also discuss regularity properties of the solution. In § 3 we obtain information about the shape of the minimizer and, in § 4, by removing the constraint, we show existence of a heteroclinic connection in the case of two minima. The second part consists of § 5, where we consider a model example and for $N = 2, 3$ and in the presence of symmetry we establish existence of connections for three or more minima. Finally, in § 6 we give a sufficient condition that guarantees existence of connections for general potentials with three minima and $N \geqslant 2$.

We conclude this section with some comments regarding the transformation of (1.1) to the one with $A^2 = I$. For $V = AU$ we set $F_0(V) = F(A^{-1}V)$ or, equivalently, $F(U) = F_0(AU)$. Then $\nabla_U F(U) = A^{\mathrm{T}} \nabla_V F_0(AU)$; hence, equation (1.1) is transformed to

$$(AU)'' - A^{-1}A^{\mathrm{T}}\nabla_V F_0(AU) = 0 \text{ or, equivalently, } V'' - \nabla_V F_0(V) = 0,$$

since A is self-adjoint. The minima of F_0 are attained at the points $\{A\xi_i\}_{i=1}^n$ and, moreover, it can be easily checked that conditions (H1)–(H3) are satisfied. Possible symmetries of the potential F are transferred to F_0, that is, if S is an orthogonal matrix satisfying $AS = SA$ and $F(SU) = F(U)$, then we have

$$F_0(SV) = F(A^{-1}SV) = F(SA^{-1}V) = F(A^{-1}V) = F_0(V).$$

We point out, however, that the non-constant coefficient case $(A(x)U')' - \nabla F(U) = 0$ cannot be transformed to an isotropic case and, although this is a different problem, it would be of some interest to check to what extent the unilateral constrained method handles this case.

2. The constrained problem

Via condition (H1) on F it follows that $E(U) \geqslant 0$, while $E(\xi_i) = 0$, for $i = 1, \dots, n$. Hence, the trivial solutions $U(x) = \xi_i$ of the equations in (1.1) are *global minimizers* of the action E. In their presence and due to lack of compactness, since these equations are autonomous, it is difficult to construct a connection between distinct minima of F by minimizing E. This difficulty in [2] is surpassed by introducing a certain type of constraints that are removed later, thus yielding a solution to (1.1). Moreover, it can be proved that this solution is a *local minimizer* of the action E (see § 4).

The heteroclinic connection joining the global minima ξ_p and ξ_q is trapped inside appropriate *cylinders* constructed below. Given $\xi \in \mathbb{R}^n$, $\ell > 0$ and $L > 0$ fixed, we define

$$\left.\begin{aligned} \mathcal{Z}^-_{L,\ell}(\xi) &:= \{U \in W^{1,2}_{\mathrm{loc}}(\mathbb{R};\mathbb{R}^n) : |A(U(x) - \xi)| \leqslant \ell \text{ for } x \leqslant -L\}, \\ \mathcal{Z}^+_{L,\ell}(\xi) &:= \{U \in W^{1,2}_{\mathrm{loc}}(\mathbb{R};\mathbb{R}^n) : |A(U(x) - \xi)| \leqslant \ell \text{ for } x \geqslant +L\}. \end{aligned}\right\} \tag{2.1}$$

Proposition 2.1. *Let $\xi_p \neq \xi_q$ be global minima of F. If ℓ and L are positive, arbitrary and fixed constants, we define $\mathcal{Z}^\ell_L(\xi_p, \xi_q) := \mathcal{Z}^-_{L,\ell}(\xi_p) \cap \mathcal{Z}^+_{L,\ell}(\xi_q)$, where $\mathcal{Z}^-_{L,\ell}(\xi_p)$, and $\mathcal{Z}^+_{L,\ell}(\xi_q)$ are as in (2.1). Then the constrained problem*

$$\min_{\mathcal{Z}^\ell_L(\xi_p,\xi_q)} \int_{\mathbb{R}} \{\tfrac{1}{2}|AU'|^2 + F(U)\}\,\mathrm{d}x \tag{2.2}$$

has a solution U_α, where $\alpha = (p, q)$, that is

$$0 \leqslant \inf_{\mathcal{Z}^\ell_L(\xi_p,\xi_q)} E = E(U_\alpha) < \infty. \tag{2.3}$$

Moreover, for $\ell < \frac{1}{2}|A(\xi_p - \xi_q)|$ we have that $E(U_\alpha) > 0$.

Proof. For a fixed positive L_0 with $L_0 < L$ we consider the control function

$$U_0(x) = \begin{cases} \xi_p & \text{if } x \leqslant -L_0, \\ \xi_p \dfrac{L_0 - x}{2L_0} + \xi_q \dfrac{L_0 + x}{2L_0} & \text{if } -L_0 \leqslant x \leqslant L_0, \\ \xi_q & \text{if } x \geqslant L_0. \end{cases} \tag{2.4}$$

Note that U_0 is independent of L and that $U_0 \in \mathcal{Z}_L^\ell(\xi_p, \xi_q)$. Moreover, $E(U_0) < \infty$; hence, using $F \geqslant 0$ on $\mathbb{R}^n$ yields

$$0 \leqslant \inf_{\mathcal{Z}_L^\ell(\xi_p,\xi_q)} E \leqslant E(U_0) < \infty.$$

If $\{U_j\} \subset \mathcal{Z}_L^\ell(\xi_p, \xi_q)$ is a minimizing sequence, that is $E(U_j) \to \inf E$, assuming, without loss of generality, that $E(U_j) \leqslant E(U_0)$, for all j, we obtain the following *a priori* estimate:

$$\frac{1}{2}\int_{\mathbb{R}} |AU_j'|^2 \, \mathrm{d}x \leqslant E(U_j) \leqslant E(U_0) < \infty, \tag{2.5}$$

which, via Morrey's inequality

$$|AU_j(x_1) - AU_j(x_2)| \leqslant |x_1 - x_2|^{1/2}\biggl(\int_{\mathbb{R}} |AU_j'|^2 \, \mathrm{d}x\biggr)^{1/2},$$

leads to

$$|AU_j(x_1) - AU_j(x_2)| \leqslant |x_1 - x_2|^{1/2}\{2E(U_0)\}^{1/2}. \tag{2.6}$$

On the other hand, we have

$$|AU_j(x)| \leqslant \max\{|A\xi_p|, |A\xi_q|\} + \ell, \quad |x| \geqslant L, \tag{2.7}$$

by the definition of $\mathcal{Z}_L^\ell(\xi_p, \xi_q)$ and the U_j. Moreover, for $x \geqslant -L$, via (2.6) one also obtains $|AU_j(x)| \leqslant |AU_j(-L)| + |x + L|^{1/2}\{2E(U_0)\}^{1/2}$; hence,

$$|AU_j(x)| \leqslant |A\xi_p| + \ell + 2\sqrt{LE(U_0)}, \quad |x| \leqslant L. \tag{2.8}$$

It then follows that the sequence $\{AU_j\}$ is equicontinuous and uniformly bounded on every bounded interval. Hence, by the Ascoli–Arzelà theorem, this is relatively compact in $C([-a, a])$, for any $a \in \mathbb{R}$. We can thus obtain a subsequence, again denoted by $\{AU_j\}$, which converges uniformly on compact sets to some $AU_\alpha \in W^{1,2}_{\mathrm{loc}}$. By weak compactness in $L^2(\mathbb{R})$, via (2.5), we have that $AU_j' \rightharpoonup AU_\alpha'$ weakly in $L^2(\mathbb{R})$, where U_α' is understood in the sense of distributions. Also, $E(U_j) \to \inf E$. By weak lower semicontinuity in L^2, on the one hand, we have

$$\varliminf_{j\to\infty} \int_{\mathbb{R}} |AU_j'|^2 \, \mathrm{d}x \geqslant \int_{\mathbb{R}} |AU_\alpha'|^2 \, \mathrm{d}x, \tag{2.9}$$

while, on the other hand, by Fatou's lemma, via the pointwise convergence $U_j(x) \to U_\alpha(x)$ on $\mathbb{R}$, we have

$$\varliminf_{j\to\infty} \int_{\mathbb{R}} F(U_j) \, \mathrm{d}x \geqslant \int_{\mathbb{R}} F(U_\alpha) \, \mathrm{d}x. \tag{2.10}$$

Finally, combining (2.9) and (2.10), we obtain $E(U_\alpha) \leqslant \varliminf_{j\to\infty} E(U_j) = \inf E$. By the imbedding $W^{1,2}_{\mathrm{loc}} \hookrightarrow C$, U_α is a continuous function joining two distinct states over the finite interval $[-L, L]$. Hence, $E(U_\alpha)$ is strictly positive. □

REMARK 2.2. For a function $U : \mathbb{R} \to \mathbb{R}^n$ and $\xi \in \mathbb{R}^n$ we can write

$$U(x) - \xi = |A(U(x) - \xi)| \frac{U(x) - \xi}{|A(U(x) - \xi)|} =: \rho(x)\boldsymbol{n}(x), \tag{2.11}$$

where $\rho(x) \geqslant 0$, and the vector $\boldsymbol{n}$ is normalized so that $|A\boldsymbol{n}(x)| = 1$. We call the expression $U - \xi = \rho(x)\boldsymbol{n}(x)$ the *polar form* of $U - \xi$. Note that ρ is defined for all x, and that the polar form of U is well defined for $\rho \neq 0$, that is, $\rho > 0$. For $U \in W^{1,2}_{\mathrm{loc}}$ and on the set $\{x : \rho(x) > 0\}$, it follows that $\rho, \boldsymbol{n} \in W^{1,2}_{\mathrm{loc}}$. Moreover,

$$\begin{aligned} |AU'|^2 &= \langle A^2U', U'\rangle \\ &= \langle A^2(\rho'\boldsymbol{n} + \rho\boldsymbol{n}'), \rho'\boldsymbol{n} + \rho\boldsymbol{n}'\rangle \\ &= (\rho')^2 + \rho^2|A\boldsymbol{n}'|^2, \end{aligned}$$

since $\langle A^2\boldsymbol{n}, \boldsymbol{n}'\rangle = 0$. On $\{x : U(x) = \xi\}$, on the other hand, we have $|U'| = 0$, in the $W^{1,2}$ sense. Therefore, if Q is any measurable set, then

$$\int_Q |AU'|^2 \, \mathrm{d}x = \int_{Q\cap\{\rho>0\}} [(\rho'(x))^2 + \rho^2(x)|A\boldsymbol{n}'(x)|^2] \, \mathrm{d}x,$$

and in what follows an integral like the one on the left will be interpreted in this way.

If U_α is a solution of (2.2), then a consequence of proposition 2.1 is that

$$U_\alpha(x) = \begin{cases} \xi_p + \rho_p(x)\boldsymbol{n}_p(x) & \text{if } x \leqslant -L, \\ \xi_q + \rho_q(x)\boldsymbol{n}_q(x) & \text{if } x \geqslant +L, \end{cases} \tag{2.12}$$

with $0 \leqslant \rho_i \leqslant \ell$, for $i = p, q$. We now derive necessary conditions for U_α to be a global minimizer of the constrained problem.

PROPOSITION 2.3. *Let U_α be a solution to (2.2) of the form (2.12) with $|A\boldsymbol{n}_i(x)| = 1$, $i = p, q$. Then the following hold:*

$$\rho_q'' - \rho_q|A\boldsymbol{n}_q'|^2 - \langle\nabla F(U_\alpha), \boldsymbol{n}_q\rangle \geqslant 0 \quad \textit{weakly} \tag{2.13}$$

on $(L, \infty) \cap \{x \geqslant L : \rho_q(x) > 0\}$, and with an analogous condition for $x \leqslant -L$. Moreover,

$$\rho_q'' - \rho_q|A\boldsymbol{n}_q'|^2 - \langle\nabla F(U_\alpha), \boldsymbol{n}_q\rangle = 0 \quad \textit{classically} \tag{2.14}$$

in a neighbourhood of any point x_0, where $\rho_q(x_0) \in (0, \ell)$.

Proof. We give the proof for $i = q$; the other case is similar. We consider appropriate variations about ρ_q so that the condition $0 \leqslant \rho(x) \leqslant \ell$ is preserved. So let $r(x) \geqslant 0$ be in C^∞_{c} with support in $(L, \infty) \cap \{x \geqslant L : \rho_q(x) > 0\}$. By the imbedding $W^{1,2}_{\mathrm{loc}} \hookrightarrow C$ the set $\{x \geqslant L : \rho_q(x) > 0\}$ is open in $[L, \infty)$. We introduce the variations $U_\epsilon(x) = U_\alpha(x) - \epsilon r(x)\boldsymbol{n}_q(x)$, that is,

$$U_\epsilon(x) = \begin{cases} U_\alpha(x) & \text{if } x < L, \\ \xi_q + (\rho_q(x) - \epsilon r(x))\boldsymbol{n}_q(x) & \text{if } x \geqslant L, \end{cases}$$

which satisfy the constraint for $\epsilon > 0$ and sufficiently small. Therefore, the function $\epsilon \to E(U_\epsilon)$ is defined on $[0, \epsilon_0]$ and satisfies the condition $E(U_\epsilon) \geqslant E(U_\alpha)$ for $0 \leqslant \epsilon \leqslant \epsilon_0$. Thus,

$$\left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} E(U_\epsilon) \geqslant 0. \tag{2.15}$$

As in remark 2.2 we obtain

$$\begin{aligned}|AU_\epsilon'|^2 &= \langle A^2[(\rho_q' - \epsilon r')\boldsymbol{n}_q + (\rho_q - \epsilon r)\boldsymbol{n}_q'], (\rho_q' - \epsilon r')\boldsymbol{n}_q + (\rho_q - \epsilon r)\boldsymbol{n}_q'\rangle \\ &= (\rho_q' - \epsilon r')^2 + (\rho_q - \epsilon r)^2\langle A^2\boldsymbol{n}_q', \boldsymbol{n}_q'\rangle\end{aligned}$$

for $x \geqslant L$. Therefore,

$$\begin{aligned}E(U_\epsilon) = \int_{x<L} \{\tfrac{1}{2}|AU_\alpha'|^2 + F(U_\alpha)\}\,\mathrm{d}x \\ + \int_{x\geqslant L} \{\tfrac{1}{2}[(\rho_q' - \epsilon r')^2 + (\rho_q - \epsilon r)^2|A\boldsymbol{n}_q'|^2] + F(U_\alpha - \epsilon r\boldsymbol{n}_q)\}\,\mathrm{d}x.\end{aligned}$$

Hence, we compute

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0} E(U_\epsilon) = -\int_{x\geqslant L} \{\rho_q' r' + \rho_q r|A\boldsymbol{n}_q'|^2 + \langle\nabla F(U_\alpha), r\boldsymbol{n}_q\rangle\}\,\mathrm{d}x.$$

This implies via (2.15) that the integral above is non-positive for all test functions $r \geqslant 0$ defined as above, which is equivalent to (2.13).

Suppose now that $\rho_q(x_0) \in (0, \ell)$, for some $x_0 > L$. Then, by continuity, there exists $\delta > 0$ so that $\rho_q(x) \in (0, \ell)$ for all $x \in \bar{B}(x_0, \delta)$. Take $r \in C_{\mathrm{c}}^\infty(B(x_0, \delta))$ and note that the variations $U_\epsilon = U_\alpha + \epsilon r(x)\boldsymbol{n}(x)$ are in $\mathcal{Z}_{L,\ell}^+(\xi_q)$, for $|\epsilon|$ small enough. Thus, $\epsilon \to E(U_\epsilon)$ is defined on $(-\epsilon_0, \epsilon_0)$ and $E(U_\epsilon) \geqslant E(U_\alpha)$, for $-\epsilon_0 \leqslant \epsilon \leqslant \epsilon_0$. Therefore, (2.15) holds as an equality. Then

$$\int_{x\geqslant L} \{\rho_q' r' + \rho_q r|A\boldsymbol{n}_q'|^2 + \langle\nabla F(U_\alpha), r\boldsymbol{n}_q\rangle\}\,\mathrm{d}x = 0$$

for all $r \in C_{\mathrm{c}}^\infty(B(x_0, \delta))$. This is, however, equivalent to (2.14) in the weak sense in $W^{1,2}(B(x_0, \delta))$ or, equivalently,

$$A^2U_\alpha'' - \nabla F(U_\alpha) = 0 \quad \text{in } B(x_0, \delta) \tag{2.16}$$

weakly. Using the fact that $F \in C^2$ and bootstrap arguments we conclude that U_α is C^3 on $B(x_0, \delta)$. Thus, U_α satisfies (2.16) classically. Since $\rho_q > 0$ on $B(x_0, \delta)$, it follows that (2.14) is satisfied classically on $B(x_0, \delta)$. The proof of the proposition is complete. □

3. On the minimizer of the constrained problem

We denote by $\|A\|$ the induced norm of the matrix A, that is, the one defined by $\|A\| = \sup\{|A\xi|/|\xi| : \xi \neq 0\}$. Observe that for $|A\xi| = 1$ we have $\lambda_{\max}^{-1} \leqslant |\xi| \leqslant \lambda_{\min}^{-1}$, where $\lambda_{\min}$ and $\lambda_{\max}$ are the minimum and maximum eigenvalues of A. Therefore, condition (H3) on F implies the following.

(H3′) There exists a constant $\beta' := \beta(\lambda_{\min}/\lambda_{\max})$ such that

$$0 < t < \beta'\|A\| \quad \text{and} \quad |A\xi| = 1 \Longrightarrow \langle\nabla F(\xi_i + t\xi), \xi\rangle > 0, \tag{3.1}$$

for all global minima ξ_i of F, $i = 1, \dots, n$.

We set $\ell_0 := \beta'\|A\|$ and we may assume that $2\ell_0 < \min\{|A(\xi_i - \xi_j)| : i, j = 1, \dots, n\}$.

LEMMA 3.1. *Let $\ell < \ell_0$. If U_α is a minimizer of the constrained problem (2.2), then for $|x| \geqslant L$ it is $U_\alpha(x) = \xi_i + \rho_i(x)\boldsymbol{n}_i(x)$, $i = p, q$, with $\rho(x) \leqslant \ell < \ell_0$. Then, dropping subscripts, ρ satisfies*

$$\rho'' > 0 \text{ weakly} \tag{3.2}$$

on $\{|x| \geqslant L : \rho(x) > 0\}$.

Proof. By (2.13), (2.12) and on $\{|x| \geqslant L : \rho(x) > 0\}$ we have

$$\rho'' - \rho|A\boldsymbol{n}'|^2 \geqslant \langle \nabla F(\xi + \rho\boldsymbol{n}), \boldsymbol{n}\rangle,$$

whence (3.2) follows via (3.1), since $\rho \leqslant \ell$. □

LEMMA 3.2. *Let ℓ and U_α be as in lemma 3.1. Suppose that*

(i) *$\rho_1 < \rho_2 < \ell$ and $\rho(a) = \rho(b) = \rho_1$ for $L \leqslant a < b$ (respectively, $b < a \leqslant -L$),*

(ii) *$\rho(x) \leqslant \rho_2$ on $[a, b]$ (respectively, $[b, a]$).*

Then $\rho(x) < \rho_1$ on (a, b) (respectively, (b, a)).

Proof. Since $U_\alpha \in W^{1,2}_{\text{loc}} \hookrightarrow C$, the boundary conditions $\rho(a) = \rho(b) = \rho_1$ are well defined. Moreover, by continuity the set $\{x : \rho(x) > \rho_1\}$ is open and we may assume that (a, b) is a connected component of this set. By (3.2) $\rho'' \geqslant 0$ on (a, b) and so, by the maximum principle, ρ attains its maximum at a or at b. Thus, $\rho(x) \leqslant \rho_1$ on (a, b). The strict inequality follows by the strong maximum principle, since ρ is continuous on $[a, b]$ and C^2 on (a, b), as implied by proposition 2.3. The proof is complete. □

LEMMA 3.3. *Let ℓ and U_α be as in lemma 3.1. Then ρ can attain the value ℓ, if at all, at $x = \pm L$. Moreover, ρ is strictly monotonically decreasing to 0 in $x \geqslant L$, with an analogous result for $x \leqslant -L$.*

Proof. We begin by showing that the equation

$$\rho(x) = \rho^*, \quad 0 < \rho^* < \ell < \ell_0, \tag{3.3}$$

has at most one solution in $x \geqslant L$. We argue by contradiction, so assume that there exist $a < b$ such that $\rho(a) = \rho(b) = \rho^*$.

CASE 1. Assume that there exists $c \in (a, b)$ such that $\rho(c) > \rho^*$. Thus, if (a^*, b^*) is the maximal connected component of the set $\{x \in (a, b) : \rho(x) > \rho^*\}$ containing c, the following hold:

$$a^* < b^*, \quad \rho(a^*) = \rho(b^*) = \rho^*, \quad \rho(x) > \rho^*, \quad x \in (a^*, b^*). \tag{3.4}$$

This behaviour though is excluded by lemma 3.2.

CASE 2. We assume now that $\rho(x) \leqslant \rho^*$ in (a, b) and $\rho(a) = \rho(b) = \rho^*$. Since $\rho^* < \ell$, locally near b the minimizer U_α does not realize the constraint and satisfies the equation $A^2 U''_\alpha - \nabla F(U_\alpha) = 0$ classically. In particular, it is smooth near b; hence, ρ is defined and is smooth near b. Let $d \in (a, b)$ be such that $\rho > 0$ on (d, b).

On (d,b) ρ satisfies $\rho'' > 0$ by (3.2); hence, $\rho'(b) > 0$ by the Hopf boundary lemma. Therefore, $\rho(x) > \rho^*$ in a right neighbourhood of b. On the other hand, from (2.3) we deduce that

$$\int_{|x|\geqslant L} F(U_\alpha)\,\mathrm{d}x < \infty.$$

In light of (H1) and (H3′) we conclude that, for the integral to be finite, we must have $\rho(x_j) \to 0$ along a sequence $x_j \to \infty$. But then, by continuity, we deduce the existence of a $c > b$ such that $\rho(b) = \rho(c) = \rho^*$ and $\rho(x) > \rho^*$ on (b,c), which contradicts lemma 3.2. Consequently, the case under discussion $\rho(a) = \rho(b) = \rho^*$, $\rho(x) \leqslant \rho^*$ on (a,b) cannot occur either. Thus, we have proved that (3.3) has at most one solution.

Suppose now that $\rho(\bar{x}) = \ell$, for some $\bar{x} > L$. If $\rho(L) < \ell$, we arrive at a contradiction by choosing $\rho^* \in (\rho(L), \ell)$ in (3.3) and recalling that $\rho(x) \to 0$ as $x \to \infty$. Thus, necessarily, $\rho(x) \equiv \ell$ on $[L, \bar{x}]$. But then U_α is smooth on $[L, \bar{x}]$ and $\rho''(x) = 0$ there, violating the condition that $\rho'' > 0$ by (3.2). Thus, this option also leads to a contradiction. The proof is complete. □

The following lemma is especially significant because it can be used to control the minimizer outside the cylinders.

Lemma 3.4. *Let U_α be a minimizer of the constrained problem and let $\xi_k \in \{\xi_p, \xi_q\}$. Let $\hat{\rho}$ be a constant with $2\hat{\rho} < \ell_0$, and assume that, for some $x_1 < x_2$,*

$$|A(U_\alpha(x_1) - \xi_k)| = |A(U_\alpha(x_2) - \xi_k)| = \hat{\rho}. \tag{3.5}$$

Then, for $x \in [x_1, x_2]$, the following holds:

$$|A(U_\alpha(x) - \xi_k)| \leqslant 2\hat{\rho}. \tag{3.6}$$

Proof. Set $I = [x_1, x_2]$, and define $G = \{x \in I : |A(U_\alpha(x) - \xi_k)| > \hat{\rho}\}$. If $G = \varnothing$, then (3.6) holds trivially, so we may assume that $G \neq \varnothing$. Let $U_\alpha(x) = \xi_k + \rho(x)\boldsymbol{n}(x)$ be the polar form of U_α on I. Then, because of the normalization of $\boldsymbol{n}$, we have that $\rho = |A(U_\alpha - \xi_k)|$, and hence

$$G = \{x \in I : \rho(x) > \hat{\rho}\}. \tag{3.7}$$

U_α is continuous, via the imbedding $W^{1,2}_{\mathrm{loc}} \hookrightarrow C$, and so is ρ. Thus, G is an open set. For an arbitrary but fixed $\delta > 0$ satisfying $2\hat{\rho} + \delta < \ell_0$ we split G into

$$\begin{aligned} G_+ &= \{x \in I : \rho(x) > 2\hat{\rho} + \delta\}, \\ G_- &= \{x \in I : \hat{\rho} < \rho(x) \leqslant 2\hat{\rho} + \delta\}. \end{aligned}$$

We will show that the measure $|G_+|$ of G_+ is zero. Observe that $x_1, x_2 \in \partial G$ and that, trivially, U_α is a global minimizer of the localized problem

$$\min_{\substack{u \in W^{1,2}(G;\mathbb{R}^n),\\ |A(u(x_i)-\xi_k)|=\hat{\rho},\ i=1,2}} \int_G \{\tfrac{1}{2}|Au'|^2 + F(u)\}\,\mathrm{d}x.$$

Considering the cut-off function

$$h(s)=\begin{cases}1 & \text{if } s\leqslant\hat\rho,\\ \dfrac{2\hat\rho+\delta-s}{\hat\rho+\delta} & \text{if } \hat\rho\leqslant s\leqslant 2\hat\rho+\delta,\\ 0 & \text{if } s\geqslant 2\hat\rho+\delta,\end{cases} \tag{3.8}$$

we define for $x\in[x_1,x_2]$ the modified function

$$\hat U_\alpha(x)=\xi_k+\hat\rho h(\rho(x))\boldsymbol{n}(x). \tag{3.9}$$

Note that $0=h(2\hat\rho+\delta)\leqslant h(s)\leqslant h(\hat\rho)=1$. Moreover, $\hat U_\alpha$, being the composition of a $W^{1,2}$ function with a Lipschitz function, belongs to $W^{1,2}(G)$. For this result we refer the reader to [8].

Claim 3.5. *$E(\hat U_\alpha;G)<E(U_\alpha;G)$, that is*

$$\int_G\{\tfrac12|A\hat U_\alpha'|^2+F(\hat U_\alpha)\}\,\mathrm{d}x<\int_G\{\tfrac12|AU_\alpha'|^2+F(U_\alpha)\}\,\mathrm{d}x. \tag{3.10}$$

Proof of claim 3.5. We first show that

$$|A\hat U_\alpha'|<|AU_\alpha'|\quad\text{on } G. \tag{3.11}$$

Recalling that $|AU_\alpha'|^2=(\rho')^2+\rho^2|A\boldsymbol{n}'|^2$ (see remark 2.2), in analogy we compute

$$\begin{aligned}|A\hat U_\alpha'|^2&=[(\hat\rho h(\rho))']^2+[\hat\rho h(\rho)]^2|A\boldsymbol{n}'|^2\\ &\leqslant\frac{\hat\rho^2}{(\hat\rho+\delta)^2}(\rho')^2+\hat\rho^2|A\boldsymbol{n}'|^2 && (h\leqslant1)\\ &<(\rho')^2+\rho^2|A\boldsymbol{n}'|^2 && \text{by (3.7)}\\ &=|AU_\alpha'|^2.\end{aligned}$$

Therefore, (3.11) is verified. Next we show that

$$F(\hat U_\alpha(x))<F(U_\alpha(x))\quad\text{on } G_- \tag{3.12}$$

or, equivalently, $F(\xi_k+\hat\rho h(\rho(x))\boldsymbol{n})<F(\xi_k+\rho(x)\boldsymbol{n})$ on $\hat\rho<\rho(x)\leqslant 2\hat\rho+\delta$. Since $h\leqslant1$, we have $\hat\rho h(\rho(x))\leqslant\hat\rho<\rho(x)$. Therefore, (3.12) follows from the fact that the function $g(t)=F(\xi_k+t\boldsymbol{n})$, $0<t<\ell_0$, is strictly increasing since, via (3.1), $g'(t)=\langle\nabla F(\xi_k+t\boldsymbol{n}),\boldsymbol{n}\rangle>0$, and $\hat\rho+\delta<\ell_0$. Noting that, on G_+, $\hat U_\alpha=\xi_k$, and hence $F(\hat U_\alpha)=0<F(U_\alpha)$, finally, we obtain

$$\begin{aligned}&\int_G[\tfrac12|A\hat U_\alpha'|^2+F(\hat U_\alpha)]\,\mathrm{d}x\\ &\quad\overset{(3.11)}{\leqslant}\int_G[\tfrac12|AU_\alpha'|^2+F(\hat U_\alpha)]\,\mathrm{d}x\\ &\quad=\int_{G_-}[\tfrac12|AU_\alpha'|^2+F(\hat U_\alpha)]\,\mathrm{d}x+\int_{G_+}\tfrac12|AU_\alpha'|^2\,\mathrm{d}x\end{aligned}$$

$$\overset{(3.12)}{\leqslant} \int_{G_-} [\tfrac{1}{2}|AU'_\alpha|^2 + F(U_\alpha)]\,\mathrm{d}x + \int_{G_+} \tfrac{1}{2}|AU'_\alpha|^2\,\mathrm{d}x$$

$$< \int_{G_-} [\tfrac{1}{2}|AU'_\alpha|^2 + F(U_\alpha)]\,\mathrm{d}x + \int_{G_+} [\tfrac{1}{2}|AU'_\alpha|^2 + F(U_\alpha)]\,\mathrm{d}x.$$

The proof of the claim is complete. □

Since (3.10) violates the condition that U_α is a global minimizer, we conclude that $|G_+| = 0$ or, equivalently, $|A(U_\alpha - \xi_k)| \leqslant 2\hat{\rho} + \delta$ holds almost everywhere on G, and hence everywhere because U_α is regular. This result is true for every $\delta > 0$. Therefore, $|A(U_\alpha - \xi_k)| \leqslant 2\hat{\rho}$ on G. Since $\rho(x) \leqslant \hat{\rho}$, for $x \in I \setminus G$, (3.6) holds on all of $[x_1, x_2]$. □

From the proof of lemma 3.4 we obtain the following lemma.

Lemma 3.6. *Let ξ_k be a global minimum of F, let $\hat{\rho}$ be a constant with $2\hat{\rho} \leqslant \ell_0$, and let $U \in W^{1,2}([x_1, x_2]; \mathbb{R}^n)$ with polar form $U(x) = \xi_k + \rho(x)\boldsymbol{n}(x)$ be such that*

(i) $|A(U(x_1) - \xi_k)| = |A(U(x_2) - \xi_k)| = \hat{\rho}$,

(ii) *there exists $x_0 \in (x_1, x_2)$ such that $\rho(x_0) = |A(U(x) - \xi_k)| > \hat{\rho}$.*

There then exists $\hat{U} \in W^{1,2}([x_1, x_2]; \mathbb{R}^n)$ satisfying

(a) $\hat{U}(x_1) = U(x_1)$, $\hat{U}(x_2) = U(x_2)$,

(b) $|A(\hat{U}(x) - \xi_k)| < \hat{\rho}$, $x \in (x_1, x_2)$,

(c) $E(\hat{U}; (x_1, x_2)) < E(U; (x_1, x_2))$.

Note that, as opposed to the previous cases, the function U is not necessarily a minimizer of the constrained problem. This result will be used in later sections.

4. The existence theorem for two minima

The solution of the constrained problem (2.2) is not a solution of (1.1) unless the constraint is not realized. In the following theorem we show that if the potential has exactly two minima, then the constraint can be removed yielding a heteroclinic connection.

Theorem 4.1. *Let F be a $C^2(\mathbb{R}^n)$ potential function with only two equal minima at ξ_1 and ξ_2 satisfying the conditions (H1), (H2) and (H3′). There then exists a connection between ξ_1 and ξ_2.*

Proof. Let ℓ be such that $\frac{1}{2}\ell_0 \leqslant \ell < \ell_0$, where $\ell_0 = \beta'\|A\|$, and β' is as in (H3′). For $\alpha = (1, 2)$, let U_α be a solution of the constrained problem. Then $U_\alpha(x) = \xi_i + \rho_i(x)\boldsymbol{n}_i(x)$, $i = 1, 2$, for $|x| \geqslant L$ with $\rho_i(x) \leqslant \ell$. We need to show that the constraint can be avoided for L sufficiently large. We recall, by lemma 3.3, that this may realized at $x = \pm L$.

Case 1. Either (i) $\rho(-L) < \ell$ and $\rho(L) = \ell$ or (ii) $\rho(-L) = \ell$ and $\rho(L) < \ell$.

(i) By translating $U_\alpha(x)$ slightly to the left we can avoid the constraint. So, for $\tau > 0$ and sufficiently small, $U_\alpha(x+\tau)$ provides a solution to (1.1). Case (ii) is treated similarly.

CASE 2. Assume that $\rho(-L) = \rho(L) = \ell$.

(i) We show that $U_\alpha(x)$ is outside $B(\xi_1, \frac{1}{4}\beta') \cup B(\xi_2, \frac{1}{4}\beta')$ for $|x| < L$. To prove this claim we argue by contradiction. First we take $B(\xi_2, \frac{1}{4}\beta')$. Suppose that there exists $x_1 \in (-L, L)$ such that $U_\alpha(x_1) \in B(\xi_2, \frac{1}{4}\beta')$. Clearly, there is also a $x_2 > L$ such that $U_\alpha(x_2) \in B(\xi_2, \frac{1}{4}\beta')$ since, by lemma 3.3, $U_\alpha(x)$ approaches ξ_2 as $x \to \infty$. Thus, $|U_\alpha(x_i) - \xi_2| < \frac{1}{4}\beta'$, for $i = 1, 2$, and therefore, via the definition of the norm, $|A(U_\alpha(x_i) - \xi_2)| < \ell_0/4$. Now, applying lemma 3.4, we conclude that $\rho(x) < \frac{1}{2}\ell_0$ on $[x_1, x_2]$. In particular, $\ell = \rho(L) < \frac{1}{2}\ell_0$, which is a contradiction by the choice $\ell \geqslant \frac{1}{2}\ell_0$. Thus, there is no such x_1. The case $B(\xi_1, \frac{1}{4}\beta')$ is treated analogously.

(ii) Making use of the fact that F has exactly two global minima, via (H1) and (H2) it follows that there exists $c_0 > 0$ such that

$$F(\xi) \geqslant c_0 > 0, \qquad |\xi - \xi_i| \geqslant \tfrac{1}{4}\beta', \quad i = 1, 2. \tag{4.1}$$

Consequently, using (i), we find the estimate

$$\int_{-L}^{L} F(U_\alpha(x))\,\mathrm{d}x \geqslant 2Lc_0. \tag{4.2}$$

Recalling that the function U_0 in (2.4) is independent of L, as long as $L > L_0$, and that $E(U_\alpha) \leqslant E(U_0) < \infty$, via (4.2) we obtain

$$E(U_0) \geqslant E(U_\alpha) \geqslant \int_{-L}^{L} F(U_\alpha(x))\,\mathrm{d}x \geqslant 2Lc_0.$$

This leads to a contradiction if L is taken so that $2Lc_0 > E(U_0)$. Thus, case 2 is impossible for large L. The proof is complete. □

REMARK 4.2. Let U_{12} be the connection provided by theorem 4.1. It can be proved that U_{12} is a minimizer of the action in the class

$$\mathcal{A} = \left\{ U \in W^{1,2}_{\mathrm{loc}}(\mathbb{R}; \mathbb{R}^n) : \exists x_1 < x_2 \text{ such that } \begin{array}{ll} |A(U(x) - \xi_1)| \leqslant \ell & \text{for } x \leqslant x_1, \\ |A(U(x) - \xi_2)| \leqslant \ell & \text{for } x \geqslant x_2, \end{array} \right\}$$

where $\ell < \ell_0$. Thus, it is a *local minimum* of the action. The proof is similar to the one in [2] and is omitted. We take for definiteness $\ell = \frac{1}{2}\ell_0$ and we choose c_0 such that $F(\xi) \geqslant c_0$ for $\xi \in \mathbb{R}^n \setminus B(\xi_1, \frac{1}{4}\beta') \cup B(\xi_2, \frac{1}{4}\beta')$. Let $L_0^* = E(U_0)/c_0$ and assume without loss of generality that $L_0^* > L_0$. Simplifying the notation of proposition 2.1, we set $\mathcal{Z}_L = \mathcal{Z}^-_{L,\ell}(\xi_1) \cap \mathcal{Z}^+_{L,\ell}(\xi_2)$ and we observe the following. If $L_1 < L_2$, then $\mathcal{Z}_{L_1} \subset \mathcal{Z}_{L_2} \subset \mathcal{A}$, and hence

$$\inf_{\mathcal{A}} E(U) \leqslant \inf_{\mathcal{Z}_{L_2}} E(U) \leqslant \inf_{\mathcal{Z}_{L_1}} E(U).$$

For $L > L_0^*$ (and $\ell = \frac{1}{2}\ell_0$), theorem 4.1 implies that the solution U_α of the constrained problem in $\mathcal{Z}_L$ cannot touch the rim of both cylinders. Thus, it renders a solution U_{12} of (1.1) and hence a minimizer of E in $\mathcal{A}$. Hence, for each $\delta > 0$, we have

$$E(U_{12}) = \inf_{\mathcal{Z}_{L+\delta}} E(U) = \inf_{\mathcal{A}} E(U).$$

A reading of the equality above is that, as L increases, the solution of the constrained problem is stabilized, and hence for L sufficiently large it becomes independent of L.

Corollary 4.3. *Let F be a $C^2(\mathbb{R}^n)$ potential function with three equal minima at ξ_1, ξ_2 and ξ_3 satisfying the conditions (H1), (H2) and (H3′). Let U_{12} be a solution of the constrained problem joining ξ_1 and ξ_2, and assume that there exists $\varepsilon_1 > 0$ so that U_{12} does not intersect $B(\xi_3, \varepsilon_1)$ for sufficiently large L. There then exists a connection between ξ_1 and ξ_2.*

Proof. This follows from the proof of theorem 4.1 and is omitted. □

5. An application

In this section we discuss a model example proposed in [6] to study the structure of interface boundaries in crystals. The potential $F = F(X, Y, Z)$, where X, Y, Z are order parameters, represents the bulk free energy, and hence respects the symmetries of the crystal. In particular, it is invariant under any permutation of the variables. It is a fourth degree polynomial ($F(X, Y, Z) = 2(X^2 + Y^2 + Z^2) - 12XYZ + (X^4 + Y^4 + Z^4) + (X^2Y^2 + Y^2Z^2 + Z^2X^2)$) with global minima at $\xi_1 = (0, 0, 0)$, $\xi_2 = (1, 1, 1)$, $\xi_3 = (-1, -1, 1)$, $\xi_4 = (1, -1, -1)$ and $\xi_5 = (-1, 1, -1)$. In our analysis we do not use the particular form of F; however, we keep and use the symmetries of the potential that are, at any rate, dictated by the underline lattice. These symmetries are described by $F(S\xi) = F(\xi)$, where S is an orthogonal matrix belonging to the group $G = G_1G_2$, where

$$\left.\begin{aligned} G_1 &= \{S : S \in \mathrm{SO}_3 \text{ and } S \text{ is diagonal}\},\\ G_2 &= \{S : S \text{ is a permutation matrix of order 3}\}.\end{aligned}\right\} \tag{5.1}$$

In this model the matrix A^2 is written as

$$A^2 = \begin{bmatrix} n_1^2 & 0 & 0 \\ 0 & n_2^2 & 0 \\ 0 & 0 & n_3^2 \end{bmatrix} + \lambda^2 \begin{bmatrix} n_2^2 + n_3^2 & 0 & 0 \\ 0 & n_1^2 + n_3^2 & 0 \\ 0 & 0 & n_1^2 + n_2^2 \end{bmatrix},$$

where $\boldsymbol{n} = (n_1, n_2, n_3)$ is the unit normal to the interface separating an ordered from a disordered phase, and λ is the anisotropy parameter. The isotropic case is the one in which the coefficients in the resulting system are independent of the orientation of $\boldsymbol{n}$. This occurs if and only if $\lambda^2 = 1$ (see also (5.3), below), leading to $A^2 = I$.

5.1. The two-dimensional case

Certain simplifications compatible with the symmetries of the potential may reduce the dimension by 1. Taking, for example, $n_2 = n_3$, the symmetry $Y = Z$ is

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preserved through the transition and the corresponding profile is restricted to the plane $Y = Z$ [4]. Thus, for $\boldsymbol{n} = (\cos\epsilon, \sin\epsilon/2^{1/2}, \sin\epsilon/2^{1/2})$, $0 \leqslant \epsilon \leqslant \pi$, and

$$f(u,v) = F\biggl(u, \frac{v}{\sqrt{2}}, \frac{v}{\sqrt{2}}\biggr) \tag{5.2}$$

with $u = X$, $v = \sqrt{2}Y = \sqrt{2}Z$, the system (1.1), (5.2) is reduced to

$$\left.\begin{aligned} (\cos^2\epsilon + \lambda^2 \sin^2\epsilon)u'' &= f_u(u,v),\\ (\lambda^2\cos^2\epsilon + (1+\lambda^2)/2\sin^2\epsilon)v'' &= f_v(u,v). \end{aligned}\right\} \tag{5.3}$$

The choices $\epsilon = 0$ and $\epsilon = \frac{1}{2}\pi$ lead, after rescaling, respectively to the systems

$$u'' = f_u(u,v), \quad \lambda^2 v'' = f_v(u,v),$$

and

$$v'' = f_v(u,v), \quad \lambda^2 u'' = f_u(u,v),$$

which were actually the departure point for this work. In this setting, the minima of f are attained at $(0,0)$ and $(1, \pm 2^{1/2})$. At this point we note that the cases above correspond to planar cuts of the crystal in the normal directions $\boldsymbol{n} = (1,0,0)$ and $\boldsymbol{n} = (0, 1/2^{1/2}, 1/2^{1/2})$, respectively. For $\lambda \ll 1$, the extreme anisotropic case, existence of connections for both systems is established in [4, 5, 10, 11] via singular perturbation techniques. Motivated by these two examples we consider the 2-system

$$A^2 U'' - \nabla f(U) = 0, \tag{5.4}$$

where A^2 is a diagonal matrix with positive entries, and the function $f : \mathbb{R}^2 \to \mathbb{R}$ satisfies hypotheses (H1), (H2) and (H3′), with minima at $z_1 = (0,0)$, $z_2 = (r_0, s_0)$ and $z_3 = (r_0, -s_0)$, $r_0 > 0$, $s_0 > 0$, and additionally satisfies the following symmetry condition.

(H4) $f(r,s) = f(r,-s)$ for all $r, s \in \mathbb{R}$.

If $U = (u_1, u_2)^{\mathrm{T}}$, we write its reflection as $\bar{U} = (u_1, -u_2)^{\mathrm{T}}$. Via (H4) and the form of A^2 it follows that if U is a solution of (5.4), then $\bar{U}$ is also a solution, and $E(U) = E(\bar{U})$.

PROPOSITION 5.1. *Let f be as above and let z_2 and z_3 be the symmetric minima of f. There then exists a connection between z_1 and z_2, and hence, by symmetry, also between z_1 and z_3.*

Proof. Let U_{12}^L be a minimizer of the constrained problem. By corollary 4.3 it is sufficient to show that U_{12}^L stays bounded away from z_3 for sufficiently large L, that is, there exists $\varepsilon_1 > 0$ so that $U_{12}^L(x)$ stays outside $B(z_3, \varepsilon_1)$. Dropping the superscripts, we proceed by contradiction, so we assume that U_{12} intersects $B(z_3, \varepsilon)$, where ε is arbitrarily small. We may take ε so that $B(z_3, \varepsilon\|A\|)$ is contained in the lower open half-plane. Let x_2 be such that $|A(U_{12}(x_2) - z_3)| = \varepsilon\|A\|$, and $|A(U_{12}(x) - z_3)| > \varepsilon\|A\|$, whenever $x > x_2$. Similarly, let x_3 be such that $|A(U_{12}(x_3) - z_2)| = \varepsilon\|A\|$, and $|A(U_{12}(x) - z_2)| < \varepsilon\|A\|$, whenever $x > x_3$. Then

$x_2 < x_3$. By continuity of U_{12} there exists a point $x_0 \in (x_2, x_3)$ such that $U_{12}(x_0)$ is on the r-axis. By symmetry of f it follows that $U_{12}(x_0) = \bar{U}_{12}(x_0)$. Defining

$$\tilde{U}_{12}(x) = \begin{cases} \bar{U}_{12}(x) & \text{if } x \leqslant x_0, \\ U_{12}(x) & \text{if } x \geqslant x_0, \end{cases} \tag{5.5}$$

we see that $\tilde{U}_{12}$ joins z_1 to z_2 and satisfies the constraints and, moreover, that $E(U_{12}) = E(\tilde{U}_{12})$. Next, modifying $\tilde{U}_{12}$ in $[x_2, x_3]$, as in lemma 3.6, we obtain a $W^{1,2}_{\text{loc}}(\mathbb{R})$ function $\hat{U}_{12}$ satisfying $E(\hat{U}_{12}) < E(\tilde{U}_{12})$. This contradicts the condition that U_{12} is a minimizer. Therefore, U_{12} stays bounded away from z_3. The proof of the proposition is complete. □

Remark 5.2. The existence of the connection between the symmetric minima z_2 and z_3 is not guaranteed. In [3] an example is given where a three-well potential f is symmetric with respect to the s-axis. The symmetric minima are at $z_2 = 1$ and $z_3 = -1$, while the third, z_1, is on the s-axis. The connection between z_2 and z_3 exists if and only if $|z_1 - z_2| > [2(3^{1/2} - 1)]^{1/2}$. This phenomenon is analysed in detail in [2].

Remark 5.3. Let S be the transformation $S : (r, s) \to (r, -s)$. Then, by identifying U_{12} with a curve γ joining z_1 to z_2, we may write $\gamma = \gamma_+ + \gamma_-$, where γ_- is in the lower half-plane. Then, referring to the proof of proposition 5.1, we may instead take the curve $\tilde{\gamma} = \gamma_+ + S\gamma_-$. Hence, $\tilde{\gamma}$ is contained in the upper half-plane and satisfies $E(\gamma) = E(\tilde{\gamma})$. We then modify $\tilde{\gamma}$ to obtain $\hat{\gamma}$ with $E(\hat{\gamma}) < E(\tilde{\gamma})$.

Remark 5.4. For general dimension N, if S is an orthogonal matrix satisfying $f(SU) = f(U)$ and $AS = SA$, then the following hold.

(i) $E(U) = E(SU)$, since $|ASU'| = |SAU'| = |AU'|$.

(ii) If U is a solution of (1.1) joining the minima ξ_k and ξ_l, with $\xi_k \neq \xi_l$, then SU is a solution of the same equation joining the minima $S\xi_k$ and $S\xi_l$. Indeed,

$$A^2 U'' = \nabla_U F(U) = S^{\mathrm{T}} \nabla_{SU} F(SU) \implies SA^2 U'' = A^2 (SU)'' = \nabla_{SU} F(SU).$$

In the two-dimensional case, the only orthogonal matrices that commute with the diagonal matrix A are the following:

$$S_1 = I_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad S_2 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \qquad S_3 = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad S_4 = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Thus, the result of proposition 5.1 holds if the matrix S_2, which is the case there, is replaced by S_3 or S_4 provided that $f(S_i z) = f(z)$, $i = 3, 4$.

5.2. The three-dimensional case

Let A^2 be a diagonal matrix with positive entries and let $f : \mathbb{R}^3 \to \mathbb{R}$ be a potential function satisfying the conditions (H1), (H2) and (H3′), with minima at the points $\xi_1 = (0, 0, 0), \dots, \xi_5$, and also satisfying the following symmetry condition.

(H4) $f(S\xi) = f(\xi)$.

Here S is an orthogonal matrix belonging to the group $G = G_1 G_2$, defined in (5.1). We note at this point that only the elements of G_1 commute with A^2.

It turns out that in this case there are at least four connections, namely the $\mathrm{O}\xi_2$, $\mathrm{O}\xi_3$, $\mathrm{O}\xi_4$ and $\mathrm{O}\xi_5$, where $\mathrm{O} = \xi_1$ is the origin. First we prove a general result.

LEMMA 5.5. *Let $f : \mathbb{R}^N \to \mathbb{R}$ be a C^2 potential with three equal minima at ξ_1, ξ_2 and ξ_3 satisfying the conditions (H1), (H2) and (H3′) in addition to the symmetry condition $f(SU) = f(U)$, where S is an orthogonal matrix that commutes with A and satisfies $S\xi_1 = \xi_1$. There then exist heteroclinic connections joining ξ_1 to ξ_2 and ξ_1 to ξ_3.*

Proof. We show that a connection between ξ_1 and ξ_2 exists. Let U_{12} be a minimizer of the constrained problem. We claim, as before, that U_{12} stays bounded away from ξ_3. We argue by contradiction, so we assume that for $\varepsilon > 0$ and arbitrarily small, U_{12} intersects $B(\xi_3, \varepsilon)$. We fix δ with $0 < \delta < |\xi_2 - \xi_3|$ and we take $\varepsilon \ll \delta$. Let x_0 be such that

$$|U_{12}(x_0) - \xi_3| = \min\{|U_{12}(x) - \xi_3| : U_{12}(x) \in \bar{B}(\xi_3, \delta)\}.$$

Then $|U_{12}(x_0) - \xi_3| < \varepsilon$. We may assume without loss of generality that $U_{12}(x_0) \neq \xi_3$. (If $U_{12}(x_0) = \xi_3$, then $x_0 < L$, since $U_{12}(x)$ is close to ξ_2 for $x \geqslant L$. Defining

$$\tilde{U}_{12}(x) = \begin{cases} SU_{12}(x) & \text{if } x \leqslant x_0, \\ \xi_2 & \text{if } x \geqslant x_0, \end{cases}$$

we have

$$E(\tilde{U}_{12}) = \int_{-\infty}^{x_0} \{|ASU_{12}'|^2 + f(SU_{12})\}\,\mathrm{d}x = \int_{-\infty}^{x_0} \{|AU_{12}'|^2 + f(U_{12})\}\,\mathrm{d}x < E(U_{12}),$$

by symmetry. But this contradicts the fact that U_{12} is a minimizer.) We set $\xi_0 = SU_{12}(x_0)$ and observe that $|\xi_2 - \xi_0| = |S\xi_3 - SU_{12}(x_0)| = |\xi_3 - U_{12}(x_0)| < \varepsilon$. Then we define the function

$$\tilde{U}_{12}(x) = \begin{cases} SU_{12}(x) & \text{if } x \leqslant x_0, \\ \xi_2 \dfrac{x - x_0}{\varepsilon_1} + \xi_0 \dfrac{x_0 - x + \varepsilon_1}{\varepsilon_1} & \text{if } x_0 < x < x_0 + \varepsilon_1, \\ \xi_2 & \text{if } x \geqslant x_0 + \varepsilon_1, \end{cases}$$

where $\varepsilon_1 > 0$ is to be chosen later. For $x_0 < x < x_0 + \varepsilon_1$ we compute

$$\begin{aligned} |A\tilde{U}_{12}'(x)| &= |A(\xi_2 - \xi_0)/\varepsilon_1| \\ &\leqslant \|A\|\varepsilon/\varepsilon_1, \end{aligned} \tag{5.6}$$

since $\xi_0 \in B(\xi_2, \varepsilon)$. Let $M = \max\{F(\xi) : |\xi - \xi_2| \leqslant \delta\}$. Since $\delta > \varepsilon$, we have

$$\int_{x_0}^{x_0+\varepsilon_1} \{|A\tilde{U}_{12}'(x)|^2 + F(\tilde{U}_{12})\}\,\mathrm{d}x \leqslant \|A\|^2\varepsilon^2/\varepsilon_1 + M\varepsilon_1; \tag{5.7}$$

hence,

$$E(\tilde{U}_{12}) = \int_{-\infty}^{x_0} \{|A\tilde{U}_{12}'(x)|^2 + F(\tilde{U}_{12})\}\,dx + \int_{x_0}^{x_0+\varepsilon_1} \{|A\tilde{U}_{12}'(x)|^2 + F(\tilde{U}_{12})\}\,dx$$
$$\leqslant \int_{-\infty}^{x_0} \{|AU_{12}'(x)|^2 + F(U_{12})\}\,dx + \|A\|^2\varepsilon^2/\varepsilon_1 + M\varepsilon_1. \tag{5.8}$$

Next we show that ε_1 can be chosen so that

$$\|A\|^2\varepsilon^2/\varepsilon_1 + M\varepsilon_1 < \int_{x_0}^{\infty} \{|AU_{12}'(x)|^2 + F(U_{12})\}\,dx := M_1, \tag{5.9}$$

where $M_1 > 0$, by the choice of δ, or, equivalently, that $M\varepsilon_1^2 - M_1\varepsilon_1 + \|A\|^2\varepsilon^2 < 0$. Since ε is arbitrarily small, the discriminant of the binomial is positive, so (5.9) is achieved by choosing ε_1 between the positive zeros $[M_1 \pm (M_1^2 - 4M\|A\|^2\varepsilon^2)^{1/2}]/2M$. Combining (5.8) and (5.9), we arrive at $E(\tilde{U}_{12}) < E(U_{12})$, which is a contradiction since U_{12} is a minimizer. Thus, U_{12} stays bounded away from ξ_3. The result then follows by corollary 4.3. □

PROPOSITION 5.6. *Let $f : \mathbb{R}^3 \to \mathbb{R}$ be a C^2 potential with equal minima at $\xi_1 = (0,0,0)$, $\xi_2, \dots, \xi_5$ satisfying hypotheses (H1), (H2) and (H3′) and the symmetry conditions $f(SU) = f(U)$, where S is an orthogonal matrix in the group G_1 defined in (5.1). There then exist heteroclinic connections joining ξ_1 to ξ_k, $k = 2, \dots, 5$.*

Proof. We show that a connection between ξ_1 and ξ_2 exists. The proof for the other cases is similar. Let U_{12} be a minimizer of the constrained problem. We claim that U_{12} stays bounded away from ξ_i, $i = 3, 4, 5$. We argue by contradiction, so let $\xi_p \in \{\xi_3, \xi_4, \xi_5\}$ be the first point so that U_{12} intersects $B(\xi_p, \varepsilon)$, where ε is arbitrarily small. Let $S \in G_1$ be such that $S\xi_p = \xi_1$. Then, as in lemma 5.5, we construct a function $\tilde{U}_{12}$ satisfying $E(\tilde{U}_{12}) < E(U_{12})$, contradicting the fact that U_{12} is a minimizer. Hence, there exists $\varepsilon_1 > 0$ so that U_{12} does not intersect $\bigcup_{i=3}^{5} B(z_i, \varepsilon_1)$. The proof then is concluded by using corollary 4.3. □

6. The general case for three minima

In the previous section, the symmetry of the potential played an important role in establishing existence of connections in the case of three or more minima. In this section, however, we obtain a quite general sufficient condition for such an existence for general F with three minima. As mentioned in § 1, a condition of this type, with $N = 2$, is also considered in [1] for symmetric potentials and in [2] for geodesic distances defined by the Jacobi functional. In [2] it is proved that for a certain class of potentials this condition is also necessary.

THEOREM 6.1. *Let $F : \mathbb{R}^N \to \mathbb{R}$ be a C^2 potential with three equal minima at ξ_1, ξ_2 and ξ_3, satisfying the conditions (H1), (H2) and (H3′). Denote by e_{pq} the minimum of the constraint problem (2.2), $p, q \in \{1, 2, 3\}$. If*

$$e_{pq} < e_{pr} + e_{rq}, \tag{6.1}$$

for sufficiently large L, then there exists a connection between ξ_p and ξ_q.

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Proof. Assume for definiteness that $p = 1$ and $q = 2$. Then, by hypothesis, there exists $\delta > 0$ such that

$$e_{12} < e_{13} + e_{32} - \delta. \tag{6.2}$$

Assume, also that e_{12} is realized by U_{12}, then $e_{12} = E(U_{12})$. We claim that U_{12} stays bounded away from ξ_3. We argue by contradiction, so we assume that for $\varepsilon > 0$ and small (there exists L such that) U_{12} intersects $B(\xi_3, \varepsilon)$. We may assume that $\varepsilon \ll \delta$ and that $0 < \delta < \min\{|\xi_3 - \xi_1|, |\xi_3 - \xi_2|\}$. Let x_0 be such that $|U_{12}(x_0) - \xi_3| < \varepsilon$. We set $\xi_0 = U_{12}(x_0)$ and define the function

$$\tilde{U}_{13}(x) = \begin{cases} U_{12}(x) & \text{if } x \leqslant x_0, \\ \xi_3 \dfrac{x - x_0}{\varepsilon_1} + \xi_0 \dfrac{x_0 - x + \varepsilon_1}{\varepsilon_1} & \text{if } x_0 < x < x_0 + \varepsilon_1, \\ \xi_3 & \text{if } x \geqslant x_0 + \varepsilon_1, \end{cases}$$

where $\varepsilon_1 > 0$ is to be chosen later. For $x_0 < x < x_0 + \varepsilon_1$, as in (5.6) and (5.7), we compute

$$|A\tilde{U}_{13}'(x)| \leqslant \|A\|\varepsilon/\varepsilon_1,$$

$$\int_{x_0}^{x_0+\varepsilon_1} \{|A\tilde{U}_{13}'(x)|^2 + F(\tilde{U}_{13})\}\,\mathrm{d}x \leqslant \|A\|^2\varepsilon^2/\varepsilon_1 + M\varepsilon_1,$$

where, as before, $M = \max\{F(\xi) : |\xi - \xi_3| \leqslant \delta\}$. Then

$$E(\tilde{U}_{13}) \leqslant E(U_{12}; x \leqslant x_0) + (\|A\|^2\varepsilon^2/\varepsilon_1^2 + M)\varepsilon_1. \tag{6.3}$$

Defining, in a similar fashion,

$$\tilde{U}_{32}(x) = \begin{cases} \xi_3 & \text{if } x \leqslant x_0 - \varepsilon_1, \\ \xi_3 \dfrac{x_0 - x}{\varepsilon_1} + \xi_0 \dfrac{x - x_0 + \varepsilon_1}{\varepsilon_1} & \text{if } x_0 - \varepsilon_1 < x < x_0, \\ U_{12}(x) & \text{if } x \geqslant x_0, \end{cases}$$

we also get

$$E(\tilde{U}_{32}) \leqslant E(U_{12}; x \geqslant x_0) + (\|A\|^2\varepsilon^2/\varepsilon_1^2 + M)\varepsilon_1. \tag{6.4}$$

By the definition of the e_{ij}, (6.3) and (6.4), we have

$$\begin{aligned} e_{12} = E(U_{12}) &= E(U_{12}; x \leqslant x_0) + E(U_{12}; x \geqslant x_0) \\ &\geqslant e_{13} + e_{32} - 2(\|A\|^2\varepsilon^2/\varepsilon_1^2 + M)\varepsilon_1. \end{aligned} \tag{6.5}$$

Combining (6.2) and (6.5), we obtain

$$2M\varepsilon_1^2 - \delta\varepsilon_1 + 2\|A\|^2\varepsilon^2 > 0. \tag{6.6}$$

However, the choice of

$$\varepsilon < \frac{\delta}{4\|A\|\sqrt{M}}$$

and ε_1 between the positive zeros of the binomial above leads to a contradiction of (6.6). Thus, U_{12} stays bounded away from ξ_3. The conclusion of the theorem then follows by corollary 4.3. □

What follows is actually lemma 5.5, the proof of which is significantly simplified when the sufficient condition discussed is used.

COROLLARY 6.2. *Let* $F : \mathbb{R}^N \to \mathbb{R}$ *be a* C^3 *potential with three equal minima at* ξ_1*,* ξ_2 *and* ξ_3 *satisfying the conditions (H1), (H2) and (H3′) in addition to the symmetry condition* $F(SU) = F(U)$*, where* S *is an orthogonal matrix satisfying* $SA = AS$ *and* $S\xi_1 = \xi_1$*. There then exist at least two heteroclinic connections.*

Proof. By symmetry, $e_{12} = e_{13}$. On the other hand, e_{32} is realized by a continuous function joining different states, and hence $e_{32} > 0$. Therefore, $e_{12} < e_{13} + e_{32}$ and $e_{13} < e_{12} + e_{23}$, and the conclusion follows from theorem 6.1. □

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