

# Computational Solution for the Double Well Nondilute Pair Configuration\*

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## Abstract

We show numerically the existence and stability at coincidence of the nondilute, multi-instanton pair configuration in the  $(1+0)$ -dimensional, double well model, defined according to a theory presented elsewhere [1]. This follows up an earlier proof that the multi-instanton pair is an effective critical point of the classical action if it exists, and is stable if it is unique [2]. We do not prove numerical uniqueness, but find no indication of nonuniqueness. The coincident pair action has a minimum at coincidence which is a factor 0.82047 times the dilute pair action, which is the maximum, and we find no other local minimum.

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## 1. Introduction

We present here a numerical study of the kink pair solution for the (1+0)-dimensional classical Euclidean  $\phi^4$  double well field equation (one-dimensional anharmonic oscillator in quantum mechanics). The multi-instanton formalism is that developed in [1], for which we proved in [2] that the coincident pair configuration is an effective critical point of the classical action, if it exists, and is stable if it is unique. Further references may be found in those works, to which this paper is a sequel.

We demonstrate the numerical existence of a family of pair solutions parametrized by the kink-antikink separation; and while we do not demonstrate numerical uniqueness, we do find the coincident pair (zero separation) to be stable. It is the only local minimum of the action evaluated on the pair solutions; considered as a function of the pair separation, the action increases monotonically to its asymptotic maximum value at the dilute pair (far separated) solution, which is of course twice the single instanton action.

We have not actually checked that our numerical solutions do *not* obey the zero mode orthogonality constraint for instanton number  $2n$  with  $n > 1$ ; but that seems clear from the structure of the curves presented in Sect. 4, given the smooth, positive pulse shape of the zero mode function.

In Sect. 2, we describe our parametrization of the problem for numerical analysis; and in Sect. 3 we describe the program algorithms and implementation.

Finally, in Sect. 4 we present plots of the results.

**Acknowledgements.** It is a pleasure to thank Leonard Sander for introducing me to the simplex method of minimization, and for supplying software to implement it.

## 2. Parametrization

The double well classical field equation with source  $J$  is

$$-\ddot{\phi} - \mu^2\phi + \lambda\phi^3 = J, \quad \lambda, \mu^2 > 0. \quad (2.1)$$

We scale this to dimensionless units by defining

$$\phi'(t') \equiv \frac{\sqrt{\lambda}}{\mu} \phi(t), \quad t' \equiv \frac{\mu}{\sqrt{2}} t, \quad J'(t') \equiv \frac{2\sqrt{\lambda}}{\mu^3} J(t). \quad (2.2)$$

The action becomes

$$\begin{aligned}
S(\phi) &= \int_{-\infty}^{\infty} \left[ \frac{1}{2} \dot{\phi}^2 + \frac{\lambda}{4} \left( \phi^2 - \frac{\mu^2}{\lambda} \right)^2 \right] dt \\
&= \frac{\mu^3}{\sqrt{2}\lambda} \int_{-\infty}^{\infty} \left[ \frac{1}{2} \dot{\phi}'^2 + \frac{1}{2} (\phi'^2 - 1)^2 \right] dt' \\
&\equiv \frac{\mu^3}{\sqrt{2}\lambda} S'(\phi').
\end{aligned} \tag{2.3}$$

From now on we suppress primes and write

$$-\ddot{\phi} - 2\phi + 2\phi^3 = J, \quad S = \frac{1}{2} \int_{-\infty}^{\infty} \left[ \dot{\phi}^2 + (\phi^2 - 1)^2 \right] dt. \tag{2.4}$$

The one-kink solution located at  $t = s$  is

$$\phi^s(t) = \tanh(t - s), \quad S(\phi^s) = 4/3; \tag{2.5}$$

and the corresponding zero mode is

$$\xi^s(t) = \text{sech}^2(t - s). \tag{2.6}$$

The nondilute kink pair with positive, finite action boundary conditions, located at  $s_1, s_2$ , is the solution  $\phi^{s_1, s_2}$  of (2.1) with source

$$J(t) = \alpha_1 \xi^{s_1}(t) + \alpha_2 \xi^{s_2}(t), \tag{2.7}$$

with the Lagrange multipliers  $\alpha_1, \alpha_2$  determined by the constraints

$$\langle \phi^{s_1, s_2}, \xi^{s_1} \rangle = \langle \phi^{s_1, s_2}, \xi^{s_2} \rangle = 0, \tag{2.8}$$

and with boundary conditions  $\phi^{s_1, s_2}(\pm\infty) = 1$ . Because of time translation invariance, it is sufficient to consider centered pairs with  $s_1 = -s_2$ . If the solution is unique, the reflection invariance of (2.4) implies that the pair solution is an even function. We consider only that case, and write

$$\phi_+^s(t) \equiv \phi^{s, -s}(t). \tag{2.9}$$

The zero mode source may also be taken as even:

$$\begin{aligned}
J &= \alpha_+ \xi_+^s, \\
\xi_+^s(t) &\equiv \frac{\xi^s(t) + \xi^{-s}(t)}{2}.
\end{aligned} \tag{2.10}$$

The entire problem may now be restricted to the interval  $0 \leq t < \infty$ . Then only one constraint is required. For future reference, we define the constraint function and action at finite time:

$$C^s(T) \equiv \int_0^T \phi_+^s \xi_+^s dt, \quad S^s(T) \equiv \frac{1}{4} \int_0^T \left[ \dot{\phi}^{s^2} + (\phi^{s^2} - 1) \right] dt. \tag{2.11}$$

The constraint is then  $C^s(\infty) = 0$ , and the action is  $S = S^s(\infty)$ .

We mostly suppress the kink position label  $s$  in what follows.

### 3. Algorithm and Implementation

The problem of solving the field equation (2.4), including constraints, for the even pair configuration on the interval  $0 \leq t < \infty$  can be formulated in the following way.

First, we write the system, including the evaluation of the action, as a four-dimensional, time-dependent vector,

$$y = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} \dot{\phi}_+ \\ \ddot{\phi}_+ \\ \dot{C} \\ \dot{S} \end{pmatrix}, \quad (3.1)$$

the components of which obey the first-order differential equations:

$$\begin{aligned} \dot{y}_1 &= \dot{\phi}_+, \\ \dot{y}_2 &= \ddot{\phi}_+ = 2(\phi_+^2 - 1)\phi_+ - \alpha_+\xi_+, \\ \dot{y}_3 &= \dot{C} = \phi_+\xi_+, \\ \dot{y}_4 &= \dot{S} = [\dot{\phi}_+^2 + (\phi_+^2 - 1)]/4. \end{aligned} \quad (3.2)$$

The initial and final values for the vector differential equation at  $t = 0$  and  $t = \infty$  are

$$y(0) = \begin{pmatrix} \phi_+(0) \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad (3.3)$$

$$y(\infty) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ S(\infty) \end{pmatrix}. \quad (3.4)$$

The final value of the component  $y_4 = S(t)$  is not actually constrained; it just integrates to whatever the action  $S(\infty)$  is. It is a major output of the calculation.

To handle the final value problem, we introduce an implicit parameter  $T_\infty$ , which is a finite approximation to  $t = \infty$ , and which is kept fixed in the calculation for a given pair separation  $2s$ . Typically  $T_\infty$  is several kink widths larger than the rightmost kink position  $s$ . In our dimensionless units, one kink width is about unity, corresponding to the width of  $|\tanh t|$  at half maximum. At  $t = T_\infty$  we define a norm  $N_\infty$  by

$$N_\infty^2 = w_1 (y_1 - 1)^2 + w_2 y_2^2 + w_3 y_3^2 + w_4 y_4^2, \quad (3.5)$$

where the positive weights  $w_i$  are fixed input parameters to the calculation, to be adjusted by hand to optimize the numerical convergence of the minimization

procedure.<sup>1</sup> The problem is then to minimize

$$N_\infty = N_\infty [\phi_+(0), \alpha_+], \quad (3.6)$$

considered as a function of the initial value  $\phi_+(0)$  and the source coefficient  $\alpha_+$ . The numerical procedure is to integrate the differential equations from  $t = 0$  to  $t = T_\infty$  for given  $\phi_+(0)$  and  $\alpha_+$ , varying those two parameters until  $N_\infty$  falls within a prescribed tolerance of a minimum.<sup>2</sup>

As for implementation, the program was coded in double precision Fortran, using differential equations subroutines maintained by the University of Michigan Computing Center, based on the Gear [3] method.<sup>3</sup> The simplex method [4] was used for the minimization.<sup>4</sup>

Finding starting values for a given kink separation that would lead to a convergent simplex minimization was sensitive, and required a certain amount of trial and error. Our basic approach was to work inward from the far separated to the coincident pair, attempting to use the results of one minimization as starting values for the next. Once found, starting values that lead to convergent minimization typically required 70-100 iterations. The calculation would have been quite tedious on a less than main frame equivalent computer, and interactiveness would have been nonexistent.

We chose  $T_\infty = s + 8$ , about eight kink widths larger than the rightmost kink position. Our results for the action were not sensitive, at more than five significant figures, to increasing this number; and the agreement with the exact action in the case of far separated kinks ( $2s > 8$ ) was considerably better than five figures. The typical weights in the norm (3.6) were

$$w_1 = 10, \quad w_2 = 1, \quad w_3 = 20, \quad w_4 = 0, \quad (3.7)$$

with typical values of the norm better than

$$N_\infty \leq 10^{-4}. \quad (3.8)$$

## 4. Plots

At the end of this section, we show a sampling of plots of the nondilute pair solution for several separations, and a plot of the kink pair action as a function of separation. The plots were done with Timothy van Zandt's PSTricks package for L<sup>A</sup>T<sub>E</sub>X.

The pair solutions are shown in Figs. 1 and 2, beginning with the coincident pair (separation  $2s = 0$ ) in the uppermost plot of Fig. 1, and ending with a far-separated pair in the last plot of Fig. 2. For comparison, we also show

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<sup>1</sup>Although included in the program, the weight  $w_4$  of the action component was actually set to zero in all runs.

<sup>2</sup>Actually zero in our case, where we put the weight of the action component to zero.

<sup>3</sup>The subroutine source dates from 1975, and was initially provided by the National Energy Software Center.

<sup>4</sup>Fortran source for the simplex subroutine was supplied by Leonard Sander.

the corresponding approximate pair configuration  $\tanh(t-s)\tanh(t+s)$ , the dashed curve on each plot.

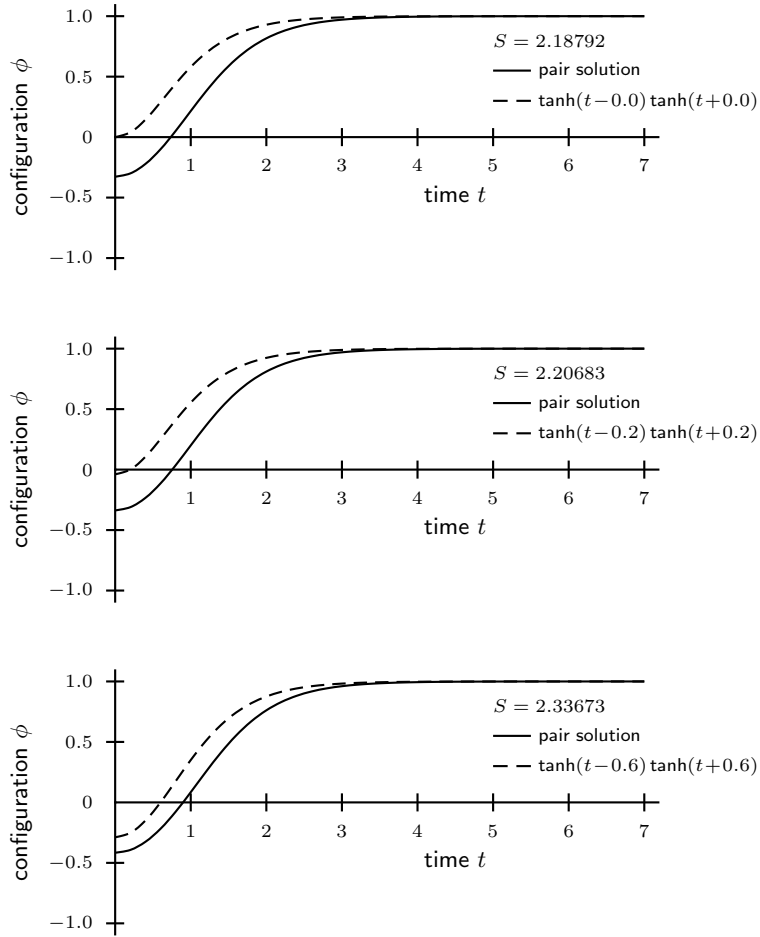
The coincident pair shows a significant deepening compared to the approximate pair configuration, but what is perhaps reassuring is that the approximate configuration is as good as it is. By the time the pair separation has reached  $2s = 4$ , about four kink widths, the topmost curve in Fig. 2, the approximate pair solution nearly coincides with the exact solution, while the action at  $S = 2.6614$  agrees with the dilute pair value  $S = 8/3$  to three significant figures. The approximate and exact solutions are visually indistinguishable at the separation  $2s = 5.2$ , in the middle graph of Fig. 2, where the action agrees with the dilute pair to four figures.

Finally, Fig. 3 shows the action as a function of pair separation, collected from a number of runs like those shown in Figs. 1 and 2. The coincident pair is clearly the minimum, and the only local minimum. We believe our numbers for the action to about five significant figures, possibly better. The attraction of the kink pair makes the pair action stable at coincidence,

$$S(0) = 2.1879 = 0.82047 S(\infty), \quad (4.1)$$

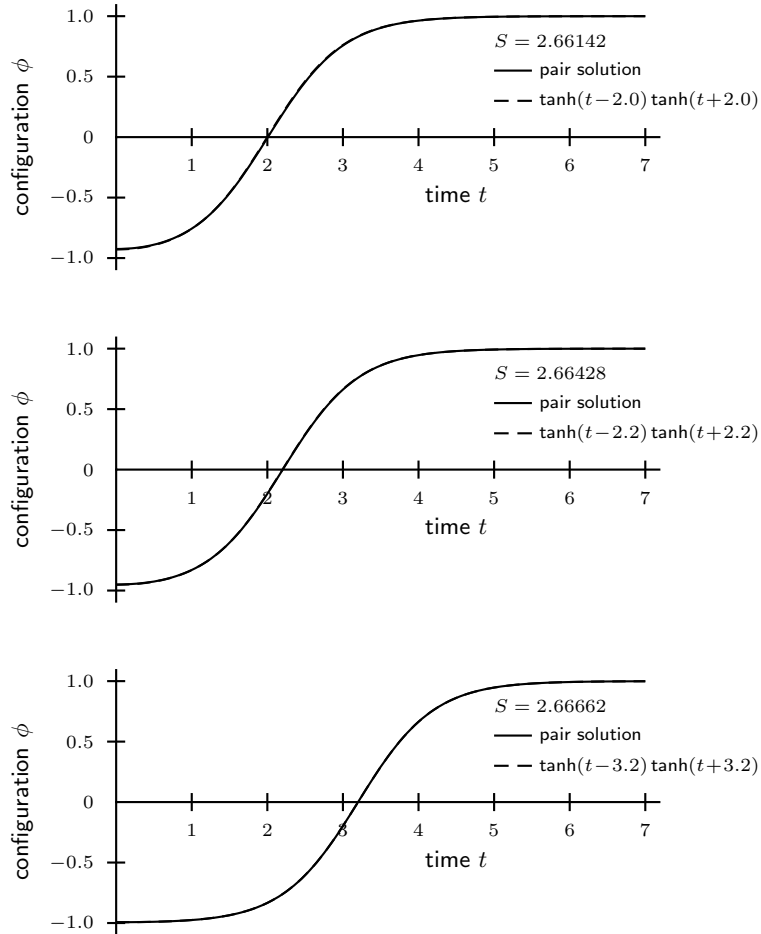
about 0.8 times the dilute pair value. As we explained in [2], the systematics of this effect on the instanton gas remains to be elucidated, but it is clearly *a priori* as large as dilute pair effects which are traditionally included.

### Kink Pair Solutions

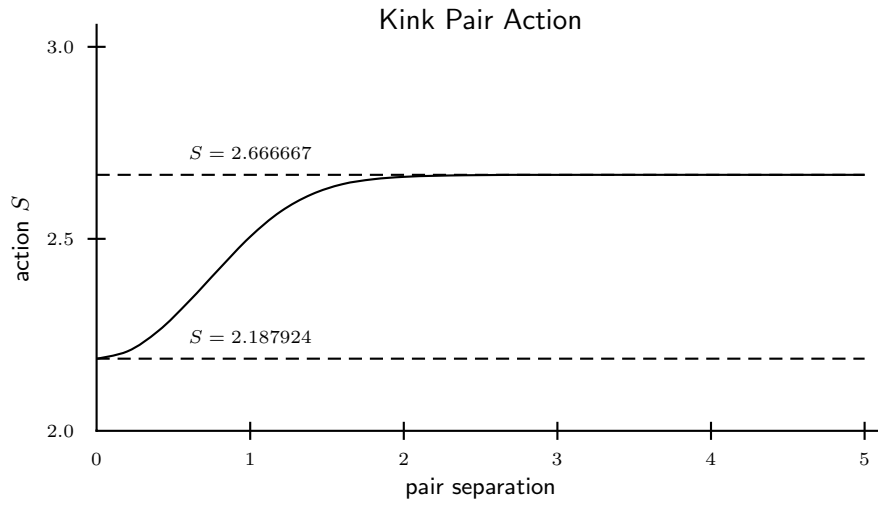


**Figure 1:** Numerical solutions for symmetrically located, nondilute kink pairs at dimensionless separations 0.0, 0.4, and 1.2, respectively, plotted for positive  $t$  only. The functions are even in  $t$ . For comparison, the dotted curves represent the corresponding dilute gas configurations, valid only at large separations. The action  $S$  in the upper right corner of each plot is that of the nondilute solution.

### Kink Pair Solutions



**Figure 2:** The same as Fig. 1, but with separations 4.0, 4.4, and 6.4, respectively. Note that the separations are large enough in all cases that the approximate dilute gas configurations are nearly the same as the exact solutions.



**Figure 3:** The action  $S$  for nondilute pair solutions in dimensionless units as a function of kink separation, twice the rightmost kink position in Figs. 1 and 2. This plot is based on a sample of solutions at 17 separations.

## Bibliography

- [1] D. N. Williams, “Instanton Gas Parameters in the Double Well Model”, *Mathematical Problems in Theoretical Physics*, Proceedings of the VIth International Conference on Mathematical Physics, Berlin (West), August 11–20, 1981, R. Schrader, R. Seiler, D. A. Uhlenbrock, eds. (Springer-Verlag, Heidelberg, 1982), pp. 295–297.
- [2] D. N. Williams, “Effective Criticality and Stability of the Double Well Coincident Pair Configuration”, University of Michigan, Randall Laboratory of Physics Preprint UM-TH-82-11, 1989.
- [3] C. W. Gear, *Numerical Initial Value Problems in Ordinary Differential Equations*, (Prentice-Hall, Englewood Cliffs, N.J., 1971).
- [4] J. A. Nelder and R. Mead, *Computer Journal* **7** (1965) 308.