

Master of Science in Advanced Mathematics and Mathematical Engineering

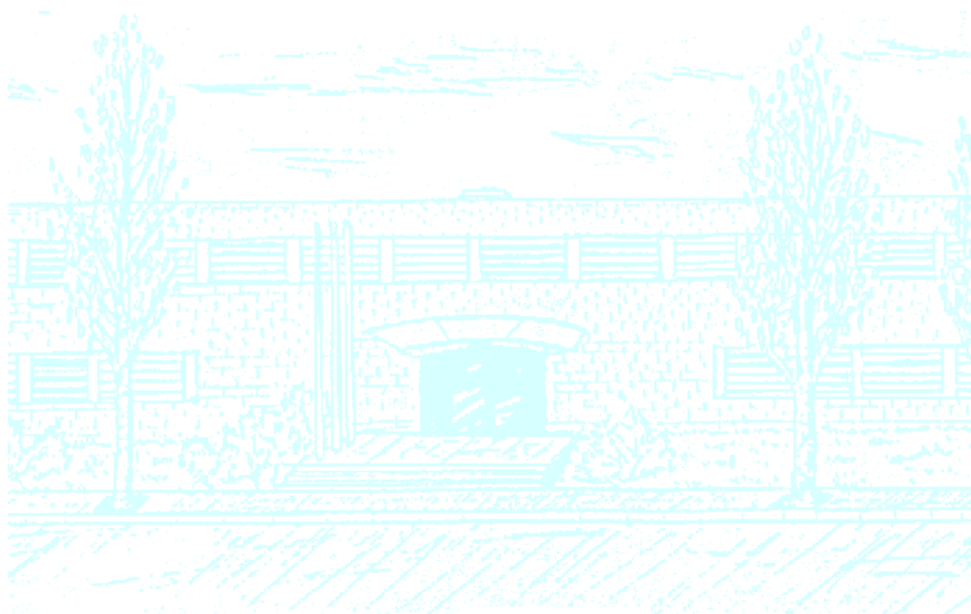
Title: Critical velocity in kink solutions of the sine-Gordon equation

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Critical velocity in kink solutions of the sine-Gordon equation

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Abstract

The sine-Gordon equation is a well-known partial differential equation that features soliton solutions. Here, a perturbed version of the equation is studied. In particular, this perturbed equation is known to admit soliton-like solutions. These solutions present rich dynamics, including the presence of a critical value of the velocity.

The goal of this work is to present a way to deduce the value of this critical velocity. To do so, an ODE system is obtained from the perturbed sine-Gordon equation using a variational approach, following the work of Fei et al. [3] and Goodman and Haberman [8]. The resulting Hamiltonian system is then studied. From that, a Melnikov integral formula for the critical velocity is deduced via an energy balance reasoning, as outlined in [8]. Finally, the problem is approached from a geometrical point of view that allows for an interpretation of the previous results in terms of intersections of invariant manifolds of periodic orbits.

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1. Introduction

1.1 The sine-Gordon equation

The sine-Gordon equation is a non-linear partial differential equation in two dimensions, a spatial one and a temporal one. For a real variable $u(x, t)$, it reads

$$u_{tt} - u_{xx} + \sin u = 0 \tag{1.1}$$

where u_{tt} , u_{xx} refer to the second derivatives with respect to time and space, respectively. The sine-Gordon equation was rediscovered in 1939 by Frenkel and Kontorova [1] in the course of their study of crystal dislocations, after being first obtained by Edmond Bour in 1862 in the context of surfaces of constant negative curvature [2]. The name of the equation is a reference to the Klein-Gordon equation, a similar equation well-known in the field of Quantum Mechanics.

Soliton solutions of the sine-Gordon equation

The sine-Gordon equation attracted a considerable amount of attention in the 1970s due to the fact that it admits soliton solutions.

Although a mathematically rigorous definition of a soliton can be formulated, in essence solitons are *localized solitary waves or pulses that propagate at a constant speed while maintaining their shape*. In particular, solitons arise when the properties of a medium are such that the wave dispersion is precisely counteracted by nonlinear effects. Soliton solutions are known to exist in numerous nonlinear partial differential equations that model physical systems.

A particular set of soliton solutions of the sine-Gordon equation are known as *kinks* and are of the form

$$u_{soliton}(x, t) = 4 \arctan \left(e^{\gamma(x-vt)+\delta} \right) \tag{1.2}$$

Where

$$\gamma^2 = \frac{1}{1-v^2}$$

With $|v| < 1$. Assuming, specifically, $v > 0$, those kink solutions correspond to a wavefront propagating to the right as time increases, with velocity v , and that takes the system from $u(x, t) = 2\pi$ to $u(x, t) = 0$, as Figure 1.1 shows.

Note that the differential equation is 2π -periodic in u , i.e. if $u(x, t)$ is a solution then so is $u(x, t) + 2\pi$. In other words, $u = 2\pi$ essentially identifies with $u = 0$, making the domain of u equivalent to a cylinder.

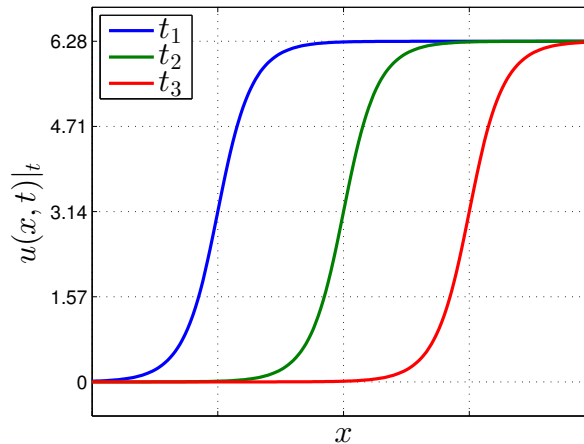


Figure 1.1: Schematic plot of the propagation of kink solitons of the sine-Gordon equation as a function of x , for various values of t ($t_1 < t_2 < t_3$). Note how the front propagates to the right as time increases for $v > 0$.

1.2 The perturbed sine-Gordon equation

The subject of this work is a perturbed form of the sine-Gordon equation. This perturbation corresponds to a nonlinear defect localized at the origin:

$$u_{tt} - u_{xx} + \sin u = \varepsilon \delta(x) \sin u \quad (1.3)$$

Where $\delta(x)$ is a Dirac delta and models said localized defect. The equation is expressed in terms of a small parameter $\varepsilon \ll 1$. The perturbed equation shows a much richer behavior than the sine-Gordon equation, the integrability of which largely constrains its dynamics.

Numerical simulations. Critical velocity

Fei et al. [3] studied the behavior of the perturbed sine-Gordon equation using numerical simulations. In particular, kink solitons are initialized far from the origin of x , propagating to the right at different constant velocities. Then, as they approach the origin, they interact with the defect, at which point the behavior depends on the initial propagating velocity. For initial velocities above a certain threshold value, which will be referred to as the *critical velocity*, the kink continues propagating towards infinity after the interaction. On the other hand, kinks moving towards the origin under said value can either get “trapped” at the origin, remaining there for all time, or can get reflected by the defect and proceed on propagating towards negative values of x . This last behavior happens only for particular bands of values of the initial velocity. These bands are known as *resonance windows*. Phenomenological explanations for these resonance windows have been given in [4, 5, 6, 7].

The described behavior is shown in Figure 1.2, taken from [3]. In it, the velocity after the interaction, v_{out} , is plotted against the initial velocity v_{in} . Note how $v_{out} > 0$ only for values of v_{in} above a certain threshold value (numerical value around $v_{in} \approx 0.166$), and how for particular values of v_{in} (within the resonance windows), v_{out} is negative, meaning that the kink gets reflected and proceeds to propagate to the left.

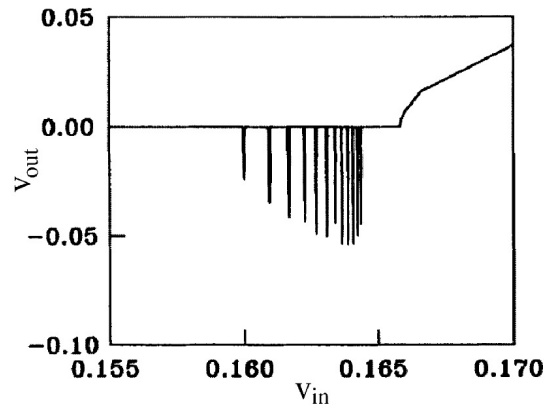


Figure 1.2: Velocities before and after the interaction with a defect at the origin for kinks of the perturbed sine-Gordon equation. Reproduced from [3].

The focus of this work will be *to present a way to deduce the value of the aforementioned critical velocity*. To do so, an ODE system is obtained from the perturbed sine-Gordon equation using a variational approach, following the work of Fei et al. [3] and Goodman and Haberman [8]. The resulting Hamiltonian system is then studied. From that, a Melnikov integral formula for the critical velocity is deduced via an energy balance reasoning, as outlined in [8]. Finally, the problem is approached from a geometrical point of view that allows for an interpretation of the previous results in terms of intersections of invariant manifolds of periodic orbits.

2. The variational approximation

2.1 Soliton solutions of the sine-Gordon equation

As stated in the previous chapter, the sine-Gordon equation

$$u_{tt} - u_{xx} + \sin u = 0 \quad (2.1)$$

has well-known soliton solutions. To obtain them, we fix the (x, t) dependence as

$$u(x, t) = U(x - vt) =: U(r) \quad (2.2)$$

Then, substituting (2.2) in (2.1) yields

$$(v^2 - 1)U'' + \sin U = 0$$

Or, equivalently,

$$(1 - v^2)U'' - \sin U = 0 \quad (2.3)$$

Where $U'' := \frac{d^2U}{dr^2}$. To simplify (2.3), the variable r is rescaled: let

$$\begin{aligned} r &\mapsto s = \gamma r \\ \frac{dU}{dr} &= \gamma \frac{dU}{ds} \end{aligned} \quad (2.4)$$

for some $\gamma \in \mathbb{R}$. Then (2.3) becomes

$$(1 - v^2)\gamma^2 \frac{d^2U}{ds^2} - \sin U = 0$$

which by taking

$$\gamma^2 = \frac{1}{1 - v^2} \quad , \quad \text{for } |v| < 1 \quad (2.5)$$

simplifies to

$$\ddot{U} - \sin U = 0 \quad (2.6)$$

Where now $\ddot{U} := \frac{d^2U}{ds^2}$. The ODE (2.6) is the well-known equation of the nonlinear pendulum, which can be written as a 2D Hamiltonian system by introducing the conjugate variable

$$W(s) := \dot{U}(s)$$

so that (2.6) becomes the system

$$\begin{cases} \dot{U} &= W \\ \dot{W} &= \sin U \end{cases} \quad (2.7)$$

Which corresponds to a Hamiltonian

$$H(U, W) = \frac{W^2}{2} + \cos U - 1 \quad (2.8)$$

(the constant term in a Hamiltonian is arbitrary, in this case it is fixed so that $H(0, 0) = 0$). Note that this system (2.7) is 2π -periodic in U , and therefore the phase space only needs to be studied for $U \in [0, 2\pi]$. Within these values, (2.7) has equilibrium points at $(U, W) = (0, 0)$ (which identifies with the point $(U, W) = (2\pi, 0)$) and at $(U, W) = (\pi, 0)$. By computing the Jacobian matrix of the system

$$J(U, W) = \begin{pmatrix} 0 & 1 \\ \cos U & 0 \end{pmatrix} \quad (2.9)$$

One can obtain that the equilibria at $(0, 0)$, $(2\pi, 0)$ correspond to saddle points, whereas the point $(U, W) = (\pi, 0)$ is a center. Thus, as shown in Figure 2.1, the phase portrait features two homoclinic orbits joining the saddle points, which split the phase space in a region of bound periodic orbits around the center and one of unbound periodic orbits, above and below these homoclinic orbits.

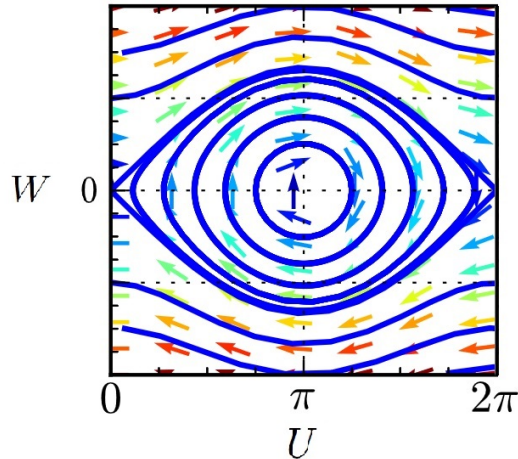


Figure 2.1: Schematic plot of the phase portrait of the nonlinear pendulum in (U, W) variables.

It is for these homoclinic orbits that we want to obtain an explicit expression, since these are the ones that correspond to the the soliton solutions of the sine-Gordon equation (2.1).

The expression for these orbits, $(U_h(s), W_h(s))$, can be obtained by taking advantage of the fact that the system (2.7) is Hamiltonian, and therefore has $H(U, W)$ as a first integral. Thus, given that $H(0, 0) = 0$, and since the homoclinic orbits tend to the origin as $t \rightarrow \pm\infty$, then by continuity $H(U_h(s), W_h(s)) = 0, \forall t$.

Therefore, we have an implicit equation for these orbits:

$$\frac{W_h^2}{2} + \cos U_h - 1 = 0 \quad (2.10)$$

From which we can obtain an time-explicit expression: applying the trigonometric identity

$$\sin^2 \left(\frac{\theta}{2} \right) = \frac{1 - \cos(\theta)}{2} \quad (2.11)$$

to equation (2.10) and rearranging, we get

$$W_h^2 = 4 \sin^2 \left(\frac{U_h}{2} \right) \quad (2.12)$$

And by recalling now that $W = \frac{dU(s)}{ds}$, then (2.12) becomes an ODE for $U_h(s)$. By taking now square roots and applying a further change of variables

$$\begin{aligned} V(s) &:= \frac{1}{2}U(s) \\ \dot{V} &= \frac{1}{2}\dot{U} \end{aligned} \quad (2.13)$$

We get the ODE

$$\dot{V}_h = \pm \sin V_h \quad (2.14)$$

(note the \pm sign, which comes from taking square roots on (2.12) and that accounts for the two symmetric homoclinic orbits). This ODE is separable and solves for

$$\ln \left(\cot \left(\frac{V_h}{2} \right) \right) = \mp s + C$$

with $C \in \mathbb{R}$ an integration constant to determine. Taking exponentials and inverting,

$$\tan \left(\frac{V_h}{2} \right) = e^{\pm s + C}$$

From which

$$V_h = 2 \arctan \left(\exp(\pm s + C) \right)$$

And reverting the change of variables (2.13) we get the explicit expression for the homoclinic orbits:

$$U_h(s) = 4 \arctan \left(\exp(\pm s + C) \right) \quad (2.15)$$

Finally, to obtain from that the expression of the kink soliton solutions of (2.1), we revert the initial changes of variables (2.2, 2.4, 2.5):

$$U(s) = U(\gamma r) = u \left(\pm \frac{x - vt}{\sqrt{1 - v^2}} \right)$$

Yielding

$$u_k(x, t) = 4 \arctan \left(\exp \left(\frac{x - vt - x_0}{\sqrt{1 - v^2}} \right) \right) \quad , \quad |v| < 1 \quad (2.16)$$

Where we fixed the integration constant $C = -\frac{x_0}{\sqrt{1 - v^2}}$ by imposing the (space) derivative at $t = 0$ to have a maximum at $x = x_0$ (which makes $x = x_0$ correspond to the central position of the propagating soliton when $t = 0$). The subindex in u_k stands for “kink”.

2.2 Small amplitude solutions of the perturbed sine-Gordon equation

We consider now the system with a localized, nonlinear impurity at the origin. This is modeled by the perturbed Sine-Gordon equation:

$$u_{tt} - u_{xx} + \sin u = \varepsilon \delta(x) \sin u \quad (2.17)$$

In particular, we begin by looking for solutions of small amplitude, i.e. $|u| \ll 1$. Then, these solutions will approximately satisfy the linearized equation, in which we can substitute $\sin u$ by u itself:

$$u_{tt} - u_{xx} + u = \varepsilon \delta(x) u \quad (2.18)$$

This can be solved by assuming separation of variables: let

$$u(x, t) = a(t) b(x) \quad (2.19)$$

Substituting (2.19) into (2.18) and rearranging, one gets

$$\frac{a''(t)}{a(t)} = \varepsilon \delta(x) + \frac{b''(x)}{b(x)} - 1 \quad (2.20)$$

And since the left hand side of (2.20) only depends on t , whereas the right hand side only depends on x , the only way the equality holds in general is by being equal to a constant. This means (2.20) is decoupled in two, second order ODEs:

$$a''(t) = D a(t) \quad (2.21)$$

$$b''(x) = (1 + D - \varepsilon \delta(x)) b(x) \quad (2.22)$$

For a common constant $D \in \mathbb{R}$ to determine. Looking first at (2.22), one can notice that, away from the origin, the ODE essentially corresponds to that of a real exponential. With that, and taking into account that $b(x)$ is expected to not diverge for $x \in \mathbb{R}$, the following ansatz is formulated:

$$b(x) = e^{-\sqrt{1+D}|x|}$$

Then, derivating:

$$\begin{aligned} b'(x) &= -\sqrt{1+D} \operatorname{sgn}(x) b(x) \\ b''(x) &= (1+D)b(x) - \sqrt{1+D}(2\delta(x))b(x) \end{aligned}$$

Where $\operatorname{sgn}(x)$ is the sign function, which appears from derivating the absolute value; in turn, its derivative is $2\delta(x)$.

Therefore, by substituting this expression for $b''(x)$ into (2.22), one immediately obtains that the ansatz is valid if

$$2\sqrt{1+D} = \varepsilon$$

And thus (2.22) admits as a solution

$$b(x) = e^{-\varepsilon|x|/2} \quad (2.23)$$

Provided that $D = \frac{\varepsilon^2}{4} - 1$. Then, taking this value for D , (2.21) solves for

$$a(t) = a_0 \cos \left(\sqrt{1 - \frac{\varepsilon^2}{4}} t + \theta_0 \right) \quad (2.24)$$

Therefore, putting it all together, the small-amplitude perturbed sine-Gordon equation (2.18) admits the following solutions (the subindex in u_s stands for “small”):

$$u_s(x, t) = a(t) b(t) = a_0 \cos(\Omega t + \theta_0) e^{-\varepsilon|x|/2} \quad (2.25)$$

Where we define

$$\Omega = \sqrt{1 - \frac{\varepsilon^2}{4}} \quad (2.26)$$

2.3 Variational derivation of a Hamiltonian ODE approximation

Using the previous results, one can derivate a Hamiltonian ODE system that approximates the behavior of the perturbed sine-Gordon equation. It is obtained using a variational approximation.

Specifically, we will assume, a priori, that the system admits a solution that is a superposition of two modes: a kink-like mode, for which we generalize the expression in equation (2.16) by substituting $x_0 + vt$ by a function $X(t)$; and a mode akin to (2.25) with an unknown function $a(t)$. That is, we take the following ansatz, where $X(t)$, $a(t)$ are unknown:

$$u(x, t) = 4 \arctan \left(\exp(x - X(t)) \right) + a(t) e^{-\varepsilon|x|/2} \quad (2.27)$$

Two remarks are important at this point:

- The generalization into $X(t)$ and $a(t)$ can be understood as assuming $x_0 + vt$ and $a_0 \cos(\Omega t + \theta_0)$, respectively, to be the first terms in their corresponding series expansion. In other words, we are implying that by substituting them by $X(t)$, $a(t)$ we are taking into account more terms from said series:

$$\begin{aligned} X(t) &= (x_0 + vt) + X_1(t) + X_2(t) + \dots \\ a(t) &= a_0 \cos(\Omega t + \theta_0) + a_1(t) + a_2(t) + \dots \end{aligned}$$

And, furthermore, we know that $a(t) = 0$ in the $\varepsilon \rightarrow 0$ limit, since it is the solution of the perturbed equation.

- Related to that last point, recall that equation (2.18) is valid under the assumption of small amplitude. Therefore, the second term in (2.27), and in particular $a(t)$, is assumed to be small compared to the first one; this means that it admits an interpretation as a small perturbation.

This ansatz, then, is substituted into the Lagrangian of the perturbed sine-Gordon equation (2.17):

$$L = \int_{-\infty}^{+\infty} \left[\frac{1}{2} u_t^2 - \frac{1}{2} u_x^2 - (1 - \varepsilon \delta(x)) (1 - \cos u) \right] dx \quad (2.28)$$

To obtain this integral, we compute the terms u_x^2 , u_t^2 using expression (2.27) (for simplicity, we note $s := x - X$):

$$u_t^2 = 4\dot{X}^2 \operatorname{sech}^2(s) - 4\dot{X}\dot{a} \operatorname{sech}(s) e^{-\varepsilon|x|/2} + \dot{a}^2 e^{-\varepsilon|x|} \quad (2.29)$$

$$u_x^2 = 4 \operatorname{sech}^2(s) - 2a\varepsilon \operatorname{sgn}(x) \operatorname{sech}(s) e^{-\varepsilon|x|/2} + \frac{\varepsilon^2}{4} a^2 e^{-\varepsilon|x|} \quad (2.30)$$

Where, again, the $\operatorname{sgn}(x)$ term in (2.30) refers to the sign of x . Furthermore, we use the aforementioned fact that we assume $a(t)$ to be small, and therefore the second term in (2.27) can be thought of as a perturbation in terms of which we can expand functions of u . More specifically, we will use the property that, for a small δ :

$$\cos(\theta + \delta) = \cos \theta - \delta \sin \theta - \frac{1}{2} \delta^2 \cos \theta + \mathcal{O}(\delta^3)$$

To expand the $(1 - \cos u)$ term of (2.28) in terms of $a(t) e^{-\varepsilon|x|/2}$; for ease of notation, let $\alpha := 4 \arctan \left(\exp(x - X(t)) \right)$:

$$\begin{aligned} 1 - \cos u &= 1 - \cos \left(\alpha + a(t) e^{-\varepsilon|x|/2} \right) = \\ &= 1 - \cos \alpha + \sin \alpha a(t) e^{-\varepsilon|x|/2} + \frac{1}{2} \cos \alpha a^2(t) e^{-\varepsilon|x|} + \mathcal{O}(a^3(t)) \end{aligned} \quad (2.31)$$

So we will substitute the computed results (2.29), (2.30), (2.31) (this last one truncating out the $\mathcal{O}(a^3(t))$) into the Lagrangian (2.28). Before doing that, however, we take an additional assumption: we assume that the two modes that we take to compose the solution (2.27) are only coupled through the defect at the origin, and therefore we will ignore all terms consisting in the product between the two of them except for those including the $\varepsilon \delta(x)$ term. In practice, this implies ignoring the cross-product terms in u_t^2 (2.29), u_x^2 (2.30). We'll speak, then, in terms of an *effective* Lagrangian, L_{eff} , to reflect the fact that some terms have been ignored.

Thus, overall, this effective Lagrangian reads

$$\begin{aligned} L_{\text{eff}} &= \int_{-\infty}^{+\infty} \left[\frac{1}{2} u_t^2 - \frac{1}{2} u_x^2 - (1 - \varepsilon \delta(x)) (1 - \cos u) \right] dx = \\ &= 2\dot{X}^2 \int_{-\infty}^{+\infty} \operatorname{sech}^2(s) dx + \frac{\dot{a}^2}{2} \int_{-\infty}^{+\infty} e^{-\varepsilon|x|} dx - 2 \int_{-\infty}^{+\infty} \operatorname{sech}^2(s) dx - \frac{\varepsilon^2 a^2}{8} \int_{-\infty}^{+\infty} e^{-\varepsilon|x|} dx - \\ &- \int_{-\infty}^{+\infty} (1 - \cos \alpha) dx - a \int_{-\infty}^{+\infty} \sin \alpha e^{-\varepsilon|x|/2} dx - \frac{a^2}{2} \int_{-\infty}^{+\infty} \cos \alpha e^{-\varepsilon|x|} dx + \\ &+ \varepsilon \int_{-\infty}^{+\infty} (1 - \cos \alpha) \delta(x) dx + \varepsilon a \int_{-\infty}^{+\infty} \sin \alpha e^{-\varepsilon|x|/2} \delta(x) dx + \frac{\varepsilon a^2}{2} \int_{-\infty}^{+\infty} \cos \alpha e^{-\varepsilon|x|} \delta(x) dx \end{aligned} \quad (2.32)$$

At this point, the following properties

$$\cos \alpha = \cos \left(4 \arctan \left(\exp(x - X(t)) \right) \right) = 1 - 2 \operatorname{sech}^2(x - X(t))$$

$$\sin \alpha = \sin \left(4 \arctan \left(\exp(x - X(t)) \right) \right) = -2 \tanh(x - X(t)) \operatorname{sech}(x - X(t))$$

Are used to compute the integrals:

$$\int_{-\infty}^{+\infty} \operatorname{sech}^2(s) dx = \int_{-\infty}^{+\infty} \operatorname{sech}^2(x - X(t)) dx = 2$$

$$\int_{-\infty}^{+\infty} e^{-\varepsilon|x|} dx = \frac{2}{\varepsilon}$$

$$\int_{-\infty}^{+\infty} (1 - \cos \alpha) dx = \int_{-\infty}^{+\infty} \left(1 - (1 - 2 \operatorname{sech}^2(x - X(t))) \right) dx = 2 \int_{-\infty}^{+\infty} \operatorname{sech}^2(x - X(t)) dx = 4$$

$$\int_{-\infty}^{+\infty} \sin \alpha e^{-\varepsilon|x|/2} dx = -2 \int_{-\infty}^{+\infty} \tanh(x - X(t)) \operatorname{sech}(x - X(t)) e^{-\varepsilon|x|/2} dx = 0$$

$$\int_{-\infty}^{+\infty} \cos \alpha e^{-\varepsilon|x|} dx = \int_{-\infty}^{+\infty} \left(1 - 2 \operatorname{sech}^2(x - X(t)) \right) e^{-\varepsilon|x|} dx = \frac{2}{\varepsilon} - 4$$

With that, and using the property $\int_{-\infty}^{+\infty} f(x)\delta(x) dx = f(0)$ and rearranging, (2.32) reads

$$\begin{aligned} L_{\text{eff}} &= 4\dot{X}^2 + \frac{\dot{a}^2}{\varepsilon} - \left(\frac{1}{\varepsilon} - \frac{\varepsilon}{4} \right) a^2 + 2\varepsilon \operatorname{sech}^2(X) - 2\varepsilon a \tanh(X) \operatorname{sech}(X) + 2a^2 - \varepsilon a^2 \operatorname{sech}^2(X) - 8 = \\ &= 4\dot{X}^2 + \frac{1}{\varepsilon} (\dot{a}^2 - \Omega^2 a^2) + 2\varepsilon \operatorname{sech}^2(X) - 2\varepsilon a \tanh(X) \operatorname{sech}(X) + 2a^2 - \varepsilon a^2 \operatorname{sech}^2(X) - 8 \end{aligned}$$

We recall that $\Omega = \sqrt{1 - \frac{\varepsilon^2}{4}}$.

As a further simplification, the $2a^2$ and $-\varepsilon a^2 \operatorname{sech}^2(X)$ terms, which are of higher order than the $-\frac{\Omega^2}{\varepsilon} a^2$ and the $2\varepsilon \operatorname{sech}^2(X)$ ones, respectively, are neglected; together with the constant term, which is irrelevant in a Lagrangian. Then, finally, we obtain the effective Lagrangian for the perturbed sine-Gordon equation given in [3, 8]:

$$L_{\text{eff}}(X, \dot{X}, a, \dot{a}) = 4\dot{X}^2 + \frac{1}{\varepsilon} (\dot{a}^2 - \Omega^2 a^2) - \varepsilon U(X) - \varepsilon a F(X) \quad (2.33)$$

Where

$$U(X) = -2 \operatorname{sech}^2(X) \quad (2.34)$$

$$F(X) = -2 \tanh(X) \operatorname{sech}(X) \quad (2.35)$$

From this Lagrangian, the associated dynamical system is obtained applying the Euler-Lagrange equations:

$$\left\{ \begin{array}{l} \frac{\partial L_{\text{eff}}}{\partial X} - \frac{d}{dt} \frac{\partial L_{\text{eff}}}{\partial \dot{X}} = 0 \end{array} \right. \quad (2.36a)$$

$$\left\{ \begin{array}{l} \frac{\partial L_{\text{eff}}}{\partial a} - \frac{d}{dt} \frac{\partial L_{\text{eff}}}{\partial \dot{a}} = 0 \end{array} \right. \quad (2.36b)$$

Which after computing and rearranging read

$$\begin{cases} 8\ddot{X} + \varepsilon U'(X) + \varepsilon a F'(X) = 0 & (2.37a) \\ \ddot{a} + \Omega^2 a + \frac{1}{2}\varepsilon^2 F(X) = 0 & (2.37b) \end{cases}$$

This is a Hamiltonian system, with a Hamiltonian

$$H(X, \dot{X}, a, \dot{a}) = 4\dot{X}^2 + \frac{1}{\varepsilon}(\dot{a}^2 + \Omega^2 a^2) + \varepsilon U(X) + \varepsilon a F(X) \quad (2.38)$$

Numerical simulations [8] show that this ODE system captures many of the key features of the original one, including the resonance windows and the presence of a critical velocity for the propagation of traveling kinks.

2.4 Rescaling. Conjugate variables. Energy partitioning

At this point we rewrite system (2.37) in preparation for the next sections. In particular, we rescale the time variable, $t \rightarrow \sqrt{\varepsilon/2} t$ (although in an abuse of notation we keep the same symbols for the time derivatives), so that (2.37) becomes

$$\begin{cases} 4\ddot{X} + U'(X) + aF'(X) = 0 & (2.39a) \\ \ddot{a} + \lambda^2 a + \varepsilon F(X) = 0 & (2.39b) \end{cases}$$

where

$$\lambda^2 = \frac{2}{\varepsilon} - \frac{\varepsilon}{2} \quad (2.40)$$

Note how this removes the dependence of the first equation on ε . We say that this rescaling fixes the leading-order time scale. Furthermore, it will be convenient to express (2.39) as a 4-dimensional, 1st order system of equations: by defining the conjugated variables

$$\begin{aligned} Y &= \dot{X} \\ b &= \frac{1}{4\varepsilon} \dot{a} \end{aligned}$$

And applying a further rescaling to the time variable, we arrive at the ODE system

$$\begin{cases} \dot{X} = 4Y & (2.41a) \\ \dot{Y} = -(U'(X) + aF'(X)) & (2.41b) \\ \dot{a} = 16\varepsilon b & (2.41c) \\ \dot{b} = -\left(\frac{\lambda^2}{\varepsilon} a + F(X)\right) & (2.41d) \end{cases}$$

which is a Hamiltonian system with Hamiltonian

$$H(X, Y, a, b) = 2Y^2 + U(X) + \frac{\lambda^2}{2\varepsilon} a^2 + 8\varepsilon b^2 + aF(X) \quad (2.42)$$

Note how only the last term in (2.42) couples the two modes; in these variables (X, Y) and (a, b) . To reflect this, we introduce the following notation:

$$H(X, Y, a, b) = E(X, Y) + G(a, b) + aF(X) \quad (2.43)$$

With

$$E(X, Y) = 2Y^2 + U(X) \quad (2.44)$$

$$G(a, b) = \frac{\lambda^2}{2\varepsilon} a^2 + 8\varepsilon b^2 \geq 0 \quad (2.45)$$

I.e. $E(X, Y)$ corresponds to the energy of the kink mode and $G(a, b)$ to the energy of the oscillator mode, with a term $aF(X)$ coupling them.

Furthermore, note that, since both $U(X)$ and $F(X)$ tend to zero exponentially as $|X| \rightarrow \infty$, then the Hamiltonian can be asymptotically partitioned into positive definite components:

$$\lim_{X \rightarrow \pm\infty} H(X, Y, a, b) = 2Y^2 + G(a, b) \quad (2.46)$$

meaning that the aforementioned two modes are coupled only in a neighborhood of the origin. Indeed, as $|X| \rightarrow \infty$, it can be immediately seen in (2.41) that $Y(t)$ tends to a constant, i.e. $X(t)$ evolving at a constant velocity, while the (a, b) variables decouple from $X(t)$ and correspond, in essence, to a harmonic oscillator; both modes evolving independently from each other. Only in a neighborhood of $X = 0$ do the equations become coupled and the modes exchange energy.

2.5 Uncoupled system

It is insightful to consider the projection of the dynamics onto the (X, Y) phase space. In particular, for $\varepsilon = 0$ it can be shown that the dynamics in (X, Y) decouple from those in (a, b) , and then orbits in (X, Y) lie on the level curves of $E(X, Y)$.

The decoupled (X, Y) system has an elliptic fixed point at the origin and degenerate saddle fixed points at $X = \pm\infty$. These saddle points are connected by two separatrix heteroclinic orbits, which split the phase space in three distinct regions, as shown in Figure 2.2. In R_1 and R_3 we have unbounded orbits that reach $X = +\infty$ and $X = -\infty$, respectively, at constant velocity. On the other hand, in R_2 orbits are bounded, oscillating clockwise around the elliptic point.

As stated, without the coupling with the (a, b) mode, the energy of the (X, Y) mode, $E(X, Y) = 2Y^2 + U(X)$, is invariant along trajectories in (X, Y) . In particular, $E = 0$ in the separatrix orbits, while the bounded orbits correspond to $E < 0$ and the unbounded ones, to $E > 0$.

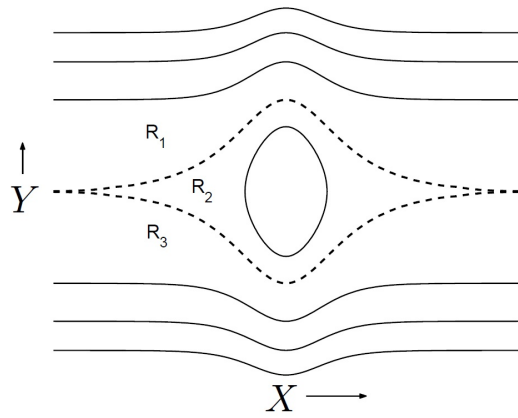


Figure 2.2: The (X, Y) phase space with decoupled dynamics (modified from [8]).

3. Computation of the critical velocity

Upon recovering the coupling with the oscillator mode by setting $\varepsilon \neq 0$, the regions R_1 , R_2 , R_3 are no longer invariant and solutions are able to cross over the separatrix. Furthermore, $E(X, Y)$ is no longer a first integral, since energy can be transferred from the (X, Y) mode to the (a, b) mode. The change of the value of $E(X, Y)$ along an orbit is precisely what will be used to compute the value of the critical velocity, which in terms of the variables used here will be noted as y_c .

Let a kink propagating from $X \rightarrow -\infty$ at constant positive speed, y_- , with no energy in the oscillator mode:

$$\begin{aligned} \lim_{t \rightarrow -\infty} X(t) &= -\infty \\ \lim_{t \rightarrow -\infty} Y(t) &= y_- > 0 \\ \lim_{t \rightarrow -\infty} a(t) &= 0 \\ \lim_{t \rightarrow -\infty} b(t) &= 0 \end{aligned} \tag{3.1}$$

In this situation, then, all the initial energy is in the kink mode. We call that energy E_- :

$$\lim_{t \rightarrow -\infty} H(X(t), Y(t), a(t), b(t)) = E_- = 2y_-^2 > 0 \tag{3.2}$$

As $X(t)$ approaches the origin, the kink mode will be able to exchange energy with the oscillator mode. It is assumed at this point that, after the interaction, the kink is able to continue towards $X \rightarrow +\infty$. It does so with a velocity approaching a constant $y_+ > 0$, while $(a(t), b(t))$ tend to steady oscillations, which is equivalent to stating that the energy of the oscillator mode tends to a constant that we refer to as G_+ :

$$\begin{aligned} \lim_{t \rightarrow +\infty} X(t) &= +\infty \\ \lim_{t \rightarrow +\infty} Y(t) &= y_+ > 0 \\ \lim_{t \rightarrow +\infty} G(a(t), b(t)) &= \lim_{t \rightarrow +\infty} \left(\frac{\lambda^2}{2\varepsilon} a^2(t) + 8\varepsilon b^2(t) \right) = G_+ \geq 0 \end{aligned} \tag{3.3}$$

Therefore, as $t \rightarrow +\infty$, the Hamiltonian tends to a constant value

$$\lim_{t \rightarrow +\infty} H(X(t), Y(t), a(t), b(t)) = E_+ + G_+ = 2y_+^2 + G_+ \tag{3.4}$$

And so, given that the Hamiltonian is a first integral, we equate (3.2) and (3.4), obtaining:

$$E_- = E_+ + G_+ \tag{3.5}$$

This immediately implies that $E_- \geq E_+$, since all the terms in (3.5) are non-negative. In turn, that means that (3.5) only has solutions for $E_- \geq G_+$, with the equality for $E_+ = 0$. That

is, there is a minimum value of the initial energy in the kink mode that still allows for $X(t)$ to reach infinity after the interaction. Recalling that $E(X, Y)$ uniquely determines Y at $X \rightarrow \pm\infty$, then this minimum energy corresponds to the smallest initial velocity y_- for which the kink can reach $+\infty$ after interacting with the defect. This is precisely the way the critical velocity, y_c , is defined. At the same time, this reasoning in terms of energies allows us to define the critical velocity as *the value of the initial velocity, y_- , such that*

$$\left\{ \begin{array}{l} \lim_{t \rightarrow +\infty} X(t) = +\infty \\ \lim_{t \rightarrow +\infty} E(X(t), Y(t)) = E_+ = 0 \end{array} \right. \quad (3.6a)$$

$$\left. \right\} \quad (3.6b)$$

This definition gives an explicit way of computing y_c . The approach is the following: if we compute the value of the (time) derivative of $E(X, Y)$ along an orbit, we can then integrate it to obtain the total energy transferred away from the kink mode to the oscillator mode, $\Delta E = E_+ - E_-$. Then, since we impose that $E_+ = 0$, it follows that the equation to solve for y_c is

$$E_-(y_c) = 2y_c^2 = |\Delta E| \quad (3.7)$$

For notation, let $e(t) := E(X(t), Y(t))$. Then, for any given solution of (2.41), $(X(t), Y(t))$, we can compute the time derivative using equation (2.44):

$$\frac{de(t)}{dt} = 4Y(t)\dot{Y}(t) + U'(X(t))\dot{X}(t) \quad (3.8)$$

Which we can rewrite using the system (2.41), obtaining

$$\frac{de(t)}{dt} = -4a(t)F'(X(t))Y(t) \quad (3.9)$$

We can then integrate that with respect to the time variable to obtain the total energy lost by the soliton mode along a given orbit:

$$\Delta E = \int_{-\infty}^{+\infty} \frac{de(t)}{dt} dt = -4 \int_{-\infty}^{+\infty} a(t)F'(X(t))Y(t) dt \quad (3.10)$$

Which, notably, takes the form of a Melnikov integral, albeit obtained through a completely different reasoning. Now, of course, to integrate that we need, in principle, the solutions $a(t)$, $X(t)$, $Y(t)$. However, by expanding them in powers of the parameter ε , one can find that, to obtain ΔE up to first order in ε , we need much less information. Expanding:

$$\begin{aligned} X(t) &= X_h(t) + \varepsilon X_1(t) + \mathcal{O}(\varepsilon^2) \\ Y(t) &= Y_h(t) + \varepsilon Y_1(t) + \mathcal{O}(\varepsilon^2) \\ a(t) &= \varepsilon a_1(t) + \mathcal{O}(\varepsilon^2) \\ b(t) &= \varepsilon b_1(t) + \mathcal{O}(\varepsilon^2) \end{aligned} \quad (3.11)$$

Where, crucially,

- The zero-order terms of $X(t)$, $Y(t)$ correspond to the heteroclinic orbits of the unperturbed (X, Y) phase space (see Figure 2.2), $(X_h(t), Y_h(t))$, for which we have an explicit expression;

- The zero-order terms of $a(t)$, $b(t)$ correspond to an harmonic oscillator; and since we're imposing as initial conditions that they tend to zero as $t \rightarrow -\infty$, then they are zero for all time. Note that, in turn, this is consistent with the property that $\lim_{\varepsilon \rightarrow 0} a(t) = 0$, stated in the argumentation to derive the system (2.37).

Therefore, expanding ΔE itself in powers of ε

$$\Delta E = \Delta E_0 + \varepsilon \Delta E_1 + \mathcal{O}(\varepsilon^2) \quad (3.12)$$

And equating expression (3.12) with with (3.10) and matching the terms of the same order yields:

$$\Delta E_0 = 0 \quad (3.13)$$

$$\Delta E_1 = -4 \int_{-\infty}^{+\infty} a_1(t) F'(X_h(t)) Y_h(t) dt \quad (3.14)$$

The first equation, (3.13), implies that the energy exchanged without taking the defect into account is zero, which is exactly what should be expected, since this decouples the two modes and thus no energy exchange can happen. Furthermore, equation (3.7) tells us then that the critical velocity for the unperturbed case is zero. This is also the expected value, since in the decoupled system, the orbit that reaches infinity with zero velocity is precisely the level curve of $E = 0$ (the separatrix in Figure 2.2), corresponding to both initial and final zero velocities.

On the other hand, the second equation, (3.14), is the one that will allow us to compute ΔE up to first order. Crucially, the only unknown in this expression is the function $a_1(t)$, the first-order term in $a(t)$. This allows to compute an approximation for ΔE without needing the full expressions of $X(t)$, $Y(t)$, $a(t)$.

The explicit expression of the separatrices $(X_h(t), Y_h(t))$, reads

$$\begin{cases} X_h(t) = \pm \operatorname{arcsinh}(t) & (3.15a) \\ Y_h(t) = \pm \frac{1}{\sqrt{1+t^2}} & (3.15b) \end{cases}$$

We then use (3.15a) to compute the term

$$F'(X_h(t)) = -4 \operatorname{sech}^3(X_h(t)) + 2 \operatorname{sech}(X_h(t)) = -\frac{4}{(1+t^2)^{3/2}} + \frac{2}{(1+t^2)^{1/2}} \quad (3.16)$$

And so substituting (3.15b) and (3.16) into (3.14) we obtain the expression

$$\Delta E_1 = -4 \int_{-\infty}^{+\infty} \left(-\frac{4}{(1+t^2)^2} + \frac{2}{1+t^2} \right) a_1(t) dt \quad (3.17)$$

Computation of $a_1(t)$

To compute $a_1(t)$, we substitute the expansions of $a(t)$ and $X(t)$ in terms of ε

$$\begin{aligned} a(t) &= \varepsilon a_1(t) + \mathcal{O}(\varepsilon^2) \\ X(t) &= X_h(t) + \varepsilon X_1(t) + \mathcal{O}(\varepsilon^2) \end{aligned} \quad (3.18)$$

Into the ODE (2.39b), yielding

$$\varepsilon \ddot{a}_1 + \lambda^2 \varepsilon a_1 + \varepsilon F(X_h + \varepsilon X_1 + \mathcal{O}(\varepsilon^2)) + \mathcal{O}(\varepsilon^2) = 0$$

Which after dividing all terms by ε reads, to first order:

$$\ddot{a}_1 + \lambda^2 a_1 + F(X_h) = 0 \quad (3.19)$$

Remark An important point that needs to be made explicit is that in this analysis, the fact that λ depends on ε is not taken into account, but rather λ is treated as a constant. This is a simplification that is acknowledged; the calculation taking this ε -dependence into account is significantly more complex.

Then, by recalling that we have an explicit expression for $F(X_h)$,

$$F(X_h) = -\frac{2t}{1+t^2}$$

the ODE (3.19) can be integrated by variation of parameters, yielding

$$a_1(t) = \frac{2}{\lambda} \int_{-\infty}^t \sin(\lambda(t-\tau)) \frac{\tau}{1+\tau^2} d\tau \quad (3.20)$$

(Where the condition that $a(t) = 0$ at $t \rightarrow -\infty$ has been imposed in the computation of $a_1(t)$). A useful simplification can be taken at this point. By recalling that computing ΔE_1 involves an integral for $t \in (-\infty, \infty)$ (3.17), then it is apparent that, in fact, only the even part of $a_1(t)$, noted as $a_{1,e}(t)$, needs to be computed, since the odd part will vanish upon integration. Thus, we need only to compute

$$a_{1,e}(t) = \frac{1}{2}(a_1(t) + a_1(-t)) = \frac{1}{\lambda} \int_{-\infty}^{+\infty} \sin(\lambda(t-\tau)) \frac{\tau}{1+\tau^2} d\tau \quad (3.21)$$

Where note that now we integrate for $\tau \in (-\infty, \infty)$, which actually makes the integration easier.

In particular, this integral is carried out in the complex domain. First, (3.21) is expressed in terms of complex exponentials:

$$\begin{aligned} a_{1,e}(t) &= \frac{1}{\lambda} \int_{-\infty}^{+\infty} \frac{e^{i\lambda(t-\tau)} - e^{-i\lambda(t-\tau)}}{2i} \frac{\tau}{1+\tau^2} d\tau \\ &= \frac{e^{i\lambda t}}{2\lambda i} \int_{-\infty}^{+\infty} e^{-i\lambda\tau} \frac{\tau}{1+\tau^2} d\tau - \frac{e^{-i\lambda t}}{2\lambda i} \int_{-\infty}^{+\infty} e^{+i\lambda\tau} \frac{\tau}{1+\tau^2} d\tau \\ &= -\frac{1}{i\lambda} \cos(\lambda t) I \end{aligned} \quad (3.22)$$

Where I is the integral

$$I = \int_{-\infty}^{+\infty} e^{i\lambda z} \frac{z}{1+z^2} dz, \quad z \in \mathbb{C} \quad (3.23)$$

Integrating first by parts, it yields

$$I = -\frac{1}{i\lambda} \int_{-\infty}^{+\infty} e^{i\lambda z} \frac{1-z^2}{(1+z^2)^2} dz = -\frac{1}{i\lambda} \int_{-\infty}^{+\infty} f(z) dz \quad (3.24)$$

With

$$f(z) = e^{i\lambda z} \frac{1 - z^2}{(1 + z^2)^2} = e^{i\lambda z} \frac{1 - z^2}{(z + i)^2(z - i)^2} = \frac{1}{(z - i)^2} g(z) \quad (3.25)$$

I will be computed using results from complex analysis. Consider the following closed path Γ in \mathbb{C} , for $R > 1$, $R \in \mathbb{R}$:

i.e. $z \in [-R, R] \in \mathbb{R}$ in γ_1 and $z = R e^{i\theta}$, $\theta \in [0, \pi]$ along γ_2 .

Then, by the residue theorem, integrating $f(z)$ along this closed curve yields:

$$\int_{\gamma_1} f(z) dz + \int_{\gamma_2} f(z) dz = 2\pi i \operatorname{Res}(f, z_p) \quad (3.26)$$

And we can immediately see that this provides a way to compute I , since

$$I = -\frac{1}{i\lambda} \lim_{R \rightarrow \infty} \int_{\gamma_2} f(z) dz = -\frac{1}{i\lambda} \left[2\pi i \operatorname{Res}(f, z_p) - \lim_{R \rightarrow \infty} \int_{\gamma_1} f(z) dz \right] \quad (3.27)$$

In the expression of (3.26) we applied that $f(z)$ has only one (double) pole enclosed by Γ , located at $z_p = i$. This means that the Laurent series of $f(z)$ around $z = i$ reads

$$f(z) = \frac{a_{-2}}{(z - i)^2} + \frac{a_{-1}}{z - i} + a_0 + a_1(z - i) + \dots \quad (3.28)$$

On the other hand, $g(z)$, defined defined in (3.25), has no poles around $z = i$. This means that its Laurent series around this point is

$$g(z) = g(i) + g'(i)(z - i) + g''(i)(z - i)^2 + \dots \quad (3.29)$$

And therefore, substituting into from (3.25):

$$f(z) = \frac{g(z)}{(z - i)^2} = \frac{g(i)}{(z - i)^2} + \frac{g'(i)}{z - i} + g''(i) + \dots \quad (3.30)$$

And since, by definition, the residue of a function at a pole is the term a_{-1} of its Laurent series around this point, then it follows that

$$\operatorname{Res}(f, i) = g'(i) = \frac{d}{dz} \left(\frac{e^{i\lambda z}(1 - z^2)}{(i + z)^2} \right)_{z=i} = -e^{-\lambda} \frac{i\lambda}{2} \quad (3.31)$$

Taking the $R \rightarrow \infty$ on the integral on γ_1 , on the other hand:

$$\begin{aligned} \lim_{R \rightarrow \infty} \int_{\gamma_2} f(z) dz &= \lim_{R \rightarrow \infty} \int_0^\pi f(R e^{i\theta}) i R e^{i\theta} d\theta \\ &= i \lim_{R \rightarrow \infty} \int_0^\pi e^{i\lambda R e^{i\theta}} \frac{R - R^3 e^{2i\theta}}{1 + 2R^2 e^{2i\theta} + R^4 e^{4i\theta}} e^{i\theta} d\theta \\ &= 0 \end{aligned} \quad (3.32)$$

Therefore, substituting (3.31) and (3.32) into (3.27) yields

$$I = -\frac{1}{i\lambda} (2\pi i \operatorname{Res}(f, z_p)) = -i\pi e^{-\lambda} \quad (3.33)$$

And, in turn, substituting (3.33) into (3.22) gives

$$a_{1,e}(t) = -\frac{1}{i\lambda} I \cos(\lambda t) = \frac{\pi}{\lambda} e^{-\lambda} \cos(\lambda t) \quad (3.34)$$

Computation of ΔE_1 and critical velocity

The result for $a_{1,e}(t)$ (3.34) is now substituted into (3.17):

$$\Delta E_1 = -\frac{4\pi}{\lambda} e^{-\lambda} \int_{-\infty}^{+\infty} \left(-\frac{4}{(1+t^2)^2} + \frac{2}{1+t^2} \right) \cos(\lambda t) dt \quad (3.35)$$

This is going to be integrated in a way similar to (3.21): First, the cosine is expressed in terms of complex exponentials; after rearranging:

$$\Delta E_1 = -\frac{4\pi}{\lambda} e^{-\lambda} \int_{-\infty}^{+\infty} \left(-\frac{4}{(1+t^2)^2} + \frac{2}{1+t^2} \right) e^{i\lambda t} dt \quad (3.36)$$

And this is computed using an analogous approach of defining a closed curve in \mathbb{C} and solving for the integral along the real axis. After doing that, it can be obtained that

$$\Delta E_1 = -8\pi^2 e^{-2\lambda} \quad (3.37)$$

Therefore, we can compute the first correction term to the critical velocity: up to $\mathcal{O}(\varepsilon)$, using (3.7) we obtain that

$$y_c = \sqrt{\frac{\varepsilon |\Delta E_1|}{2}} = 2\pi e^{-\lambda} \sqrt{\varepsilon} \quad (3.38)$$

Which, after taking into account the rescalings done previously, is in good agreement with the numerical experiments from [8]. This allows us to be confident that the approximations made to compute the value of ΔE are valid.

4. Geometry. Invariant manifolds

In this last section, a geometrical interpretation is given for the energy arguments developed for the computation of the critical velocity. First, a change of variables is performed to move the equilibria at $X = -\infty$ and $X = +\infty$ to $Z = 0$ and $Z = 2\pi$, respectively; and a symplectic transformation is applied to the oscillator variables (a, b) to express them in polar coordinates. With that, a qualitative reasoning is provided for the behavior of the orbits as a function of the initial velocity in terms of manifolds of the invariant sets of the system.

4.1 Changes of variables

We will apply the following transformations to the variables (X, Y, a, b) of system (2.41):

$$(i) \quad X \mapsto Z = 4 \arctan(e^X), \quad Z \in (0, 2\pi)$$

so that

$$\begin{aligned} X \rightarrow -\infty &\implies Z \rightarrow 0 \\ X \rightarrow +\infty &\implies Z \rightarrow 2\pi \end{aligned}$$

Under this change,

$$\begin{aligned} \frac{dZ}{dX} &= \frac{1}{2} \sin\left(\frac{Z}{2}\right) \\ F(X) &= \sin(Z) \\ F'(X) &= \sin\left(\frac{3Z}{2}\right) - \sin\left(\frac{Z}{2}\right) \\ U'(X) &= 2 - \sin(Z) \sin\left(\frac{Z}{2}\right) \end{aligned} \tag{4.1}$$

(ii) Recalling equation (2.45),

$$G(a, b) = \frac{1}{2} \left(\frac{\lambda}{\varepsilon} a^2 + 16\varepsilon b^2 \right)$$

we can see that if we define the following change of coordinates (symplectic polar coordinates, $(a, b) \mapsto (r, \theta)$):

$$\begin{aligned} r &= \frac{1}{2} \left(\frac{\lambda}{\varepsilon} a^2 + 16\varepsilon b^2 \right) \\ \theta &= \frac{1}{4\lambda} \arctan\left(\frac{4\varepsilon b}{\lambda a}\right) \end{aligned} \tag{4.2}$$

Or, equivalently,

$$\begin{aligned} a &= \frac{\sqrt{2\varepsilon}}{\lambda} \sqrt{r} \cos(4\lambda\theta) \\ b &= \frac{1}{2\sqrt{2\varepsilon}} \sqrt{r} \sin(4\lambda\theta) \end{aligned} \quad (4.3)$$

Then it follows that

$$G(r, \theta) = r \quad (4.4)$$

That is, G has no θ dependence. Note that this implies that r is a first integral when the two modes decouple; we say r is an *action coordinate*.

Then, using (4.1) and (4.3) to write the system (2.41) in terms of the new coordinates (Z, Y, r, θ) , one obtains

$$\begin{cases} \dot{Z} = 2 \sin\left(\frac{Z}{2}\right) Y & (4.5a) \\ \dot{Y} = 2 \sin\left(\frac{Z}{2}\right) \left(\sin(Z) - \frac{\sqrt{2\varepsilon}}{\lambda} \sqrt{r} \cos(4\lambda\theta) \cos(Z) \right) & (4.5b) \\ \dot{r} = -4\sqrt{2\varepsilon} \sqrt{r} \sin(4\lambda\theta) \sin(Z) & (4.5c) \\ \dot{\theta} = -1 - \frac{\sqrt{2\varepsilon}}{2\lambda} \frac{1}{\sqrt{r}} \cos(4\lambda\theta) \sin(Z) & (4.5d) \end{cases}$$

Recall that, in the original (X, Y, a, b) coordinates, in the $|X| \rightarrow \infty$ limit the system decoupled; with $Y \rightarrow y_{\pm}$ a constant and (a, b) oscillating at a constant frequency. In the new coordinates, the limits $X \rightarrow \pm\infty$ correspond to $Z \rightarrow \{0, 2\pi\}$, respectively. If we take that limit on (4.5), it reduces to

$$\begin{cases} \dot{Z} = 0 & (4.6a) \\ \dot{Y} = 0 & (4.6b) \\ \dot{r} = 0 & (4.6c) \\ \dot{\theta} = -1 & (4.6d) \end{cases}$$

So $Z = \{0, 2\pi\}$ are indeed invariant sets, as expected; in which $Y(t) = Y_0$, $r(t) = r_0$ and $\theta(t) = \theta_0 - t$. In particular, as before, (r, θ) tends to steady oscillations.

Furthermore, note the following: If we take the $\varepsilon \rightarrow 0$ limit, the two modes also decouple (again, as expected; since they do in the original coordinates). In this case, (4.5a) and (4.5b) reduce to

$$\begin{cases} \dot{Z} = 2 \sin\left(\frac{Z}{2}\right) Y & (4.7a) \\ \dot{Y} = 2 \sin\left(\frac{Z}{2}\right) (\sin(Z)) & (4.7b) \end{cases}$$

Which, after dividing both equations by $2 \sin\left(\frac{Z}{2}\right)$, is the ODE system of the nonlinear pendulum shown in Figure 2.1. This means that, orbit-wise, when $\varepsilon \rightarrow 0$, the invariant subspace (Z, Y) corresponds to a pendulum, since dividing the equations in an ODE system by a common factor corresponds to a rescaling in the time variable, leaving the phase space unaltered (that is, except in the lines $Z = 0$ and $Z = 2\pi$, in which (4.7) features two lines of equilibrium points; however, this will not be of large concern since our system was restricted to $Z \in [0, 2\pi]$ to begin with).

It will also be useful to write the initial conditions that are being considered here (3.1) in the new coordinates. They read

$$\begin{aligned} \lim_{t \rightarrow -\infty} Z(t) &= 0 \\ \lim_{t \rightarrow -\infty} Y(t) &= y_- > 0 \\ \lim_{t \rightarrow -\infty} r(t) &= 0 \end{aligned} \tag{4.8}$$

Where there is no sense in imposing an initial condition on $\theta(t)$, given that θ is not defined when $r = 0$.

An additional remark is that the changes of variables applied here are not, overall, symplectic; therefore, the system is not, in general, Hamiltonian. However, it is a general property that first integrals retain their character under changes of coordinates; therefore, H evaluated in the new coordinates is still a first integral of the transformed system. This property will be used in the next section.

4.2 Geometry of the invariant sets $\{Z = 0, 2\pi\}$

We begin by describing the geometry of the invariant set $\{Z = 0\}$, corresponding to $\{X \rightarrow -\infty\}$. Since the system is of 2 degrees of freedom, $\{Z = 0, Y, r, \theta\}$ is a 3-dimensional subspace. From that, by fixing the level of energy at $H(Z = 0, Y, r, \theta) = 2Y^2 + r = h$, h a constant, we obtain a 2-dimensional set. It is useful to consider the projection of this set on the (r, θ) plane. There, given that the relationship $Y^2 + r = h$ constrains the value of r within $[0, h]$, what we have, in geometrical terms, is a *disk of radius h* , which we denote as D_h^- .

This disk is foliated by invariant circles; each of them correspond to fixing the particular value of r , which fixes the value of Y . They correspond to periodic orbits (recall that $\theta \neq 0$ when $Z = 0$) and are referred to as \mathbb{T}_r^- . We therefore note

$$D_h^- = \{(Z, Y, r, \theta) \mid Z = 0, 2Y^2 + r = h\} = \bigcup_{r \in [0, h]} \mathbb{T}_r^- \tag{4.9}$$

A particular case corresponds to $r = 0$, which implies $Y = \sqrt{\frac{h}{2}}$. In this case, the circle collapses to a point (the periodic orbit actually corresponds to an equilibrium point). Note that this is precisely the initial condition that is used throughout this work, as is been shown in the previous section (4.8). On the other hand, the perimeter of D_h^- is the circle \mathbb{T}_h^- , with $r = h$, and consequently $Y = 0$. All this is sketched in Figure 4.1.

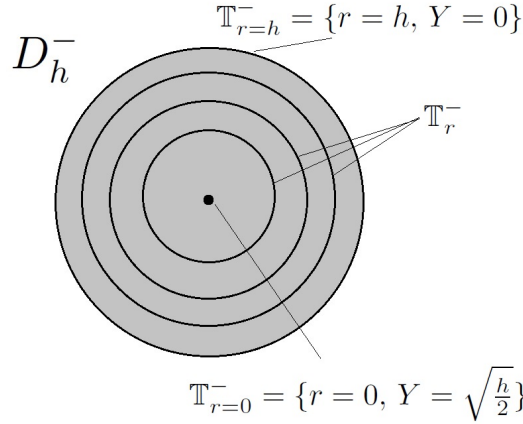


Figure 4.1: The projection of the invariant set $\{(Z, Y, r, \theta) \mid Z = 0, 2Y^2 + r = h\}$ onto (r, θ) is a disk of radius h foliated by periodic orbits, which are noted as \mathbb{T}_r^- . The figure is completely analogous for the case of D_h^+ .

For the case of $\{Z = 2\pi\}$, corresponding to $\{X \rightarrow +\infty\}$, the description is exactly the same: with the level of energy fixed at h , we define the analogous set D_h^+ , the projection of which onto (r, θ) corresponds to a disk that is foliated by periodic orbits, which we note \mathbb{T}_r^+ :

$$D_h^+ = \{(Z, Y, r, \theta) \mid Z = 2\pi, 2Y^2 + r = h\} = \bigcup_{r \in [0, h]} \mathbb{T}_r^+ \quad (4.10)$$

In this case, the set $\mathbb{T}_{r=h}^+$ corresponds to a periodic orbit at $Z = 2\pi$ with $r = h, Y = 0$ and therefore corresponds to a kink that has reached $Z = 2\pi$ with asymptotically zero velocity, all the energy having been transferred to the oscillator mode. Note that this is the orbit to which a solution starting at the critical velocity will tend to.

4.3 Invariant manifolds

The purpose of this last section is to describe and study the invariant manifolds of the equilibria of system (4.5) at $\{Z = 0, 2\pi\}$, corresponding to $\{X \rightarrow \pm\infty\}$. This will allow for describing the different behaviors of the solitons as a function of their velocity in terms of these invariant manifolds and their intersections. As exposed in the previous section, the invariant sets $\{Z = 0, 2\pi \mid H = h\}$ correspond to disks when projected onto (r, θ) , noted respectively D_h^- and D_h^+ . Each of them foliated by periodic orbits characterized by the value of r . We are going to assume the existence of invariant manifolds associated to the periodic orbits \mathbb{T}_r^\pm . Note the invariant manifold of each periodic orbit is a two-dimensional set corresponding to the surface of a cylinder; by continuity, their union will necessarily be the invariant manifold of the whole disk, geometrically a solid cylinder. Furthermore, in particular, the invariant manifolds of $\mathbb{T}_{r=0}^\pm$, which are points, will be one-dimensional curves.

Let $W^u(\mathbb{T}_r^-)$ the unstable manifold of the periodic orbit \mathbb{T}_r^- (corresponding to $Z = 0$). Let $W^u(D_h^-)$ the unstable manifold of the disk D_h^- . Then,

$$W^u(D_h^-) = \bigcup_{r \in [0, h]} W^u(\mathbb{T}_r^-) \quad (4.11)$$

And analogously for $Z = 2\pi$:

$$W^u(D_h^+) = \bigcup_{r \in [0, h]} W^u(\mathbb{T}_r^+) \quad (4.12)$$

Then, these manifolds can be continued, forward or backwards, through the flow of the system.

Invariant manifolds in the unperturbed case

We know that when $\varepsilon = 0$, the (Z, Y) and the (r, θ) dynamics become decoupled. Indeed, as noted in the previous section, the subsystem (Z, Y) behaves essentially like a nonlinear pendulum (see (4.7)), while $\dot{r}|_{\varepsilon=0} = 0$ shows that the oscillator mode evolves at a constant frequency. In particular, r being a constant implies that $\lim_{t \rightarrow -\infty} Y(t) = \lim_{t \rightarrow +\infty} Y(t)$, consistent with the pendulum phase portrait (recall that in this discussion we are assuming solutions that go from $Z = 0$ to $Z = 2\pi$). Geometrically, then, this requires that, for any solution on the energy level $H = h$ and with the initial condition $\lim_{t \rightarrow -\infty} r(t) = r_0$:

$$\begin{aligned} \lim_{t \rightarrow -\infty} (Z(t), Y(t), r(t), \theta(t)) &\in \mathbb{T}_{r_0}^- \\ \lim_{t \rightarrow +\infty} (Z(t), Y(t), r(t), \theta(t)) &\in \mathbb{T}_{r_0}^+ \end{aligned} \quad (4.13)$$

Since this verifies independently of the initial condition on $\theta(t)$, then it must follow that *the unstable manifold of $\mathbb{T}_{r_0}^-$ coincides with the stable manifold of $\mathbb{T}_{r_0}^+$* :

$$W^u(\mathbb{T}_{r_0}^-) = W^s(\mathbb{T}_{r_0}^+) , \quad r_0 \in [0, h] \quad (4.14)$$

And then all solutions with a positive velocity at $Z = 0$ can reach $Z = 2\pi$, consistently with previous descriptions.

What's more, since this is true for any $r_0 \in [0, h]$, then necessarily *the unstable manifold of D_h^- coincides with the stable manifold of D_h^+* :

$$W^u(D_h^-) = W^s(D_h^+) \quad (4.15)$$

This is schematically shown in Figure (4.2).

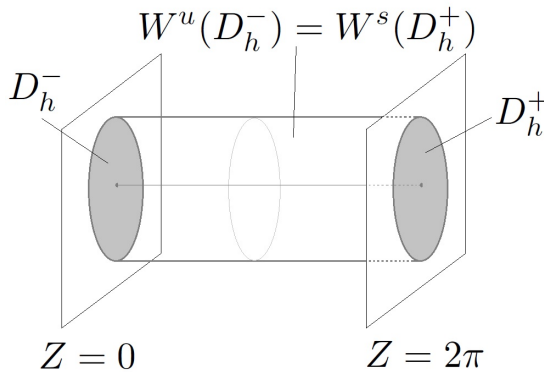


Figure 4.2: When $\varepsilon = 0$, the unstable manifold of D_h^- coincides with the stable manifold of D_h^+ . All orbits with initial $Y > 0$ at $Z = 0$ can reach $Z = 2\pi$, doing so at a velocity tending to the initial one.

Invariant manifolds in the perturbed system. Intersection of invariant manifolds. Geometrical interpretation of the critical velocity

When the coupling is restored by setting $\varepsilon \neq 0$, we know that r ceases to be a first integral and that the initial and final velocities will be different, since the two modes now exchange energy when close to $Z = \pi$ ($X = 0$). Geometrically, this corresponds to the invariant manifolds of the periodic orbits at $Z = 0$ and $Z = 2\pi$ not coinciding anymore. In dynamical terms, this means that not all solutions that start at $Z = 0$ with positive Y will be able to reach $Z = 2\pi$. The way the manifolds intersect will determine this.

For visualization purposes, we will consider the intersection of the manifolds with $Z = \pi$ (of course, any value of $Z \in (0, 2\pi)$ would be equally valid). As a reference, the schematic for the unperturbed case, in which $W^u(D_h^-) \cap \{Z = \pi\} = W^s(D_h^+) \cap \{Z = \pi\}$ is shown in Figure 4.3:

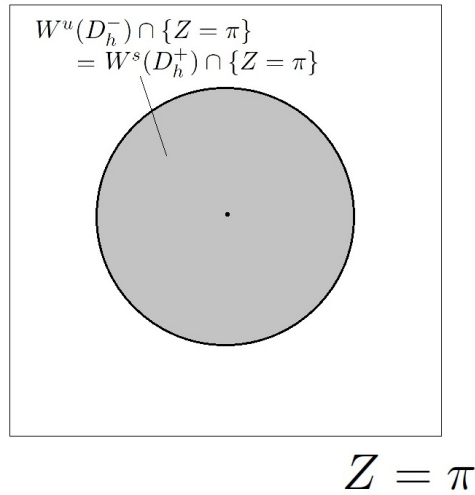


Figure 4.3: Intersection of the unstable manifold of D_h^- , which coincides with the stable manifold of D_h^+ when $\varepsilon = 0$, with $\{Z = \pi\}$.

In contrast, for $\varepsilon \neq 0$, various degrees of intersection between the manifolds are possible, depending on the value of the energy h (recall that h is the radius of the disks D_h^\pm):

- For small enough values of h , $W^u(D_h^-)$ will not intersect $W^s(D_h^+)$ at all, as shown in Figure 4.4. In dynamical terms, this implies that there is not enough initial energy for any solution coming from $Z = 0$ to be able to reach $Z = 2\pi$.
- As h increases, the two manifolds might intersect. A schematic example is shown in Figure 4.5. In it, we see a case in which the unstable manifold of D_h^- partially intersects the stable manifold of D_h^+ . This implies that there is a minimum value of $r = \bar{r}$ that this variable can have at $Z = 0$ that will allow it to reach $Z = 2\pi$; the periodic orbits with a lower value of r do not intersect $W^s(D_h^+)$.

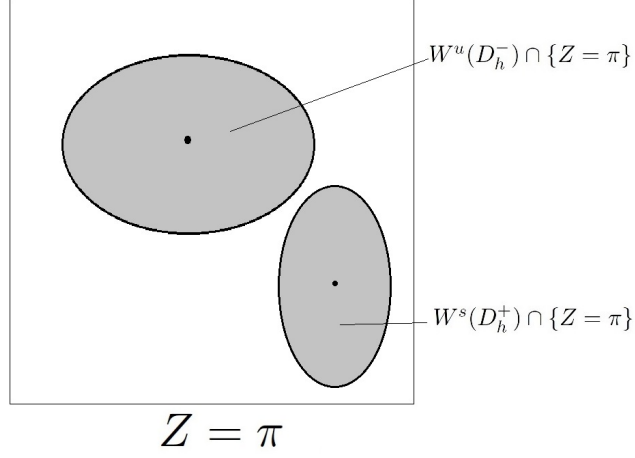


Figure 4.4: For small h , $W^u(D_h^-) \cap W^s(D_h^+) = \emptyset$ ($\varepsilon \neq 0$).

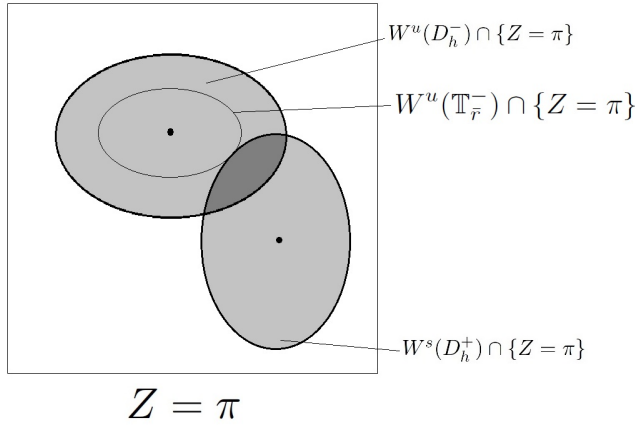


Figure 4.5: Different possible cases of intersection of the unstable and stable manifolds with $\{Z = \pi\}$, depending on the value of h ($\varepsilon \neq 0$).

At this point we can come back to the matter of the critical velocity of solitons treated in the previous section. Recall that the critical velocity was defined (using already the new variables) as the initial value for the velocity of a solution such that it reached $Z = 2\pi$ with zero velocity, under the initial condition $r = 0$ for the oscillator mode. Then, we see that this can be reinterpreted in terms of the invariant objects presented in this chapter: the initial condition $r = 0$ corresponds to the orbit tending to the equilibrium point \mathbb{T}_0^- as $t \rightarrow -\infty$, and so having an initial velocity of $y_- = \sqrt{\frac{h}{2}}$; whereas the condition of reaching $Z = 2\pi$ with zero velocity translates to the solution tending to the periodic orbit \mathbb{T}_h^+ as $t \rightarrow +\infty$, i.e. $r_+ = h$. Therefore, recalling that the energy level h is the parameter that determines the intersection of the invariant manifolds, we define the

critical energy h_c as the value of the energy h such that the unstable manifold of \mathbb{T}_0^- intersects the stable manifold of \mathbb{T}_h^+ . From this, then, the critical velocity is just $y_c = \sqrt{\frac{h_c}{2}}$.

Figure 4.6 shows this intersection at $Z = \pi$.

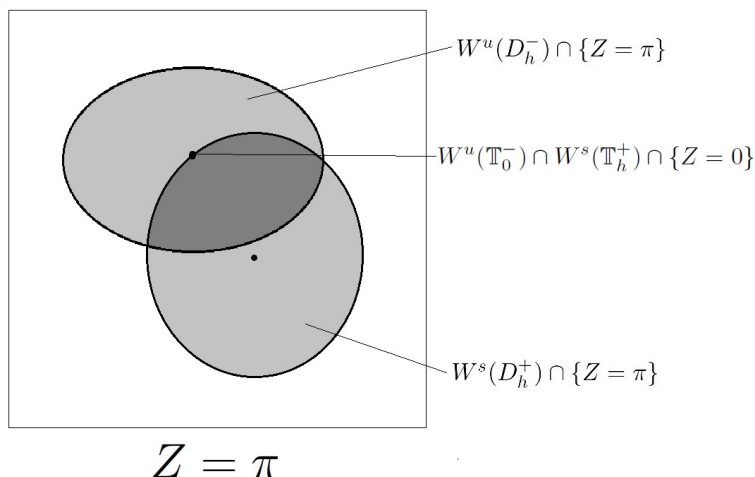


Figure 4.6: Intersection of the unstable and stable manifolds with $\{Z = \pi\}$ for $h = h_c$, so that $W^u(\mathbb{T}_0^-)$ intersects $W^s(\mathbb{T}_h^+)$ ($\varepsilon \neq 0$).

Finally, the following points are worth remarking:

- Note that, as mentioned, $W^u(\mathbb{T}_0^-)$ is 1-dimensional, as it is the invariant manifold of an equilibrium point, while $W^s(\mathbb{T}_h^+)$ is 2-dimensional, being the invariant manifold of a periodic orbit. Therefore, their intersection is a unique orbit that “wraps” around $W^s(\mathbb{T}_h^+)$.
- Aside from giving a new interpretation of the existence of the critical velocity in terms of geometrical objects, this (qualitative) formulation in terms of invariant manifolds serves an additional purpose: in a Chapter 3, in the computation of the integral to obtain ΔE to calculate the critical velocity, it was assumed that the expressions for $X(t)$, $a(t)$ could be expanded around their values for the homoclinic orbit (see (3.18)). Although not mentioned at the time, this is actually not a trivial assumption, since we are not in the context of regular perturbation theory. However, the fact that these arguments have been translated here in terms of invariant manifolds gives confidence in the aforementioned assumption; in particular, invariant manifolds are expected to behave robustly under perturbations (nevertheless, it is worth noting that specific theory would need to be applied in this case, since we are not dealing with invariant manifolds of hyperbolic points, which are the subject of the standard invariant manifolds theorems).
- The original calculation of the critical velocity in Chapter 3, a Melnikov integral is arrived at after energy considerations. Melnikov integrals measure, in fact, the distance between stable and unstable invariant manifolds in perturbed dynamical systems. Although not

developed quantitatively in this work, the author is confident that obtaining the corresponding Melnikov integral in terms of the invariant manifolds described in this chapter would yield the same integral, confirming that the two descriptions are equivalent.

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