Kink Moduli Spaces – Collective Coordinates Reconsidered

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ABSTRACT: Moduli spaces – finite-dimensional, collective coordinate manifolds – for kinks and antikinks in $\phi^4$ theory and sine-Gordon theory are reconsidered. The field theory Lagrangian restricted to moduli space defines a reduced Lagrangian, combining a potential with a kinetic term that can be interpreted as a Riemannian metric on moduli space. Moduli spaces should be metrically complete, or have an infinite potential on their boundary. Examples are constructed for both kink-antikink and kink-antikink-kink configurations. The naive position coordinates of the kinks and antikinks sometimes need to be extended from real to imaginary values, although the field remains real. The previously discussed null-vector problem for the shape modes of $\phi^4$ kinks is resolved by a better coordinate choice. In sine-Gordon theory, moduli spaces can be constructed using exact solutions at the critical energy separating scattering and breather (or wobble) solutions; here, energy conservation relates the metric and potential. The reduced dynamics on these moduli spaces accurately reproduces properties of the exact solutions over a range of energies.
1 Introduction

In field theory one often encounters particle-like solitons [1–3]. We will only consider here the type known as kinks, which are topological solitons in Lorentz-invariant theories in one space dimension, and will focus on the well-known examples of $\phi^4$ and sine-Gordon kinks. Because they are topologically distinct from the vacuum field, these kinks are stable. They can be at rest, or moving with any speed less than the speed of light (1 in our units). The energy of a kink at rest is identified with its mass, and each of these kinks has associated with it an antikink, obtained by spatial reflection, having an identical mass. A kink and antikink can exist together, as spatially separated particles in the topological vacuum sector of the theory, but because of the attractive force between them there is no static kink-antikink solution.

The fundamental distinction between field dynamics and particle dynamics is that fields have infinitely many degrees of freedom, whereas particles have finitely many. The finitely many degrees of freedom of solitons are known as collective coordinates, or moduli. Calling these coordinates moduli is a concise nomenclature derived from pure mathematics, and we will use it here in the context of kink-antikink dynamics. An interesting challenge is to
construct a finite-dimensional approximation to the field dynamics – a reduced dynamics on
moduli space – that adequately describes the dynamics of one or more kinks and antikinks.

In this paper we aim for an improved understanding of the geometry of moduli space,
and our models will combine a Riemannian metric on moduli space with a potential energy
function. This kind of model is not especially new. Generally, the moduli space is a finite-
dimensional submanifold of the infinite-dimensional field configuration space, the space
of all (static) field configurations at a given instant satisfying the boundary conditions
for finite energy, and in the desired topological sector. The field theory has kinetic and
potential terms. The kinetic energy is quadratic in time derivatives of the field and positive
definite. Restricting this to time-dependent fields moving through moduli space (i.e., static
field configurations with time-dependent moduli) gives an expression that is quadratic in
time derivatives of the moduli and positive definite. Since the field time derivatives are
tangent to the moduli space, these kinetic terms define a metric on moduli space. The field
theory potential energy (which includes the field gradient terms) restricts to a potential
energy on moduli space. The reduced dynamics on moduli space is then defined by this
metric and potential. This is a natural dynamical system in the sense of Arnol’d [4].

For certain types of soliton, usually in more than one space dimension, there are
no static forces between solitons; these are the solitons of Bogomolny (or BPS) type [5].
Examples are abelian Higgs vortices at critical coupling [6] and non-abelian Yang–Mills–
Higgs monopoles [7]. For Bogomolny solitons, there is a moduli space of static \( N \)-soliton
solutions (solitons and antisolitons never occur simultaneously here). The potential energy
is a constant proportional to the topological charge, having no effect, so the dynamics on
moduli space is controlled by the metric alone and the motion is therefore along geodesics
at constant speed [8–10]. This is usually a good approximation to the soliton dynamics in
the field theory, provided the soliton motion is not highly relativistic. For some types of
Bogomolny soliton, e.g. sigma-model lumps, the moduli space is not geodesically complete
because a lump can contract to zero size in finite time [11–13]. We shall avoid examples
with a scaling invariance that makes this behaviour possible. There are also examples of
solitons close to those of Bogomolny type, for example, vortices close to critical coupling.
The potential is then non-zero but small, and its effect is to modify the geodesic motion on
moduli space. In the examples of kink-antikink dynamics that we study here, the potential
energy is not small, and the metric and potential on moduli space play equally important
roles.

For kinks and antikinks, there is no canonically defined moduli space. It is a matter
of art rather than science to construct one. However, basic principles can be learned from
the Bogomolny examples. First, the moduli space should either be a metrically complete
submanifold of field configuration space, or the potential should be infinite on the boundary.
If not, the dynamics can reach the boundary in finite time, and it is unclear what happens
next. Second, the moduli space should be smoothly embedded in the field configuration
space, otherwise the moduli space motion cannot smoothly approximate the true field
dynamics. Apparent singularities in the moduli space metric sometimes occur, but these
can be resolved by a better choice of coordinates, as we will show.

We begin in Section 2 by introducing the notion of moduli space dynamics in \( \phi^4 \) theory,
and illustrate it with the simple example of single kink motion. A static kink interpolates between the two vacuum field values $\pm 1$, and has the simple form $\phi(x) = \tanh(x - a)$, where $a$ is the modulus representing the centre of the kink. The antikink with centre $a$ is $\phi(x) = -\tanh(x - a)$, and is the reflection of the kink. In the moduli space dynamics, $a$ becomes a function of time $t$. We defer discussion of kink-antikink dynamics in $\phi^4$ theory until Section 4, because it is relatively complicated.

Instead, in Section 3 we consider sine-Gordon (sG) theory, and construct a moduli space model for kink-antikink dynamics there. As sG theory is exactly integrable, we can compare the moduli space dynamics with the known exact solutions. Our model can be applied simultaneously to kink-antikink scattering and to the lower-energy sG breather, which can be interpreted as a bounded kink-antikink motion. Including a non-trivial metric on the moduli space is important. A model with only a potential energy depending on the kink-antikink separation is less successful. We also investigate kink-antikink-kink dynamics, where again an exact solution is known. One feature of sG theory is that for each kink and antikink we need to introduce just one collective coordinate. Our models do not identically reproduce the behaviour of the exact solutions because the field configurations we use do not vary as the soliton speeds change – the solitons do not Lorentz contract. The modelling is therefore non-relativistic in character, and yet it can cope quite well with kinks and antikinks close to annihilation, a fundamentally relativistic process, where the initial rest energy of the solitons converts entirely into kinetic energy.

In Section 4 we return to the non-integrable $\phi^4$ field theory, and its kinks and antikinks. There are field configurations with a string of well-separated, alternating kinks and antikinks along the spatial line, where the field value varies between close to $-1$ and $+1$. A kink and antikink are in some sense identical particles, because of this forced alternation. There have been numerous studies of kink-antikink dynamics in $\phi^4$ theory, starting with the pioneering work of [14–16] and others; for a review, see [17]. Although the field dynamics is complicated, there is still much interest in devising an approximate description with a finite number of moduli, modelling the kinks and antikinks as particles.

The simplest model for a kink and antikink would have just two degrees of freedom, their positions. However, it is well known that in $\phi^4$ theory, a kink has an internal vibrational degree of freedom – the shape mode – because the linearised field equation in the kink background has one localised field vibration mode, whose frequency is below the continuum of radiation modes that can disperse to spatial infinity. More sophisticated models therefore allow the kink and antikink to have two degrees of freedom each, allowing for transfer of energy between the positional dynamics and the vibrational shape modes. The moduli space dynamics conserves energy and doesn’t account for the conversion of energy into radiation. Nevertheless, a good finite-dimensional moduli space dynamics can help us understand better the mechanism by which energy is transferred in and out of the shape modes, and by coupling the moduli space dynamics to other field modes, one may understand better the mechanism and timing of the production of radiation.

It is recognised that some finite-dimensional models of $\phi^4$ kink-antikink dynamics have problems. The manifold on which the finite-dimensional dynamics takes place has not always been complete, and if complete then unsuitable coordinates have sometimes been
chosen. Problems tend to occur, not when the kink and antikink are well separated, but when they are close together and about to annihilate. We will show that these problems can nevertheless be resolved.

It might be thought that the problems are intrinsic – that the notion of kink and antikink as separate objects is bound to fail when they are about to annihilate. However this is not the case. Field simulations in $\phi^4$ theory show that in a collision of a kink and antikink, after rather dramatic behaviour while they are close together, they can emerge relatively unscathed and separate to infinity with limited transfer of energy to radiation. Even if they completely annihilate into radiation, this can be a relatively slow process. In sG theory things are simpler, because the integrability of the theory implies that kinks and antikinks never annihilate, and no radiation is produced. A kink and antikink just pass through each other, but with a positional shift.

As mentioned above, the construction of a suitable moduli space for a kink and antikink is more art than science. However, there are some rather simple formulae for kink-antikink field configurations that have been proposed, and we will use these together with some variants. The basic formula is simply to add (superpose) the exact static kink solution to the exact antikink. In $\phi^4$ theory a field shift by a constant is needed to satisfy the boundary conditions. We will also consider a variant of this formula, due to Sugiyama [14], where the shape modes for the kink and the antikink are included, with arbitrary amplitudes. We resolve the problem of the null-vector that can occur here, noted by Takyi and Weigel [18]. A further variant is to include a weight factor multiplying the usual kink and antikink profiles. The aim is not to add further moduli, but to more satisfactorily account for the field configurations where the kink and antikink are close to annihilating.

We will also consider, in Section 5, the configurations of $\phi^4$ kinks and antikinks that arise from the recently proposed iterated kink equation [19]. The $n$th iterate $\phi_n$ provides a moduli space of dimension $n$ for a total of $n$ kinks and antikinks. Iterated kinks do not allow for the usual shape mode deformations, but do allow for arbitrary kink locations, and smoothly allow a kink and antikink to pass through the vacuum configuration. The kink-antikink configurations $\phi_2$ are weighted superpositions of the usual kink and antikink, and this is part of the motivation for introducing weights.

In Section 6 we study kink-antikink-kink configurations in $\phi^4$ theory (restricted to configurations with spatial antisymmetry), using a naive superposition of profiles, a weighted superposition of profiles, and solutions $\phi_3$ in the iterated kink scheme. These field configurations differ, although they agree when the two kinks are well separated from the central antikink. We quantitatively compare these three descriptions.

One remarkable discovery, seen here in several guises, is that the dynamics of the moduli in the kink-antikink and kink-antikink-kink sectors must sometimes be interpreted as particle motions where the separation coordinate scatters from a real to an imaginary value. (In detail, this depends on whether there are weight factors or not.) This is a curious extension of the idea of 90-degree scattering of solitons. It is well known that higher-dimensional topological solitons, including vortices [10, 20], monopoles [9] and Skyrmions [21], often scatter at 90 degrees in a head-on collision. Two such solitons approach each other symmetrically along, say, the $x$-axis, collide smoothly at the origin, and emerge back-
to-back along the $y$-axis. (For the 3-dimensional solitons, the scattering plane is determined by the initial conditions, e.g., the relative orientation of Skyrmions.)

In a $\phi^4$ kink-antikink collision, the incoming centres are at $-a$ and $a$, with $a$ approaching zero. After meeting, the centres are at $i\tilde{a}$ and $-i\tilde{a}$, with $\tilde{a}$ real and increasing from zero. The field remains real. As $\tilde{a}$ increases, the potential energy becomes large, and at some point the motion stops and reverses. The relevant moduli space is complete only if one allows $a$ to become imaginary, and this is because the good coordinate is really $a^2$, which can become negative. So even for moduli space dynamics in one dimension, 90-degree scattering can occur in the complex plane of the relative position coordinate. The possibility, indeed necessity, for 90-degree scattering is because of the identity of the kinks, and the symmetry of the field configuration under interchange of $a$ and $-a$.

2 Moduli Spaces in $\phi^4$ Theory

The manifold and metric structure of the infinite-dimensional $\phi^4$ field configuration space is quite simple. We recall it here and describe how it can be used to construct the metric on a finite-dimensional moduli space of fields. We then apply this formalism to the basic example of the moduli space of a single kink. This is an opportunity to fix conventions and notation before tackling kink-antikink and kink-antikink-kink fields.

The Lagrangian of $\phi^4$ theory in one spatial dimension is

$$L = \int_{-\infty}^{\infty} \left( \frac{1}{2} \dot{\phi}^2 - \frac{1}{2} \phi''^2 - \frac{1}{2} (1 - \phi^2)^2 \right) dx,$$

where $\phi(x,t)$ is a real field taking arbitrary values. An overdot denotes a time derivative, and a prime denotes a spatial derivative. The field equation, the Euler–Lagrange equation derived from the Lagrangian, is the nonlinear Klein–Gordon equation

$$\ddot{\phi} - \phi'' - 2(1 - \phi^2)\phi = 0.$$

The Lagrangian can be split into positive definite kinetic and potential terms as $L = T - V$, where $T$ just involves the integral of $\dot{\phi}^2$, and the remaining terms contribute to $V$. The splitting of kinetic from gradient terms hides the theory’s Lorentz invariance, but this seems to be necessary to obtain a moduli space dynamics for kinks.

The theory has two vacua, $\phi = \pm 1$. We will restrict attention to field configurations with finite potential energy, which means that each configuration approaches vacuum values at spatial infinity. There are therefore four topologically distinct sectors. One is the vacuum sector where $\phi \to -1$ as $x \to \pm \infty$. The vacuum solution itself is $\phi(x) = -1$ for all $x$. Another is the kink sector, where $\phi \to -1$ as $x \to -\infty$ and $\phi \to +1$ as $x \to \infty$. There is a second vacuum sector and an antikink sector, which are similar, but we will not explicitly need these.

Field configuration space is an infinite-dimensional affine space. An affine space is modelled on a linear space, but has no natural or canonical origin. In the vacuum sector, one can express any field configuration as $\phi(x) = -1 + \chi(x)$ where $\chi \to 0$ as $x \to \pm \infty$. 

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The shifted fields $\chi$ can be linearly combined, which explains why this sector has an affine structure.

For static fields, the field equation (2.2) has the first integral

$$\phi' = 1 - \phi^2.$$  \hspace{1cm} (2.3)

The constant of integration has been chosen so that a solution can satisfy the vacuum boundary conditions $\phi \to \pm 1$ at spatial infinity, and the sign of the square root has been chosen so that the solutions are kinks rather than antikinks. The kink solutions are

$$\phi(x; a) = \tanh(x - a)$$  \hspace{1cm} (2.4)

where $a$, the further constant of integration, is arbitrary, and for the moment, real. $a$ represents the kink centre, where $\phi = 0$. $a$ is the modulus of the solution, and the moduli space of kink solutions is the real line $\mathbb{R}$ with $a$ a good coordinate everywhere, as we will verify. The kink sector of field configuration space is also an affine space, because the generic configuration in this sector can be written as $\phi(x) = \tanh(x) + \chi(x)$, where $\chi$ has the same decay properties as before, so different field configurations $\chi$ can be added. We have chosen the kink centred at the origin as the origin of the affine space, but this is just a choice.

Each sector of field configuration space has a natural Riemannian metric, an infinite-dimensional Euclidean metric. The squared distance between configurations $\phi_1$ and $\phi_2$ is given by

$$s^2 = \int_{-\infty}^{\infty} (\phi_2(x) - \phi_1(x))^2 \, dx.$$  \hspace{1cm} (2.5)

The integrand can also be written as a squared difference of $\chi$ fields, which shows that the metric structures in the vacuum and kink sectors are essentially the same. The Riemannian metric is obtained by considering field configurations with infinitesimal separation, $\phi$ and $\phi + \delta\phi$; this is

$$\delta s^2 = \int_{-\infty}^{\infty} (\delta\phi(x))^2 \, dx.$$  \hspace{1cm} (2.6)

Note the need for spatial integration in these formulae.

Suppose we now have a moduli space, a finite-dimensional submanifold of field configuration space, where the configurations depend on finitely many moduli (collective coordinates) $y^i$, denoted jointly as $y$. We write these field configurations as $\phi(x; y)$. Varying the moduli, we have the field variation

$$\delta\phi(x; y) = \frac{\partial\phi}{\partial y^i} (x; y) \delta y^i.$$  \hspace{1cm} (2.7)

The Riemannian metric restricted to the moduli space can therefore be written as $\delta s^2 = g_{ij}(y) \delta y^i \delta y^j$, where, from eq.(2.6), we see that

$$g_{ij}(y) = \int_{-\infty}^{\infty} \frac{\partial\phi}{\partial y^i}(x; y) \frac{\partial\phi}{\partial y^j}(x; y) \, dx.$$  \hspace{1cm} (2.8)
This is the key formula. It is used to define the metric on moduli spaces of kinks and antikinks, and allows one to study if the moduli space is metrically complete, and whether the coordinates have been well chosen. From this formula we immediately infer that the kinetic energy for motion restricted to the moduli space is

\[ T = \frac{1}{2} g_{ij}(y) \dot{y}^i \dot{y}^j, \]  

(2.9)
as \[ \dot{\phi} = \frac{\partial \phi}{\partial y^i} \dot{y}^i. \]

Let us apply this to the moduli space of a single kink. The field configurations here are the static solutions of the field equation, \( \phi(x; a) = \tanh(x - a) \). There is just one modulus \( a \), and the metric is \( \delta s^2 = g(a) \delta a^2 \) where

\[ g(a) = \int_{-\infty}^{\infty} \left( \frac{\partial \phi}{\partial a}(x; a) \right)^2 dx. \]  

(2.10)

For \( \phi(x; a) = \tanh(x - a) \), the derivative with respect to \( a \) can be traded for (minus) the gradient, the derivative with respect to \( x \), so

\[ g(a) = \int_{-\infty}^{\infty} \delta^2(x; a) dx, \]  

(2.11)

which is independent of the location \( a \) of the kink.

\( \delta^2 \) can be evaluated directly for the kink and integrated, but it is illuminating to note that the integral is equal to the mass \( M \) (the total potential energy) of the kink, and this result holds for any type of scalar kink in a Lorentz-invariant theory in one dimension, not just the \( \phi^4 \) kink. Recall that the potential energy is

\[ V = \int_{-\infty}^{\infty} \left( \frac{1}{2} \phi'^2 + \frac{1}{2}(1 - \phi^2)^2 \right) dx. \]  

(2.12)

This is minimised in its topological sector by the kink, and in particular is minimised under a spatial rescaling of the kink profile. This last property implies that the two integrals contributing to \( V \) are equal, and therefore \( V \) equals the integral of \( \phi'^2 \). For the \( \phi^4 \) kink, \( V = M = \frac{4}{3} \) and therefore \( g(a) = M = \frac{4}{3} \).

The kinetic energy of a moving kink, with a time-dependent modulus \( a(t) \), is therefore \( \frac{1}{2} Ma^2 \), the standard expression for the kinetic energy of a moving particle in non-relativistic physics. The moduli space approximation does not take relativistic effects into account. The potential energy is just a constant, the kink mass, so the reduced Lagrangian on moduli space for a single kink is \( L_{\text{red}} = \frac{2}{3} \dot{a}^2 \). The equation of motion is \( \ddot{a} = 0 \), and the kink moves with constant velocity. There is no Lorentz contraction of the kink, and its speed is not constrained to be less than the speed of light.

Metrically, the single kink moduli space is the real line with the standard Euclidean metric scaled by a constant factor. \( a \) is a good coordinate, because the metric \( g(a) = M \) is everywhere positive. We will see examples later where a moduli space metric appears not to be positive definite, but becomes so with a better choice of coordinates.
3 Sine-Gordon Theory

Probably the clearest laboratory where we can test our ideas is the sine-Gordon (sG) field theory [22] where the exact forms of multi-soliton solutions are known. The Lagrangian of sG theory is

\[ L = \int_{-\infty}^{\infty} \left( \frac{1}{2} \dot{\phi}^2 - \frac{1}{2} \phi'^2 - (1 - \cos \phi) \right) dx. \]  

(3.1)

The first integral is the kinetic energy \( T \) and the remaining integrals give the potential energy \( V \). The field equation,

\[ \ddot{\phi} - \phi'' + \sin \phi = 0, \]  

(3.2)

has the static kink (soliton) solutions

\[ \phi(x; a) = 4 \arctan(e^{x-a}) , \]  

(3.3)

interpolating between 0 and \( 2\pi \). The antikink is \( \phi(x; a) = -4 \arctan(e^{x-a}) \), interpolating between 0 and \(-2\pi\). Both the kink and antikink have mass \( M = 8 \).

In the moduli space dynamics, the expression for a moving kink is

\[ \phi(x, t) = 4 \arctan(e^{x-a(t)}) \]  

(3.4)

and the reduced Lagrangian is \( L_{\text{red}} = \frac{1}{2} M \dot{a}^2 = 4a^2 \). Like a \( \phi^4 \) kink, an sG kink moves at constant velocity.

3.1 Kink-antikink dynamics in sine-Gordon theory

The naive superposition of a kink centred at \(-a\) and an antikink centred at \(a\) is

\[ \phi(x; a) = 4 \arctan(e^{x+a}) - 4 \arctan(e^{x-a}). \]  

(3.5)
Applying the tangent subtraction formula to $\frac{1}{4}\phi$, this becomes

$$\phi(x; a) = 4 \arctan \left( \frac{\sinh(a)}{\cosh(x)} \right),$$

where $a$ takes any real value. This is our moduli space of field configurations representing a kink and antikink. For large positive $a$ there is a kink on the left and antikink on the right, and $\phi$ is positive; for large negative $a$ the kink and antikink are exchanged and $\phi$ is negative. When $a = 0$, the configuration is the vacuum $\phi = 0$. The configurations for various values of $a$ are shown in Fig. 1.

We wish to model kink-antikink dynamics (both scattering and oscillating solutions, i.e., breathers) using this 1-dimensional moduli space. Considering $a(t)$ as a time-dependent modulus, substituting (3.6) into the field theory Lagrangian (3.1), and integrating, we derive a reduced Lagrangian on moduli space

$$L_{\text{red}} = \frac{1}{2} g(a) \dot{a}^2 - V(a).$$

The kinetic term of the field theory Lagrangian gives the moduli space metric

$$g(a) = 16 \left( 1 + \frac{2a}{\sinh(2a)} \right)$$

and the remaining terms give the moduli space potential

$$V(a) = 16 \left[ 1 - \frac{1}{2 \cosh^2(a)} \left( 1 + \frac{2a}{\sinh(2a)} \right) \right].$$

Observe that the metric and the potential satisfy the relation

$$\frac{1}{2 \cosh^2(a)} g(a) + V(a) = 16.$$

For large $a$, $V(a) \sim 16 - 32e^{-2a}$, where the second term is the well-known interaction energy between an sG kink and antikink at large separation $2a$.

The time-dependence of the modulus $a$ can be found using the first integral of the equation of motion derived from (3.7),

$$\frac{1}{2} g(a) \dot{a}^2 + V(a) = E,$$

and then integrating once more. Both $V$ and the conserved energy $E$ include the rest energy of the kink and antikink, so the critical energy separating scattering solutions from breathers is $E = 16$. The motion on moduli space is implicitly given by

$$\pm (t - t_0) = \int \sqrt{\frac{g(a)}{2(E - V(a))}} \, da,$$

and can be calculated numerically.
Before presenting the solutions, let us recall the analogous exact solutions of the sine-Gordon theory. A breather solution is

$$\phi(x,t) = -4 \arctan \left( \frac{\sqrt{1 - \omega^2 \sin(\omega t)}}{\omega \cosh(\sqrt{1 - \omega^2} x)} \right). \quad (3.13)$$

This has frequency $\omega$ in the range $(0, 1)$ and energy

$$E = 16 \sqrt{1 - \omega^2}. \quad (3.14)$$

The configurations that define the moduli space do not allow for a change in spatial profile. To make a comparison with the moduli space dynamics we therefore ignore the factor $\sqrt{1 - \omega^2}$ in $\cosh(\sqrt{1 - \omega^2} x)$ and say that the exact breather has modulus dynamics given by

$$\sinh(a(t)) = -\frac{\sqrt{1 - \omega^2} \sin(\omega t)}{\omega}. \quad (3.15)$$

The most important property of the breather for us is the relation (3.14) between energy and frequency, and this will be compared with the prediction of the moduli space dynamics.

The kink-antikink scattering solution can be obtained by analytic continuation of the breather, when the frequency becomes imaginary. Setting $\omega = iq$ in (3.13), with $q$ real, we obtain the scattering solution

$$\phi(x,t) = -4 \arctan \left( \frac{\sqrt{1 + q^2 \sinh(qt)}}{q \cosh(\sqrt{1 + q^2} x)} \right). \quad (3.16)$$

This is not in the standard form. The reparametrisation $v = q/\sqrt{1 + q^2}$ leads to

$$\phi(x,t) = -4 \arctan \left( \frac{\sinh(\gamma vt)}{v \cosh(\gamma x)} \right), \quad (3.17)$$

where $\gamma = 1/\sqrt{1 - v^2}$ is the usual Lorentz factor and $\gamma v = q$. This is the scattering solution for a kink and antikink that approach each other with velocities $v$ and $-v$, having total energy $E = 16 \gamma = 16 \sqrt{1 + q^2}$. To make a comparison with the prediction of the moduli space dynamics, we say that the exact scattering solution has modulus dynamics

$$\sinh(a(t)) = -\frac{\sinh(\gamma vt)}{v}, \quad (3.18)$$

ignoring the $\gamma$ factor in $\cosh(\gamma x)$. The asymptotic form of the scattering solution, for large negative $t$ and $x$, is the incoming kink

$$\phi(x,t) \sim 4 \arctan(e^{\gamma(x-vt)-\log v}), \quad (3.19)$$

and the outgoing kink (with field value shifted down by $2\pi$) has the opposite positional shift.

Particularly useful and interesting for us is the exact solution with the critical energy $16$,

$$\phi(x,t) = -4 \arctan \left( \frac{t}{\cosh(x)} \right), \quad (3.20)$$
which evolves precisely through the configurations in our moduli space, with

\[ \sinh(a(t)) = -t. \quad (3.21) \]

This can be regarded either as a scattering solution where the initial incoming velocities have decreased to zero, or as a breather of infinite period, where the kink and antikink reach spatial infinity with zero velocity. Equation (3.21) must be an exact solution of the equation of motion for \( a(t) \) on the moduli space. The reason is that an exact solution of the field equation is a stationary point of the action for unconstrained field variations, and is therefore automatically a stationary point of the action for a smoothly embedded set of constrained fields (the fields in the moduli space). This result holds provided the Lagrangian of the constrained problem is the restriction of the Lagrangian of the unconstrained problem, which is the case here, since both kinetic and potential terms of the moduli space Lagrangian are obtained by restriction from the field theory Lagrangian.

This has an interesting consequence. If \( \sinh(a(t)) = -t \), then \( \cosh(a(t)) \dot{a} = -1 \). Substituting this into the energy conservation equation (3.11), we see that the relation (3.10) between the metric and potential on moduli space must hold. More generally, if there is an exact solution of the field theory which is precisely a motion through moduli space, then the potential along the trajectory through the moduli space can be deduced from the metric. Generally, the field theory solution will be at a particular energy, and it does not follow that all motions in moduli space correspond to exact solutions of the field theory.

Let us now consider the two energy regimes of the moduli space dynamics. The first is where \( E > 16 \); then \( a \to \mp \infty \) as \( t \to \pm \infty \) and there is kink-antikink scattering. The kink
effectively passes through the antikink. In Fig. 2 we compare the moduli space evolution of $a(t)$ according to (3.12) (solid line) with the nonrelativistic version of the exact evolution (3.18) (dotted line),

$$\sinh(a(t)) = -\frac{\sinh(vt)}{v}. \quad (3.22)$$

The agreement is very good. There is a very small discrepancy that grows with the velocity, shown in Fig. 3. In Fig. 4 we show the positional shift of $a$ away from a linear evolution in time, due to the collision. The solid line represents the exact, nonrelativistic shift

$$\Delta a = 2 \log v, \quad (3.23)$$

while the dotted line is our numerical result from the moduli space dynamics. The agreement is again striking.
The second regime is where $E < 16$. The modulus $a$ oscillates between turning points $\pm a_{\text{max}}$ (where the kinetic energy vanishes) given by

$$V(\pm a_{\text{max}}) = 16 \left[ 1 - \frac{1}{2 \cosh^2(a_{\text{max}})} \left( 1 + \frac{2a_{\text{max}}}{\sinh(2a_{\text{max}})} \right) \right] = E.$$  \hspace{1cm} (3.24)

This motion corresponds to a breather. Its period, as a function of $a_{\text{max}}$, is

$$\sqrt{2} \int_{-a_{\text{max}}}^{a_{\text{max}}} \frac{g(a)}{V(a_{\text{max}}) - V(a)} \, da,$$

and the frequency $\omega$ is $2\pi$ divided by this period.

In Fig. 5 we plot $E/\sqrt{1 - \omega^2}$ for the moduli space dynamics, and compare with the ratio 16 for the exact sG breather solution. The ratios agree as the energy approaches 16 (i.e., as $a_{\text{max}} \rightarrow \infty$). In Fig. 6 we plot frequency $\omega$ against energy $E$ for the breather and for the periodic solutions in the moduli space dynamics over a larger range. Again the agreement is good, especially as $E \rightarrow 16$. The poorer result for the moduli space dynamics if the variation of the metric is ignored (i.e., if it is fixed to its asymptotic value $g = 16$) is also shown.

Note that the exact breather’s frequency approaches 1 as its amplitude goes to zero, whereas in the moduli space dynamics the limiting frequency is $\sqrt{\frac{4}{3}}$. The difference is because the moduli space dynamics uses a field profile of constant width, whereas the exact breather gets arbitrarily broad. This broadening can be interpreted as the opposite (the analytic continuation) of the Lorentz contraction of a colliding kink and antikink, and is ignored in the moduli space approach.

### 3.2 Kink-antikink-kink dynamics in sine-Gordon theory

A kink-antikink-kink analogue of the naive superposition of a kink and antikink in sine-Gordon theory is

$$\phi(x; b) = 4 \arctan(e^{x+b}) - 4 \arctan(e^x) + 4 \arctan(e^{x-b}).$$  \hspace{1cm} (3.26)
To simplify the discussion, we are restricting attention to configurations that are (anti)symmetric in $x$, in the sense that $\phi(-x) = 2\pi - \phi(x)$. Using the tangent addition formula

$$\tan(\alpha + \beta + \gamma) = \frac{\tan(\alpha) + \tan(\beta) + \tan(\gamma) - \tan(\alpha)\tan(\beta)\tan(\gamma)}{1 - \tan(\alpha)\tan(\beta) - \tan(\alpha)\tan(\gamma) - \tan(\beta)\tan(\gamma)}$$

we can reexpress the superposition (3.26) as

$$\phi(x; b) = 4 \arctan \left( \frac{2 \cosh(b) - 1}{1 + (2 \cosh(b) - 1)e^{2x}} \right).$$

(3.28)

When $b = 0$ this kink-antikink-kink configuration simplifies to a single kink.

The set of field configurations (3.28) is symmetric in $b$, and $2 \cosh(b) - 1$ is nowhere less than 1. The derivative $\frac{\partial \phi}{\partial b}$ vanishes at $b = 0$, so the metric coefficient $g(b)$ vanishes there too. The moduli space is incomplete. This problem is easily resolved by extending the moduli space to the set of configurations

$$\phi(x; \mu) = 4 \arctan \left( \frac{\mu e^x + e^{3x}}{1 + \mu e^{2x}} \right),$$

(3.29)

where $\mu$ takes any real value greater than $-1$. For sufficiently large positive $\mu$ we have a chain of kink, antikink and kink, and for $\mu = 1$ we have a single kink. When $\mu = 0$ the configuration is a compressed kink $\phi(x) = 4 \arctan(e^{3x})$, and when $\mu$ is negative the configurations acquire bumps outside the usual range of field values $[0, 2\pi]$. The bumps extend down to $-\pi$ and up to $3\pi$ as $\mu \to -1$, and the configuration asymptotically looks like a half-antikink on the left (interpolating between 0 and $-\pi$), a compressed double-kink in the middle (interpolating between $-\pi$ and $3\pi$) and another half-antikink on the right (interpolating between $3\pi$ and $2\pi$). Examples of these configurations are plotted in Fig. 7.
The metric on this moduli space, in terms of \( \mu \), is
\[
 g(\mu) = \frac{16}{(\mu - 1)(\mu + 3)} \left[ 1 - \frac{4}{(\mu + 1)\sqrt{(\mu - 1)(\mu + 3)}} \text{arccoth} \left( \frac{1 + \mu}{\sqrt{(\mu - 1)(\mu + 3)}} \right) \right].
\]
(3.30)

It is smooth and positive definite, but becomes singular as \( \mu \to -1 \). The metric and potential are shown in Fig. 9 (left panel), and the reduced dynamics on the moduli space gives a reasonably good description of symmetric kink-antikink-kink motion.

However the exact sG kink-antikink-kink solutions involve somewhat different field configurations. There is an analogue of a breather solution in this sector [23],
\[
 \phi(x, t) = 4 \text{arctan} \left( \frac{(1 + \beta)e^x + (1 - \beta)e^{x+2\beta x} - 2\beta e^{\beta x} \cos(\alpha t)}{(1 - \beta) + (1 + \beta)e^{2\beta x} - 2\beta e^{x+\beta x} \cos(\alpha t)} \right),
\]
(3.31)

where the parameters \( \alpha \) and \( \beta \) must satisfy \( \alpha^2 + \beta^2 = 1 \). This breather has frequency \( \alpha \) and its amplitude depends on \( \beta \). In the limit where \( \alpha \to 1 \) and \( \beta \to 0 \) the solution reduces to a static single kink, and for small \( \beta \) the solution is known as a wobbling kink.

We are interested in the opposite limit, where \( \alpha \to 0 \) and \( \beta \to 1 \). Taking this limit
carefully, one finds an analogue of the critical breather with infinite period, the solution

\[
\phi(x, t) = 4 \arctan \left( \frac{(1 + 2t^2 + 2x)e^x + e^{3x}}{1 + (1 + 2t^2 - 2x)e^{2x}} \right). \tag{3.32}
\]

It has energy \(E = 24\), and approaches a configuration with infinitely separated kink, antikink, and kink at rest as \(|t| \to \infty\).

Notice that because of the terms \(2x\) in this formula, this solution does not match any of the naive kink-antikink-kink field configurations. We therefore consider a variant moduli space with configurations

\[
\phi(x; d) = 4 \arctan \left( \frac{(d + 2x)e^x + e^{3x}}{1 + (d - 2x)e^{2x}} \right). \tag{3.33}
\]

The solution (3.32) moves precisely in this moduli space, but only along the half-line \(d \geq 1\). For the same reason as before, we need \(d\) to extend through zero to negative real values to have a metrically complete moduli space. Again, the allowed range is \(d > -1\), because the configuration approaches an infinitely steep double-kink sandwiched between two half-antikinks as \(d \to -1\). However, for these configurations, bumps occur for positive and negative values of \(d\), see Fig. 8.

The metric \(g(d)\) and potential \(V(d)\) on the moduli space can be calculated in the usual way and are plotted in Fig. 9 (right panel). Because there is an exact solution of sG field theory moving through this moduli space, \(g\) and \(V\) are related. For the solution (3.32) there is the energy equation

\[
\frac{1}{2} g(d) \dot{d}^2 + V(d) = 24, \tag{3.34}
\]

where \(d = 1 + 2t^2\). So \(\dot{d}^2 = 16t^2 = 8(d - 1)\), and we obtain the relation

\[
4g(d)(d - 1) + V(d) = 24. \tag{3.35}
\]

Motion on the moduli space does not have to be at energy \(E = 24\). When the energy is less, we obtain a good approximation to the true breather (wobbling kink) solution. Also,
extending the moduli space to negative $d$ allows us to consider motion on the moduli space with energy greater than 24, modelling a symmetrical collision of two incoming kinks with an antikink at the origin. The exact solutions in this case can be derived from eq.(3.31) by allowing $\beta$ to be greater than 1 and $\alpha$ imaginary.

This completes our discussion of moduli spaces for selected examples of kink and antikink dynamics in sine-Gordon theory. We now return to $\phi^4$ theory.

4 Kink-Antikink Moduli Spaces in $\phi^4$ Theory

In this section we discuss candidate moduli spaces for kink-antikink configurations in $\phi^4$ theory. These configurations are topologically in the vacuum sector, but kink-antikink dynamics is still interesting and non-trivial, and has been much studied, see e.g. [14–16, 24, 25].

4.1 Naive superposition of kink and antikink

The naive superposition of a kink and antikink is a field configuration of the form

$$\phi(x; a) = \tanh(x + a) - \tanh(x - a) - 1.$$  \hspace{1cm} (4.1)

For large or modest positive values of $a$ this represents a kink centred at $-a$ and an antikink at $a$. The field is symmetric in $x$, and the centre of mass is at the origin. The centre of mass can be moved, but this is not very interesting. The field shift by $-1$ is a little awkward, but essential to satisfy the boundary condition $\phi \to -1$ as $x \to \pm \infty$. Note that $\chi(x) = \tanh(x + a) - \tanh(x - a)$ is a linear field of the type we mentioned earlier, approaching zero at spatial infinity.

A naive superposition of the form (4.1) has often been used before. By calculating the potential energy or the energy-momentum tensor for $a \gg 0$, one can find the force between a well-separated kink-antikink pair. This superposition, possibly modified to give the kink and antikink some velocity, is often taken as initial data in numerical simulations of kink-antikink collisions.

We are interested here in whether the space of field configurations $\phi(x; a)$ is a good moduli space for a kink and antikink with their centre of mass fixed. The moduli space is 1-dimensional, and the modulus $a$ runs along the whole real line $\mathbb{R}$. When $a$ is positive, there is a kink on the left and antikink on the right. When $a = 0$, the configuration is exactly the vacuum $\phi = -1$. As $a$ becomes negative, the configuration $\phi(x; a)$ is less familiar, but note that $\tanh(x + a) - \tanh(x - a)$ is antisymmetric in $a$. So as $a$ passes through zero, the kink and antikink in some sense pass through each other. For $a$ large and negative, the field interpolates from $-1$ to $-3$ close to $x = a$ and back to $-1$ near $x = -a$.

Configurations for various values of $a$ are shown in Fig. 10 (left panel).

The potential energy $V(a)$ for field configurations of the form (4.1) is

$$V(a) = \frac{8}{3} \left( 17 + 24a + 9(-1 + 8a)e^{4a} - 9e^{8a} + e^{12a} \right).$$  \hspace{1cm} (4.2)
Figure 10: Left: Naive superposition of a $\phi^4$ kink and antikink for several values of the modulus $a$. Right: The corresponding moduli space metric and potential.

It sharply distinguishes positive and negative $a$. For large positive $a$ the energy is approximately $\frac{8}{3}$, twice the kink mass, whereas for large negative $a$ it is dominated by the interval of length $2|a|$ where $\phi \approx -3$ and the potential energy density is approximately $32$. Here, the total potential energy grows linearly with $|a|$. Dynamically there is no reason for the field $\phi$ to prefer a value close to $-3$, so the field configurations that occur in kink-antikink collisions, even at high speed, are probably never close to configurations with large negative $a$ in this moduli space. $V$ has its minimum at $a = 0$, where the configuration is the vacuum.

To find the metric on the moduli space, we need the derivative with respect to $a$,

$$\frac{\partial \phi}{\partial a}(x; a) = \frac{1}{\cosh^2(x + a)} + \frac{1}{\cosh^2(x - a)}.$$  \hspace{1cm} (4.3)

This is obviously symmetric in $a$ and also a non-zero function for all $a$. According to eq.(2.8), the metric $g(a)$ on the moduli space is the integral of the square of this function, and therefore also symmetric in $a$. Its analytic formula is

$$g(a) = \frac{8}{\sinh^2(2a)} \left( -1 + \frac{2a}{\tanh 2a} \right) + \frac{8}{3},$$  \hspace{1cm} (4.4)

and is plotted with the potential $V$ in Fig. 10 (right panel).

Let us consider more carefully the configurations that occur for $a \approx 0$. Using the Taylor expansion in $a$ we find that

$$\phi(x; a) = -1 + \frac{2a}{\cosh^2(x)} + O(a^3).$$  \hspace{1cm} (4.5)

We call the function $\frac{1}{\cosh^2(x)}$ a bump, so the field changes from having a positive bump to a negative bump (around $\phi = -1$) as $a$ changes from positive to negative. The derivative of this approximation to $\phi$ with respect to $a$ agrees with eq.(4.3) at $a = 0$. The derivative is a non-zero function at $a = 0$, so the metric is positive here. The modulus $a$ is therefore a good coordinate globally. In detail,

$$g(0) = \int_{-\infty}^{\infty} \frac{4}{\cosh^4(x)} \, dx = \frac{16}{3},$$  \hspace{1cm} (4.6)
where the integral is eight times the gradient contribution to the kink mass $M$, and therefore equals $4M$.

In summary, the moduli space of the naive kink-antikink superposition is good metrically, and a motion along this moduli space represents a kink and antikink passing through each other smoothly from positive to negative separation. The reduced Lagrangian on moduli space is

$$L_{\text{red}} = \frac{1}{2} g(a) \dot{a}^2 - V(a).$$

(4.7)

The equation of motion,

$$g(a) \ddot{a} + \frac{1}{2} g'(a) \dot{a}^2 + V'(a) = 0,$$

(4.8)

has the first integral

$$\frac{1}{2} g(a) \dot{a}^2 + V(a) = E.$$

(4.9)

In a kink-antikink collision, $a$ decreases from a positive value, passes through zero, stops and then returns to a positive value. While $a$ is negative the field has a negative bump, and energy conservation determines the maximal negative value of $a$ that is reached. The time taken for this bounce process can be estimated using the equation of motion for $a$. It depends on both the metric $g(a)$ and potential $V(a)$.

Numerical exploration of solutions of the field equation for $\phi$ show that this type of moduli space dynamics is too simple-minded to capture important features of true kink-antikink dynamics. It’s not just that some energy is converted to radiation in the true dynamics. There is also transfer of energy from the positional motions of the kink and antikink into the shape modes. This can lead to capture in the potential well of $V$, i.e., to kink-antikink annihilation, or to multiple oscillations of $a$ before the kink and antikink emerge. The next moduli space candidate attempts to capture these features of the dynamics.

### 4.2 Including the shape mode

A single kink, with profile $\phi(x) = \tanh(x)$, has a small amplitude mode of oscillation

$$\phi(x, t) = \tanh(x) + A(t) \frac{\sinh(x)}{\cosh^2(x)},$$

(4.10)

where $A(t)$ oscillates harmonically with frequency $\sqrt{3}$. This discrete frequency is below the frequencies of continuum radiation modes which start immediately above 2. Large amplitude oscillations of $A$ are not exact solutions of the field equation. Energy is converted into radiation through a nonlinear process, and $A$ slowly decays.

Configurations of a single kink, including this mode, are

$$\phi(x; a, A) = \tanh(x - a) + A \frac{\sinh(x - a)}{\cosh^2(x - a)}.$$

(4.11)

This moduli space is 2-dimensional, with coordinates $a$ and $A$ that each run through $\mathbb{R}$. As the derivatives of $\phi$ with respect to $a$ and $A$ are both non-zero functions, and linearly
independent, the metric is positive definite. Its explicit form is
\[ g_{aa} = \frac{4}{3} + \frac{\pi}{2} A + \frac{14}{15} A^2, \quad g_{aA} = 0, \quad g_{AA} = \frac{2}{3}. \] (4.12)

Thus \( a \) and \( A \) are globally good coordinates. The moduli space dynamics describes a kink that oscillates indefinitely while also moving at a steady mean velocity.

A set of field configurations for a kink at \(-a\) and an antikink \(a\) that includes this mode for each of them is
\[ \phi(x; a, A) = \tanh(x + a) - \tanh(x - a) + A \left( \frac{\sinh(x + a)}{\cosh^2(x + a)} - \frac{\sinh(x - a)}{\cosh^2(x - a)} \right) - 1. \] (4.13)

This is again a 2-dimensional moduli space with coordinates \( a \) and \( A \). The centre of mass is fixed at the origin, and the amplitudes of the shape modes are related so that \( \phi \) is symmetric in \( x \). This restricted set of fields is adequate for initial kink-antikink data having this symmetry. The more general set of field configurations where the shape mode amplitudes are independent was introduced by Sugiyama [14] and has been investigated by Takyi and Weigel [18] and others.

For a well-separated kink and antikink, it is clear that \( a \) and \( A \) are good coordinates. \( a \) can be positive or negative, and the shape mode usefully allows a change of shape of the kink and antikink. However, at \( a = 0 \) there is a problem, because the shape modes cancel out and \( A \) fails to be a good coordinate there. The derivatives of \( \phi \) with respect to \( a \) and \( A \) need to be non-zero and linearly independent functions for the metric on moduli space to be positive definite (in these coordinates). This requirement is not satisfied at \( a = 0 \) because the derivative with respect to \( A \) is zero. This problem was noted by Takyi and Weigel as a null-vector problem.

The problem has a simple resolution by a change of coordinates. Replace \( A \) by \( B f(a) \), where \( f(a) \) is any antisymmetric function of \( a \) that is linear for small \( a \). One could choose \( f(a) = a \) but we prefer \( f(a) = \tanh(a) \), as \( B \) is then the amplitude of the shape mode, up to a sign, for large \(|a|\). The moduli space of field configurations is now
\[ \phi(x; a, B) = \tanh(x + a) - \tanh(x - a) + B \tanh(a) \left( \frac{\sinh(x + a)}{\cosh^2(x + a)} - \frac{\sinh(x - a)}{\cosh^2(x - a)} \right) - 1. \] (4.14)

The function of which \( B \) is the coefficient has a smooth, non-zero limit as \( a \to 0 \). Using the Taylor expansion or equivalently l'Hôpital’s rule, we find for small \( a \) the leading terms
\[ \phi(x; a, B) \approx 2a \frac{1}{\cosh^2(x)} + 2B \left( \frac{2}{\cosh^3(x)} - \frac{1}{\cosh(x)} \right) - 1. \] (4.15)

\( a \) and \( B \) are coefficients of distinct non-zero functions, so the moduli space is non-singular in these coordinates and has a smooth metric. \( a \) and \( B \) are globally good coordinates, taking values in the whole of \( \mathbb{R} \).

The metric on the Sugiyama moduli space has been calculated by Pereira et al. [25], using contour integration to evaluate the integrals. It should not be difficult to recalculate the metric on the reduced 2-dimensional moduli space in terms of the coordinates \( a \) and
B. The spatial integrals defining the metric coefficients are not affected, but they must be combined differently. Including distinct amplitudes for the two shape modes adds no further difficulties, because there is no additional null-vector when the shape modes centred at $-a$ and $a$ are added rather than subtracted.

It should be possible to model kink-antikink dynamics quite well using the dynamics in this 2-dimensional moduli space, and working with the new coordinates $a$ and $B$ should resolve earlier difficulties.

4.3 Weighted kink-antikink configurations

Here we discuss a variant of the kink-antikink superposition, where the kink and antikink amplitudes are given a weight that depends on their separation. Including a weight has the interpretation that the kink is modified by the nearby presence of the antikink, and vice versa. The field configurations now have the form

$$\phi(x; a) = \tanh(a)(\tanh(x + a) - \tanh(x - a)) - 1.$$  \hfill (4.16)

We do not include the shape modes here, although their inclusion could be explored. The choice of weight function $\tanh(a)$ is motivated by the identity

$$\tanh(a)(\tanh(x + a) - \tanh(x - a)) - 1 = \frac{c - \cosh^2(x)}{c + \cosh^2(x)},$$  \hfill (4.17)

where $c = \sinh^2(a)$. The expression on the right hand side occurs in the iterated kink scheme that we will review in the next section. The identity is verified by writing

$$\tanh(x + a) - \tanh(x - a) = \frac{\sinh(x + a)\cosh(x - a) - \cosh(x + a)\sinh(x - a)}{\cosh(x + a)\cosh(x - a)},$$  \hfill (4.18)

and then using hyperbolic analogues of trigonometrical addition and double angle formulae.

For $a$ large and positive, the weighted superposition agrees with the naive superposition we considered earlier. Curiously, it also agrees for small positive $a$, because to leading order, the weighted superposition is $\phi = \frac{2a^2}{\cosh^2(x)} - 1$ whereas the naive superposition is $\phi = \frac{2a}{\cosh^2(x)} - 1$. So the field configurations have the same form, with a positive bump, but the parameter $a$ has changed its meaning. For intermediate $a$, the configurations are slightly different, no matter how the parameters are matched.

However, the naive and weighted superpositions are metrically quite different as $a$ approaches zero, and if an attempt is made to extend beyond here. Recall that the naive superposition can be extended smoothly to negative $a$, and the positive bump becomes a negative bump. On the other hand, the weighted superposition (4.16) is symmetric in $a$, so here the moduli space of field configurations is covered twice if $a$ runs over the whole of $\mathbb{R}$. In fact, this moduli space has a boundary at $a = 0$ and is geodesically incomplete. This is because $\phi$ depends quadratically on $a$ for small $a$, so

$$\frac{\partial\phi}{\partial a} = O(a)$$  \hfill (4.19)
and the metric coefficient is \( g(a) = O(a^2) \). Therefore \( a \) is not a good coordinate near \( a = 0 \). The parameter \( c = \sinh^2(a) \) is a better coordinate, as \( c \approx a^2 \) for small \( a \), and in terms of \( c \) the metric coefficient is \( g(c) = O(1) \). This can be seen directly starting from the expression for the weighted superposition on the right hand side of (4.17). A motion in which \( a \) evolves smoothly from positive through zero to negative is not acceptable as a motion in the moduli space. Instead, a motion where \( c \) evolves smoothly through zero is acceptable.

The natural range of \( c \) is the interval \((-1, \infty)\), as \( \phi \) has a singularity at \( x = 0 \) when \( c = -1 \). The identity (4.17) is still valid for \( c < 0 \) if suitably interpreted. \( a \) becomes imaginary, so let us write \( a = i\tilde{a} \) with \( \tilde{a} \) positive. (We will comment further on the signs of \( a \) and \( \tilde{a} \) below.) Recall the relations

\[
\begin{align*}
\sinh(i\tilde{a}) &= i\sin(\tilde{a}), & \sin(i\tilde{a}) &= i\sinh(\tilde{a}), \\
\cosh(i\tilde{a}) &= \cos(\tilde{a}), & \cos(i\tilde{a}) &= \cosh(\tilde{a}).
\end{align*}
\]

(4.20)

Therefore, for negative \( c \), we have \( c = -\sin^2(\tilde{a}) \) and we can express the weighted superposition of kink and antikink (4.16) as

\[
\phi(x; \tilde{a}) = i\tan(\tilde{a})(\tanh(x + i\tilde{a}) - \tanh(x - i\tilde{a})) - 1.
\]

(4.21)

This expression is real, and symmetric in \( \tilde{a} \). Use of the subtraction formula for the \( \tanh \) function leads back to the formula for \( \phi \) in terms of \( c \).

The interpretation of (4.21) is that the kink and antikink have imaginary locations \( \mp i\tilde{a} \). The moduli space is well defined in terms of \( c \) and is smooth at \( c = 0 \). Motion through \( c = 0 \) in the moduli space is unproblematic, but it corresponds to a 90-degree scattering of the locations of the kink and antikink. Such scattering is familiar in the dynamics of solitons in higher dimensions, for example for vortices and monopoles, where the scattering occurs in a real 2-dimensional plane. Here, remarkably, the scattering occurs in the complex plane of the 1-dimensional kink position parameter \( a \). This type of scattering is only possible because the sign of \( a \) is not fixed. The kink and antikink are initially located on the real axis at \( -a \) and \( a \), but because of the weight factor, there is no effect if \( a \) is replaced by \( -a \). The kink and antikink later appear on the imaginary axis at \( \tilde{a} \) and \( -\tilde{a} \), and note that because the amplitude \( i\tan(\tilde{a}) \) is imaginary, the kink and antikink cannot now be distinguished. Therefore the scattering does not break the reflection symmetries of the complexified \( a \)-plane. A pair of points scatters from the real to the imaginary axis, in the same way that the algebraic roots of \( z^2 = c \) scatter as \( c \) passes through zero along the real axis, and rather like the way that the foci of an ellipse scatter when the major axis and minor axis swap over as the ellipse passes through a circle.

The moduli space with coordinate \( c \) is geodesically complete, for \( c \) extending to \(-1 \). This could be verified by calculating the metric factor \( g(c) \), but is easier to see as follows. The limiting (singular) field configuration when \( c = -1 \) is

\[
\phi(x; c = -1) = -1 - \frac{2}{\sinh^2(x)}.
\]

(4.22)
As the infinite-dimensional field configuration space is Euclidean, we can work out the squared distance between this configuration and the configuration \( \phi(x; c = 0) = -1 \). It is the integral of \( \frac{4}{\sinh^4(x)} \), but this is divergent. So the length of the moduli space between \( c = 0 \) and \( c = -1 \) (which is not a straight path in field configuration space) is also infinite.

In summary, the moduli space of a superposed weighted kink and antikink is an interesting alternative to the more familiar moduli space of the naive superposition. For this new moduli space to be geodesically complete, one must allow for the kink and antikink to scatter in the complexified plane of their separation. However the field remains real, and in the interpretation in terms of \( c \) the field just transitions from having a positive bump to a negative bump as \( c \) passes through zero. Further investigation is needed to see if this moduli space is better than the moduli space of the naive superposition for modelling kink-antikink dynamics in the full field theory. It is almost certainly necessary to include shape modes in either case.

5 Iterated Kinks

In this section we briefly review the iterated kink equation that was introduced by three of the present authors in [19]. It is really the sequence of ODEs,

\[
\frac{d\phi_n}{dx} = -(1 - \phi_n^2)\phi_{n-1}, \quad n = 1, 2, 3, \ldots ,
\]

(5.1)

where we fix \( \phi_0(x) = -1 \). For all \( n \) we impose the boundary condition \( \phi_n(x) \to -1 \) as \( x \to -\infty \). The equations are solved sequentially, and one can stop at any \( n \). We will only discuss the solutions in detail up to \( n = 3 \). It can be shown that for odd (even) \( n \), the generic solution \( \phi_n \) approaches \(+1\) \((-1)\) as \( x \to \infty \). For odd \( n \), let us therefore impose the boundary condition \( \phi_n(x) \to +1 \) as \( x \to \infty \); then the solution always lies between \(-1\) and \(+1\). For even \( n \), the solutions are essentially of two types: a solution either lies between \(-1\) and \(+1\), or is everywhere less than \(-1\). These types are separated by the constant solution \( \phi_n(x) = -1 \).

The iterated kink equation is a systematic extension of the idea of a kink equation with impurity \( \chi(x) \) [26–28]

\[
\frac{d\phi}{dx} = -(1 - \phi^2)\chi(x),
\]

(5.2)

which in turn is a generalisation of the basic first order ODE for a \( \phi^4 \) kink or antikink, \( \frac{d\phi}{dx} = \pm(1 - \phi^2) \).

As each equation of the iterated kink sequence is of first order, its solution has one constant of integration. If we retain all of these, the \( n \)th iterate \( \phi_n \) depends on \( n \) arbitrary constants. We will call these the moduli of the \( n \)th iterate. There is more than one way to construct solutions of these ODEs and introduce the constants of integration, but one systematic approach described in [19] shows that each constant can be regarded as an arbitrary real number, an additive constant in the solution. For even \( n \) we noted that there are two types of solution separated by the constant solution \( \phi_n(x) = -1 \). This constant solution occurs in the interior of the moduli space.
The reason that the iterated kink solutions are interesting is that a large part of the moduli space of the \( n \)th iterate consists of field configurations with \( n \) alternating kinks and antikinks at arbitrary separations (starting with a kink on the left). Other parts of the moduli space consist of configurations where a kink-antikink pair, or more than one pair, have approached each other to form a bump. The moduli space of the \( n \)th iterate therefore usefully describes configurations of \( n \) kinks and antikinks. However these configurations do not incorporate the standard shape mode deformations of a kink or antikink.

We conjecture that each of these moduli spaces has a positive definite metric and is metrically smooth and geodesically complete, almost everywhere. We have not proved this, but it is clearly true for \( n = 1 \) and \( n = 2 \), and the numerical study for \( n = 3 \) and \( n = 4 \) reported in [19] indicates that the partial derivatives of the field \( \phi_n(x) \) with respect to all moduli are almost everywhere non-zero and linearly independent. The exceptional points in moduli space are the constant configurations \( \phi_n(x) = -1 \), for even \( n \), where a rigid translation has no effect. We will focus on the relative motion of kinks, so this problem with translations does not occur.

Let us now recall the form of the first few iterates. For \( n = 1 \), we have the standard equation for a \( \phi^4 \) kink, with solution \( \phi_1(x; a) = \tanh(x - a) \). As discussed earlier, the moduli space is the real line with its Euclidean metric. For \( n = 2 \), the field \( \phi_1 \) acts as an impurity. As the modulus \( a \) shifts, the solution \( \phi_2 \) simply shifts with it. Let us therefore ignore this translational modulus, and assume that \( \phi_1(x) = \tanh(x) \). Then one way of presenting the solutions \( \phi_2 \) is

\[
\phi_2(x; c) = \frac{c - \cosh^2(x)}{c + \cosh^2(x)}. \tag{5.3}
\]

These configurations appeared in Section 4. By letting \( c \) run over the interval \((-1, \infty)\) we capture all non-singular solutions. Note that for \( c \) positive, \( \phi_2 \) is between \(-1\) and \(+1\); for \( c = 0 \), \( \phi_2(x) = -1 \); and for \( c \) negative, \( \phi_2 \) is everywhere less than \(-1\). The moduli space with coordinate \( c \) has no metric singularity at \( c = 0 \).

The third iterate \( \phi_3(x) \) is obtained from the second iterate \( \phi_2 \) by integrating the relevant ODE, and an explicit solution can be obtained. We will consider here only the resulting field configurations that are antisymmetric in \( x \), although the general \( \phi_3 \) with broken reflection symmetry is known and illustrated in [19]. The only modulus is then \( c \), arising from \( \phi_2 \). The antisymmetric solutions are kink-antikink-kink configurations when \( c \) is large, having an antikink at the origin and kinks at equal separation on either side. As \( c \) approaches zero and becomes negative, the kinks approach and annihilate the antikink, leaving a single kink modified by a variant of the shape mode. In the next section we look at the moduli space of these configurations in more detail, and compare it with a similar moduli space of explicitly superposed, weighted kinks and antikinks.

6 Kink-Antikink-Kink Moduli Spaces in \( \phi^4 \) Theory

Here we investigate three possible moduli spaces for kink-antikink-kink configurations in \( \phi^4 \) theory.
6.1 Naive superposition of kink, antikink and kink

An obvious choice for a kink-antikink-kink configuration is a generalisation of the naive kink-antikink superposition, i.e., the superposition of a kink, antikink and kink,

$$\phi(x; b) = \tanh(x + b) - \tanh(x) + \tanh(x - b),$$  \hspace{1cm} (6.1)

where $b$ parametrises the positions of the two kinks, and the antikink is at the origin. For simplicity we have chosen the field to be antisymmetric in $x$. This set of field configurations is symmetric in the single modulus $b$, and $b$ can take any real value. For large positive $b$ we get a well-separated, equally spaced chain of kink, antikink and kink. They approach and merge as $b \to 0$, and when $b = 0$ they form a configuration which is just the usual, undeformed kink located at the origin. Then, for negative $b$ they return to their original positions, so the moduli space is really just the half-line with $b$ non-negative.

To find the corresponding metric we compute the derivative with respect to $b$,

$$\frac{\partial \phi}{\partial b}(x; b) = \left(\frac{1}{\cosh^2(x + b)} - \frac{1}{\cosh^2(x - b)}\right).$$  \hspace{1cm} (6.2)

This is antisymmetric in $b$ and vanishes at $b = 0$. The resulting metric is

$$g(b) = \frac{2}{3} \frac{-24 b \cosh(2b) + 9 \sinh(2b) + \sinh(6b)}{\sinh^4(2b)},$$  \hspace{1cm} (6.3)

and also vanishes at $b = 0$. The metric on the half-line is therefore not complete and $b$ is not globally a good coordinate. However, this problem can be resolved by extending the moduli space.

Interestingly, the naive field superposition (6.1) is (up to a sign) the product of the iterated configuration $\phi_2$, given by (5.3), and the kink at the origin $\phi_1(x; 0)$,

$$\phi(x; b) = -\left(\frac{\sinh^2(b) - \cosh^2(x)}{\sinh^2(b) + \cosh^2(x)}\right) \tanh(x) = -\phi_2(x; c)\phi_1(x; 0),$$  \hspace{1cm} (6.4)

where $c = \sinh^2(b)$ and is therefore non-negative. $c$ is a good choice for the modulus, and we can straightforwardly extend the moduli space to negative values of $c$, but this requires the modulus $b$ to be extended to imaginary values $b = i\tilde{b}$, with $\tilde{b}$ positive. Here $c = -\sin^2(\tilde{b})$, so the range of $\tilde{b}$ is $0 \leq \tilde{b} < \frac{1}{2}\pi$. The new field configurations are more compressed than the undeformed kink at the origin. $\phi(x; \tilde{b})$ becomes not only steeper as $\tilde{b}$ grows, but also acquires negative and positive bumps outside the range of field values $[-1, 1]$ as $\tilde{b}$ approaches $\frac{1}{2}\pi$. Their existence is due to the large negative bump in $\phi_2$.

The field evolution is smooth as $c$ passes from positive to negative, but as $c$ approaches $-1$, the potential energy becomes large, so in a dynamical kink-antikink-kink motion $c$ will decrease, stop before it reaches $-1$, and then increase again. In the complex plane of the modulus $b$ there will be a 90-degree scattering during a kink-antikink-kink collision, which occurs in reverse as the motion reverses. From the perspective of the naive superposition, the kinks scatter but the antikink remains at rest at the origin. In Fig. 11 we plot the field configurations as well as the metric and potential on moduli space as a function of $b$. 

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Figure 11: Naive superposition of kink, antikink and kink. Left: Profiles for several values of the extended modulus $b'$. Right: The moduli space metric and potential.

We show these for the real and imaginary ranges of $b$ simultaneously by introducing a new real coordinate $b'$ defined by

$$b' = \begin{cases} 
  b & \text{for } b \in [0, \infty) \\
  -\tilde{b} & \text{for } \tilde{b} \in [0, \frac{1}{2}\pi) 
\end{cases}.$$  
(6.5)

Note that, under the replacement $b \to i\tilde{b}$, the metric (6.3) acquires an additional minus sign to compensate $\dot{b}^2$ being negative in the kinetic part of the Lagrangian. There is not a genuine sign problem, and the metric is positive if $c$ is used as the coordinate.

6.2 Iterated kink-antikink-kink

The iterated kink scheme gives an alternative moduli space of kink-antikink-kink configurations. We start from the $\phi_2$ solution, with its modulus $c$, and iterate to obtain the $\phi_3$ solution

$$\phi_3(x; c) = \tanh \left( x - 2\sqrt{\frac{c}{1 + c}} \arctanh \left( \sqrt{\frac{c}{1 + c}} \tanh(x) \right) \right).$$  
(6.6)

There is no further modulus derived from the constant of integration because we select antisymmetric configurations with equal kink-antikink-kink spacings. For the most general solution $\phi_3$ we refer to [19]. The formula (6.6) is valid for all $c > -1$, even though the square root is imaginary if $c < 0$. This is interesting because it includes the range where the standard kink (occurring for $c = 0$) is compressed, becoming steeper and steeper as $c \to -1$. So $\phi_3$ is qualitatively similar to the naive superposition with $b$ continued to imaginary values, but here the field value is always confined to $[-1, 1]$, and does not have bumps. These $\phi_3$ field configurations are shown in Fig. 12.

The metric $g(c)$ on this moduli space is shown in Fig. 13. $c$ is again a good coordinate. In particular, at $c = 0$,

$$\frac{\partial \phi}{\partial c}(x; c) = -2 \frac{\sinh(x)}{\cosh^3(x)},$$  
(6.7)

which gives $g(c = 0) = \frac{16}{15}$. The potential $V(c)$ is also shown in Fig. 13. It rapidly increases as $c$ approaches $-1$. 

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6.3 Weighted superposition of kink-antikink-kink

We noted earlier that the kink-antikink configuration $\phi_2$ can be expressed exactly as a weighted superposition of kink and antikink. This suggests that it could be interesting to find a moduli space of weighted kink-antikink-kink configurations. A suitable formula that introduces weights is

$$
\phi(x; b) = \Lambda(b) \tanh(x + b) + (1 - 2\Lambda(b)) \tanh(x) + \Lambda(b) \tanh(x - b). 
$$

The weights are arranged so that this configuration is antisymmetric in $x$ and satisfies the vacuum boundary conditions. The naive superposition has $\Lambda = 1$, but allowing non-trivial $\Lambda$ could be an improvement.

The weighted superposition is quite close to the iterated kink solution $\phi_3(x; c)$ for a suitable choice of $b$ and $\Lambda(b)$ in terms of $c$. For $c$ negative, $b$ becomes imaginary and we again introduce the extended modulus $b'$. In Fig. 14 we plot the optimal $b$ and $\Lambda(b)$, found using a least squares fit of $\phi(x; b)$ to $\phi_3(x; c)$. For large $c$, the kinks are well-separated from the antikink, so $\Lambda \approx 1$ and $b \approx \log(4c)$. When $c$ is close to zero, the best fit is with $b \approx \sqrt{\frac{2c}{3}}$ and $\Lambda = \frac{2}{7}$. Strictly speaking, $\Lambda$ is indeterminate when $c = 0$, but these values of $b$ and $\Lambda$ give the best fit nearby, giving an exact fit up to quadratic order in $c$ in the Taylor
expansion of \( \phi_3(x;c) \). \( \Lambda \) decreases towards zero as \( c \) approaches \(-1\). Here \( \phi_3 \) approaches a step function, and the fit is not very good.

These weighted kink-antikink-kink superpositions with numerically determined coefficients are probably not very useful, especially since they are close to the iterated kink configurations \( \phi_3 \). More interesting could be a moduli space of configurations of a qualitatively different type, obtained using an analytic formula for the weight \( \Lambda(b) \).

In summary, we have described three moduli spaces for kink-antikink-kink configurations, of which the last two are very similar. Which of these is best for modelling kink-antikink-kink collisions in \( \phi^4 \) theory requires further study.

7 Conclusions

We have constructed a number of moduli spaces – collective coordinate manifolds – for field configurations of kink and antikink solitons in both \( \phi^4 \) theory and sine-Gordon (sG) theory. These are smooth, finite-dimensional submanifolds of the infinite-dimensional field configuration spaces. The moduli are chosen so that the soliton dynamics can be approximately modelled as particle dynamics, and for the \( \phi^4 \) kinks we have also incorporated an amplitude for the shape mode oscillation (the discrete, normalisable kink oscillation mode whose frequency is below the continuum). For kink-antikink and also kink-antikink-kink configurations, we have assumed a spatial reflection symmetry to simplify the analysis. This implies that the centre of mass remains fixed at the origin.

By restricting the kinetic and potential terms of the field theory Lagrangian (where the potential term includes the field gradient contribution) to field evolution through moduli space, we obtain a reduced Lagrangian with kinetic and potential terms on moduli space, whose equation of motion is an ODE. The coefficient matrix of the kinetic term can be interpreted as a Riemannian metric on moduli space. (In several of our examples there is just one modulus and the metric is a single function.) Both the metric and potential are spatial integrals involving the corresponding field configuration and its derivatives. A guiding principle is that the metric on moduli space should be either metrically complete, so that free geodesic motion does not reach any boundary in finite time, or metrically
incomplete but with a potential that is infinite at the boundary, so that no dynamical trajectory reaches it.

For a single kink in $\phi^4$ or sG theory, there is a 1-dimensional moduli space, with modulus the kink position (centre) $a$. By translational invariance, the metric is Euclidean and the potential constant, so kink motion is at constant velocity. Shape mode oscillations of the $\phi^4$ kink can also be accommodated. Moduli space dynamics is a fundamentally non-relativistic approximation, so the kink is not Lorentz contracted nor is its speed constrained to be less than 1 (the speed of light).

The simplest moduli space for kink-antikink dynamics in $\phi^4$ theory is obtained using a naive superposition of the kink and antikink, with the centres at $-a$ and $a$ respectively. The modulus $a$ runs from $-\infty$ to $\infty$ and the moduli space is complete. An interesting alternative moduli space uses a weighted kink-antikink superposition. When the weight factor is $\tanh(a)$, the configurations are identical to those occurring in the iterated kink scheme [19]. This observation is useful, because the moduli space in this case is incomplete, and has a boundary at the vacuum configuration ($a = 0$) where the kink and antikink annihilate. The reason is that the weighted configurations are symmetric in $a$, so the moduli space is the half-line $a \geq 0$. The iterated kink configuration has a different parameter $c = \sinh^2(a)$, and one can extend $c$ through 0 down to $-1$. The moduli space is now complete; the potential also becomes infinite as $c \to -1$. Motion in this moduli space allows the kink and antikink to approach from large separation, smoothly pass through the vacuum configuration, stop at a configuration with a negative bump, and bounce back. In terms of the original modulus $a$, there has been scattering from real to imaginary values, which then reverses, although the field remains real. This remarkable 90-degree scattering of the complexified position coordinate $a$ is reminiscent of the 90-degree scattering in a real spatial plane that occurs for several types of soliton in two or three spatial dimensions.

We also reconsider the moduli space that includes the shape modes of the $\phi^4$ kink and antikink (still preserving a reflection symmetry). This moduli space was introduced by Sugiyama [14], and studied by a number of authors, including Takyi and Weigel [18], who clarified details of the metric structure but also reported a null-vector problem – a zero in the metric. We have shown here that this null-vector is an artifact of the coordinate choice, and disappears if the shape mode amplitude $A$ is replaced by $B = A / \tanh(a)$ (the denominator could be any function linear in $a$ near $a = 0$). There remains the possibility of a null-vector problem for the centre-of-mass translational modulus, at the point where a kink and antikink annihilate into the vacuum configuration, but we have not investigated this in detail. The inertia associated with field kinetic energy (a relativistic effect) may provide a resolution.

In the sG case, the moduli space of naive kink-antikink superpositions consists, surprisingly, of the same field configurations that occur in the exact kink-antikink solution at the critical energy 16 separating kink-antikink scattering solutions from breathers. Using the energy conservation law for the exact solution, we obtain a nice relation between the metric and potential on this moduli space (which provides a useful check on the calculations). The moduli space is complete, and the dynamics on it gives a good approximation to the true scattering and breather solutions with respective energies above and below 16.
We have verified this by comparing the energy/frequency relation for the approximate and exact breathers, and the approximate and exact positional shift that occurs in scattering.

We have also considered kink-antikink-kink moduli spaces, where the two kinks are always equidistant from the antikink at the origin. The naive moduli space of superposed solitons allows the kinks to approach and annihilate the antikink, leaving a single kink. However this moduli space is incomplete, and needs to be extended to allow the single kink to become more compressed (steeper). We have proposed a way of doing this, both in $\phi^4$ and sG theory. The kink position coordinates are imaginary in this extension, although the field again remains real. The resulting moduli spaces are still incomplete, having a boundary configuration that is a step function – an infinitely steep kink – which is at only a finite distance from a smooth kink. However, the step function has infinite potential energy, so the dynamics on moduli space does not reach the boundary and is well defined. In the sG case there is an exact solution having critical energy 24 separating the kink-antikink-kink scattering solutions from the wobbling kink solutions. Its configurations define a useful alternative moduli space, but again, this moduli space is incomplete and has to be extended to accommodate dynamics with energy larger than 24. This is another example where the metric and potential are simply related.

We have provided some tests of the moduli space approximation for kink and antikink dynamics in sG theory, where we can compare known exact solutions. Because of the theory’s integrability, there is no radiation. It would be interesting to test afresh the moduli space approximation to kink and antikink dynamics in $\phi^4$ theory, but this remains to be done. It is more complicated, because of the shape mode of the kink, and because of the radiation emitted. The field equation, a PDE, needs to be solved numerically. Despite much work in this area for more than 40 years [17], various difficulties have arisen in attempts to compare field theory solutions to moduli space dynamics. In this paper we have drawn attention to more than one way that the moduli space dynamics itself can be improved and developed, and we hope this will allow a deeper understanding of the interesting phenomena observed in $\phi^4$ kink-antikink interactions.

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