PART VI

MATHEMATICAL METHODS

COLLECTIVE COORDINATES BY A VARIATIONAL APPROACH: PROBLEMS FOR SINE GORDON AND Φ^4 MODELS

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The method of collective-coordinates obtained by a variational approach is examined for the sine-Gordon and ϕ^4 models. It is shown that the evolution equations for the collective coordinates can be ill-defined because they are obtained by projecting on a null vector. New ansatzes that do not have this problem are presented.

I. Introduction

A certain number of non-linear partial differential equations can be solved exactly by the method of inverse scattering [1]. When they are perturbed the evolution of the solution can be obtained by perturbation methods [2]. Parameters of the unperturbed problem become slowly varying because of the perturbation.

In many other cases however only a few analytical solutions are known and the equation only has a few conserved quantities so that the mathematical structure of the problem is much more limited. In those situations to obtain the evolution of collective coordinates a variational method can be used. This method introduced by Rice and Mele [3] in the study of lightly doped poly-acetylene has had some remarkable sucesses for the sine-Gordon model [4]. For kink-antikink collisions in the sine-Gordon equation, Legrand guided by an algebraic identity gave a collective coordinate ansatz which he used for the study of a perturbed breather [5]. This ode description compared well with the pde solution despite of a sign error in the Lagrangian. The correct sign as will be shown below introduces a mathematical singularity that cannot be removed. The shape mode coordinate blows up when the breather is "flat" because the Lagrange equations are obtained through a projection on a vector which becomes zero at that point.

The paper is derived from [6]. It is organised as follows. Section II presents the variational procedure in the sine-Gordon case. Section III explains the ill-definition of the collective coordinates for kink-antikink collisions in sine-Gordon and ϕ^4. Section IV shows how to fix things and introduces new ansatzes.

II. The variational approach for the sine-Gordon equation

Consider the perturbed sine-Gordon equation:

$$\phi_{tt} - \phi_{xx} + \sin\phi = F(\phi, \phi_t, t) \tag{1}$$

When $F = 0$, equation (1) can be integrated exactly and two well-known solutions are [1] : the breather

$$\phi_B(x,t) = 4arctan(\frac{k_B \sin(\omega_B t + \phi_B)}{\omega_B \cosh(k_B x)}) \tag{2}$$

where $k_B^2 = 1 - \omega_B^2$ and the kink-antikink

$$\phi_{K\bar{K}}(x,t) = 4arctan(\frac{\sinh(\gamma_L u t)}{u \cosh(\gamma_L x)}) \tag{3}$$

where $\gamma_L = \frac{1}{\sqrt{1-u^2}}$ is the Lorenz factor. Formulas (2) and (3) can be seen as special cases of:

$$\phi(x, y(t), k(t)) = 4arctan(\frac{\sinh(y(t))}{\cosh(k(t)x)}) \tag{4}$$

where y(t) and k(t) have different expressions depending on whether the solution is a kink-antikink or a breather. This ansatz relies on an algebraic identity between the sum of a soliton and antisoliton profiles and the expression in the rhs of (4) -2π. It was put forth by Legrand [5]. The collective coordinate approach is to assume that the solution has again the form (4) when the perturbation is present. In order to derive the evolution equations for y and k, one could plug (4) into (1) but there would still be an x dependance. Instead, a variational approach is used. Equation (1) with $F = 0$ can be derived from the following Lagrangian density:

$$l = \frac{1}{2}{\phi_t}^2 - \frac{1}{2}{\phi_x}^2 - (1 - cos\phi) \tag{5}$$

by writing that the variation of $\int\int l dx dt$ is zero. Assuming that the solution follows (4), the evolution of y and k is then obtained from the Lagrangian $L(y, \dot{y}, k, \dot{k}, t) = \int l dx$ where expression (4) for ϕ is used to compute (5), by writing the usual Lagrange equations. The terms in the perturbation that cannot be incorporated in the Lagrangian density such as the damping are treated separately [5]. If

$$F = \epsilon sin \omega t - \delta\phi_t \tag{6}$$

the equations of motion are :

$$P = \partial\Lambda / \partial\dot{y} \tag{7.a}$$

$$Q = \partial\Lambda/\partial\dot{k} \tag{7.b}$$

$$\frac{dP}{dt} + \delta P = \partial\Lambda/\partial y \tag{7.c}$$

$$\frac{dQ}{dt} + \delta Q = \partial\Lambda/\partial k \tag{7.d}$$

where

$$\Lambda = \dot{y}^2\frac{8}{k}(1+\frac{2y}{\sinh 2y}) - \dot{y}\dot{k}16\frac{y}{k^2} + \dot{k}^2\frac{2}{3k^3}[(\pi^2+4y^2)(1-\frac{2y}{\sinh 2y}) + 8y^2]$$
$$-8k(1-\frac{2y}{\sinh 2y}) - \frac{8}{k}(\tanh y)^2(1+\frac{2y}{\sinh 2y}) + 4\pi\frac{y}{k}\epsilon\sin\omega t \tag{7.e}$$

is the Lagrangian and P (Q) is the momentum associated to y (k) respectively.

In the original paper of Legrand, a sign error was made in the coefficient of the k_t^2 term in Λ. It was written to be $(\pi^2+4y^2)(1+\frac{2y}{\sinh 2y}) + 8y^2$. We will see that this mistake completely hid the real behavior of the solution. All the terms in Λ except for the coefficient of $\dot{y}^2$ become 0 when $y=0$. So only the y kinetic energy remains when $y=0$. Therefore numerical problems are to be expected for k when y is small.

Equations (7) can be integrated numerically by transforming them into a system of first order differential equations using as variables (y,k,P,Q). The equations for $\dot{y}$ and $\dot{k}$ come from the definition of P and Q and are obtained by inverting the system:

$$\begin{pmatrix} P \\ Q \end{pmatrix} = \begin{pmatrix} 16\frac{\alpha}{k} & -16\frac{y}{k^2} \\ -16\frac{y}{k^2} & \frac{4}{3k^3}[\gamma(2-\alpha)+8y^2] \end{pmatrix} \begin{pmatrix} \dot{y} \\ \dot{k} \end{pmatrix} \tag{8}$$
$$\alpha = 1 + \frac{2y}{\sinh 2y} \quad \gamma = \pi^2 + 4y^2$$

The equations for $\dot{P}$ and $\dot{Q}$ are given by (7.c) and (7.d). Even in the absence of perturbations problems are to be expected when $y=0$ because the rhs. matrix of (8) becomes non-invertible. To study that case δ and ϵ are set to 0. A breather initial condition was chosen and its evolution monitored through the variables y and k.

All the standard ode integrators tried failed to get across $y=0$ and maintain reasonable accuracy. A finite difference energy conserving scheme suggested by Luiz Vazquez [7] showed the same behavior. This situation is also observed by Flesch in his study of the kink-antikink collisions in the ϕ^4 model [8] even though he uses an algebraic differential equation solver which is a completely different method. From these numerical results it becomes clear that equations (7) are ill-defined when $y=0$. It turns out that this feature can be predicted from the ansatz (4).

Before going into the detail of the explaination it is worth mentioning that the agreement Legrand finds between the numerical solution of the pde and his collective coordinates odes is for the y variable only. There is very little interplay between the y and k variables except for when y=0. Computing $(y(t), k(t))$ with the wrong sign in (7.e) and a pure breather initial condition with $k = 0.1$ leads to a value of k about 10^{-3} clearly non zero but still small. The $\dot{k}$ terms in the Lagrangian are very small. Furthermore all the comparisons are shown with the perturbation term present. One situation displayed is a collision and annihilation due to damping; because of the damping it would be hard to see the difference with the pde. In the other situation where the kink and antikink pass through each other the comparison would point out the mistake. Therefore it is important in these collective coordinate studies to check the agreement of the pde with the behavior of all the variables.

III. Analysis of the singularity: the projection argument

The Lagrange equations derived from :

$$L(y, \dot{y}, k, \dot{k}, t) = \int l(\phi_t, \phi_x, \phi, t) dx \tag{9}$$

have a solution that is undetermined when $y = 0$. Legrand [5] examined in detail the procedure in which (4) is substituted into (9). The spatio-temporal dependance of ϕ in (4) can be written as: $\phi = \phi(x, a_i(t))$ where the a_i are the collective coordinates. The Lagrange equations from (9):

$$\frac{\partial L}{\partial a_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{a}_i}\right) = 0 \tag{10}$$

imply using the fact that $\frac{\partial \phi_t}{\partial \dot{a}_i} = \frac{\partial \phi}{\partial a_i}$, integrating by parts with respect to x, and assuming that $\frac{\partial \phi}{\partial \dot{a}_i}$ vanishes for $x \to \pm\infty$:

$$\int_{-\infty}^{+\infty} dx\left[\frac{\partial l}{\partial \phi} - \frac{\partial}{\partial t}\left(\frac{\partial l}{\partial \phi_t}\right) - \frac{\partial}{\partial x}\left(\frac{\partial l}{\partial \phi_x}\right)\right]\frac{\partial \phi}{\partial a_i} = 0 \tag{11}$$

Equation (11) is the key to the understanding of the ill-definition of the equations. The expression in brackets is the left hand-side of the evolution equation as obtained from the condition that the spatio-temporal variation of l is stationary. If l is the Lagrangian density associated to the sine-Gordon equation then the lhs of (11) is identically zero for an exact solution of the sine-Gordon equation. Therefore (11) can be seen as a projection of the sine-Gordon operator onto the mode $\partial\phi/\partial a_i$.

For the (y, k) variables the first mode is non-zero for all values of y but the second mode is zero when $y = 0$ so that the Lagrange equation for the evolution of k is automatically satisfied no matter what the dependance of y and k on time is. For $y = 0$, the projection is done on a zero mode, therefore giving no information. Note that this problem only occurs for a breather or kink-antikink ansatz and not for a pure kink. It has been shown in [6] that all ansatz of the type:

$$\phi(x,y(t),k(t)) = 4arctan(\frac{\sinh[f(y(t),k(t))]}{\cosh(g(y(t),k(t))x)}h(y(t),k(t))) \tag{12}$$

where f can be zero cause the y and k evolution equations to be ill-defined. This is because the partial derivatives $\frac{\partial \phi}{\partial k}$ and $\frac{\partial \phi}{\partial y}$ become proportional when f=0.

Let us now consider the case of the ϕ^4 model [1]:

$$\phi_{tt} - \phi_{xx} - (\phi - \phi^3) = 0 \tag{13}$$

which can be seen as a generalisation of an equation derived from (1) in which the sine is replaced by the two first terms of its expansion. Even though the equation is not integrable an exact solution is known: the kink (or antikink):

$$\phi(x,t) = \pm \tanh[\frac{1}{\sqrt(2)}\frac{(x-vt)}{\sqrt{1-v^2}} + \xi] \tag{14}$$

To describe collisions between kinks for this model collective coordinates have been used. In particular Flesch [8] used an ansatz:

$$\phi(x,x_0(t),y_0(t)) = 1 - \tanh[\frac{y_0(x-x_0)}{\sqrt{2}}] + \tanh[\frac{y_0(x+x_0)}{\sqrt{2}}] \tag{15}$$

where x_0 is the center of mass variable and y_0 is the inverse of the width of the kinks. The Lagrangian he obtains is very similar to (7.e) in the sense that when x_0 goes through 0 the coefficients of the terms in $\dot{y_0}^2$ and $\dot{x_0}\dot{y_0}$ got to zero. In fact

$$\phi_{y_0} = -(sech[\frac{y_0(x-x_0)}{\sqrt{2}}])^2\frac{(x-x_0)}{\sqrt{2}} + (sech[\frac{y_0(x+x_0)}{\sqrt{2}}])^2\frac{(x+x_0)}{\sqrt{2}} \tag{16}$$

is zero for $x_0 = 0$ so that again the projection is done on a null vector. The problem cannot be fixed by introducing $\dot{x_0}$ in the ansatz or by adding a radiation term because the projection on the y_0 mode is the problem. Exactly as for the (y,k) variables, the numerical simulations show that $\dot{y_0}$ blows up when $x_0 = 0$. From the hamiltonian Flesch shows [8] that $\dot{y_0}$ necessarily goes to ∞ when $x_0 = 0$ unless $\dot{x_0}$ is such that $\frac{1}{2}m_1\dot{x_0}^2 + V - H_0 = 0$ where V is the potential energy and H_0 the total energy.
Prior to the study of Flesch, Jeyadev and Schrieffer [9] had done a collective coordinate study of the ϕ^4model using an ansatz derived from the Lorenz transformed solution of the linearised ϕ^4 equation around a static kink. Because of the complication in the calculations they simplified the expression. Again they obtained a blow-up for the shape mode [6].

To complete the picture of the singularity it is shown in [6] for the sine-Gordon model that the position y and the width k of a kink can be modulated in terms of collective coordinates and that this is not the case for a breather when y is close to zero. To be more specific, consider the normal modes of the collective coordinate equations in the sine-Gordon case and ϕ^4. For both models the translation mode associated to a zero frequency is non zero both for a kink and a kink-antikink pair (or breather in the sine-Gordon case). On the contrary the shape mode which corresponds to a non-zero frequency is non-zero for the kink alone and can become zero for the kink-antikink pair.

IV. New ansatzes for sine Gordon and ϕ^4

Because the ill definition of the equations is due to the fact that the Lagrange equations are obtained by a projection on a null vector, a way to fix things is not to do a simple projection anymore. Introducing an $\dot{a}_i$ dependancy in the ansatz leads to a Lagrangian $L(a_i, \dot{a}_i, \ddot{a}_i)$ The Lagrange equation for a_i is now:

$$\frac{\partial L}{\partial a_i} - \frac{d}{dt}(\frac{\partial L}{\partial \dot{a}_i}) + \frac{d^2}{dt^2}(\frac{\partial L}{\partial \ddot{a}_i}) = 0 \tag{17}$$

Using the same sort of arguments as in the previous section it can be shown [6] that the Lagrange equation (17) is equivalent to:

$$\int_{-\infty}^{+\infty} dx[\Xi\frac{\partial \phi}{\partial a_i} - \frac{\partial}{\partial t}(\Xi\frac{\partial \phi}{\partial \dot{a}_i})] = 0 \tag{18.a}$$

where

$$\Xi = \frac{\partial l}{\partial \phi} - \frac{\partial}{\partial t}(\frac{\partial l}{\partial \phi_t}) - \frac{\partial}{\partial x}(\frac{\partial l}{\partial \phi_x}) \tag{18.b}$$

which is no longer a simple projection. Following this idea, a simple ansatz that can be introduced for the breather problem is:

$$\phi(x, y(t), k(t)) = 4arctan(\frac{\sinh[y(1+\dot{k})]}{\cosh kx}) \tag{19}$$

While this ansatz is rather arbitrary, it is very appropriate to make our point for the removal of the divergence in the equation for k. It is not also unreasonable since any shape oscillation can cause a small extension or contraction of the breather. When y is large the $\dot{k}$ term leads to a wobbling kink antikink pair. The reason for putting y as a factor is to avoid a forced time dependance of k. In the absence of perturbations $\dot{k} = 0$ so that the pure breather or kink antikink solutions still exist. For all these reasons it is hoped that this ansatz will lead to a successful quantitative comparison with the solution of the perturbed pde. The evolution equations are currently being derived.

For the ϕ^4 problem, an ansatz of the form

$$\phi(x, x_0(t), y_0(t)) = 1 - \tanh[\frac{y_0(x - x_0(1+\dot{y}_0))}{\sqrt{2}}] + \tanh[\frac{y_0(x + x_0(1+\dot{y}_0))}{\sqrt{2}}] \tag{20}$$

eliminates the singularity for $x_0 = 0$. Again, it is not unreasonable to assume that the separation of the kink antikink pair depends on the shape variable y_0. It is hoped using this ansatz to obtain a quantitative agreement with the solution of the partial differential equation.

V. Discussion and summary

The breather dynamics and its transition to a kink-antikink pair is an important source of chaos in the perturbed sine-Gordon equation. This has been shown by solving directly the partial differential equation. Such a direct approach involves long computational times and does not lead to a quantitative mechanism for the transition to chaos for sine-Gordon or the complicated resonance structure for the unperturbed but non-integrable ϕ^4 system. Several authors therefore used the collective coordinate approach [5,8,9]. In all these cases the choice of the ansatz introduced mathematical singularities.
It has been shown in section III that the source of the singularity lies on the projection on a mode that vanishes at one point in the evolution of the system. This was established by writing the Lagrange equations. At this point it should be remarked that the problem is attached to only one of the two coordinates. Introducing a relativistic effect on the problem free coordinate will not remedy the situation. For example in the (y,k) problem considered introducing $\dot{y}$ in the ansatz is useless because it is the effective mass connected with $\dot{k}^2$ in the Lagrangian that vanishes. Section IV showed the essential mathematical ingredient that a new ansatz must have. For the breather a phenomenological $\dot{k}$ dependance was introduced in the ansatz leading to a Lagrangian containing a $\ddot{k}$ dependance and a fourth order non singular evolution equation through a second order variational equation.
In the case of ϕ^4, a phenomenological dependance of the kink antikink separation was introduced. It is then clear that the evolution equation of the shape mode is not singular. The same goal could have been achieved by keeping the complete relativistic ansatz introduced in [9]. This would have introduced very complicated integrals over x the value of which could not have been calculated analytically. Following a different approach, Fei and Vazquez [10] took the Lagrangian obtained from the ansatz (15) and reduced it by some rather severe approximations to the one of a particel coupled with a harmonic oscillator. Using one adjustable parameter they were able to get a remarkable semi-quantitative agreement with the pde simulations of [11]. Using our approach we hope to get a quantitative agreement with the pde without an adjustable parameter. The price to pay is that the evolution equations will be much more complex than the ones of [11]. On the other hand it is hoped to get more insight on the collision process.

As a general conclusion we think it is important before going into the lengthy calculations for the evolution of the collective coordinates to check that the projection is not done on a null mode or on colinear modes. The calculations shown in section III despite of their formal appearance reveal a lot on the physics of the problem.

REFERENCES

[1] R. K. Dodd, J. C. Eilbeck, J. D. Gibbon and H. C. Morris
"Solitons and Nonlinear wave equations"
Academic Press (1982)

[2] A. C. Scott and D. Mclaughlin
"Perturbation analysis of fluxon dynamics"

Phys. Rev. A **18**, nb. 4 (1978)
and references 17 and 18 therein.

[3] M. J. Rice and E. J. Mele
"Phenomenelogical theory of soliton formation in lihgtly doped polyacetylene"
Solid State Comm. **35**, p. 487 (1980)

[4] G. Reinisch, J. C. Fernandez, N. Flytzanis, M. Taki and S. Pnevmatikos
"Phase lock of a weakly biased inhomogeneous long Josephson junction to an external microwave source"
Phys. Rev. B **38**, nb. 16, p. 11284 (1988)

[5] O. Legrand
"Kink-antikink dissociation and annihilation: a collective-coordinate description"
Phys. Rev. A **36**, 5068 (1987)

[6] J. G. Caputo and N. Flytzanis
"Kink-antikink collisions in sine-Gordon and ϕ^4 models: problems in the variational approach
submitted to Phys. Rev. A, December 1991

[7] L. Vazquez
"A conservative scheme for lagrangian systems"
In preparation.

[8] R. Flesch
"Collective coordinates for non-linear Klein-Gordon field theory"
PhD doctoral dissertation, USC, (1987)

[9] S. Jeyadev and J. R. Schrieffer
"Collective coordinate description of soliton dynamics in trans-polyacetylene-like systems"
Synthetic Metals **9**, p. 451 (1984)

[10] Z. Fei and L. Vazquez
"Resonance phenomena in a dynamical system with two degrees of freedom "
submitted to Physica D

[11] D. K. Campbell, J. F. Schonfeld and C. A. Wingate
"Resonance structure in kink-antikink interactions in ϕ^4 theory"
Physica **9D**, p. 451 (1983)