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LETTER TO THE EDITOR

Exact kink solutions in a new non-linear hyperbolic double-well potential

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Abstract. We propose a model of a kink bearing Hamiltonian with a new non-linear potential $V(\varphi, \mu)$ whose double-well shape can be varied continuously as a function of the parameter μ and which has the φ^4 potential as a particular case. Exact classical kink solutions that depend on μ are obtained. The rest masses and rest energies of the kinks are also determined.

In recent years non-linear monatomic chain models have been extensively used in condensed-matter physics because they provide a non-perturbation approach to strongly anharmonic systems. The governing equations frequently admit large-amplitude localized field profiles that are physically distinct from those obtainable by superposition of small-amplitude or linearized profiles. These localized large-amplitude excitations can propagate through the system without distortion of shape and are commonly referred to as solitary waves. They exhibit remarkable stability and other particle-like properties. Because of their localized nature, they have found widespread use as one-dimensional models of extended particles in non-linear quantum-field theories, dislocations in crystals, planar domain walls in ferromagnets and ferroelectrics, propagating flux quanta in Josephson transmission lines, disgyration planes in superfluid He, charge carriers in weakly pinned charge-density-wave condensates, and charged dislocations in superionic conductors, to mention only a few examples.

Various kinds of non-linear potential have been proposed to explain these phenomena. As examples, we may retain the Toda potential (1967), the Lennard-Jones potential, the Morse potential, the sine–Gordon and double sine–Gordon potentials, the φ^4, φ^6 and φ^8 fields, a double quadratic potential, the Schmidt potential (1979), the Magyari potential (1981), the Behera and Khare potential (1981) and the Remoissenet–Peyrard potential (1981).

Consider a general class of non-linear solitary wave bearing one-dimensional lattice Hamiltonians (see Currie *et al* 1980).

$$H = \sum_i lA\left(\tfrac{1}{2}\dot{\varphi}_i^2 + \frac{1}{2}\frac{C_0^2}{l}(\varphi_{i+1} - \varphi_i)^2 + \omega_0^2 V(\varphi_i)\right) \tag{1}$$

where φ_i is a one-component dimensionless field defined on a one-dimensional lattice of points with lattice constant l. The first term represents the kinetic energy carried by the field, the second represents harmonic coupling between field values at neighbouring lattice sites and the last term, $V(\varphi_i)$, is the local non-linear potential function. The constants C_0 and ω_0 are the characteristic velocity and frequency, respectively, whose ratio, $d_0 = C_0/\omega_0$, determines the fundamental length scale for variations in φ_i, while the constant A sets the energy scale. In the displacive limit $d_0 \equiv C_0/\omega_0 \gg 1$, where non-linear kinks become well-defined (Currie *et al* 1977) elementary excitations with long lifetimes, and as such behave very much like particles (Fogel *et al* 1976), the Hamiltonian (1) is transformed approximatively to

$$H = A \int_{-\infty}^{+\infty} (\tfrac{1}{2}\varphi_t^2 + \tfrac{1}{2}C_0^2\varphi_x^2 + \omega_0^2 V(\varphi))\,\mathrm{d}x \tag{2}$$

which may be regarded as the energy functional of a classical scalar field $\varphi = \varphi(x, t)$ having the Lagrange density

$$L = (A/2)\varphi_t^2 - (AC_0^2/2)\varphi_x^2 - A\omega_0^2 V(\varphi). \tag{3}$$

The corresponding Euler–Lagrange equation

$$\varphi_{xx} - (1/C_0^2)\varphi_{tt} - (1/d_0^2)\,\mathrm{d}V/\mathrm{d}\varphi = 0 \tag{4}$$

is usually called the generalized Klein–Gordon equation of the displacement field φ.

The non-linear solitary wave (kink, soliton) excitations, the periodic non-linear wave (periodon) excitations and the linear (phonon) excitations of the system arise as travelling-wave solutions $\varphi = \varphi(S)$, $S = x - vt$ to (4), i.e. as solutions to the equation

$$\varphi_{SS} = \gamma^2 d_0^2\,\mathrm{d}V/\mathrm{d}\varphi \tag{5}$$

where

$$\gamma = (1 - v^2/C_0^2)^{-1/2} \qquad \text{and } |v| \leqslant C_0.$$

We look for a kink moving with velocity v and impose appropriate boundary conditions:

$$(\mathrm{d}\varphi(S)/\mathrm{d}S)(S = \pm\infty) = 0 \qquad \varphi(S = \pm\infty) = \varphi_{1,2}.$$

$V(\varphi(S = \pm\infty)) = 0$ (a convenient energy zero). The kink solution is obtained from the first integral of equation (5)

$$\mathrm{d}\varphi/\mathrm{d}S = \pm[2(\gamma^2/d_0^2)V(\varphi)]^{1/2} \tag{6}$$

by integrating a second time yielding

$$S = \pm\gamma^{-1}(d_0/\sqrt{2}) \int_{\varphi(0)}^{\varphi(S)} (V(\varphi))^{-1/2}\,\mathrm{d}\varphi. \tag{7}$$

The relativistic dependence on v follows from the Lorentz covariant form of equation (4).

Our aim in this letter is to examine the possible non-linear excitations of a model system with a new non-linear potential whose shape can be varied as a function of a

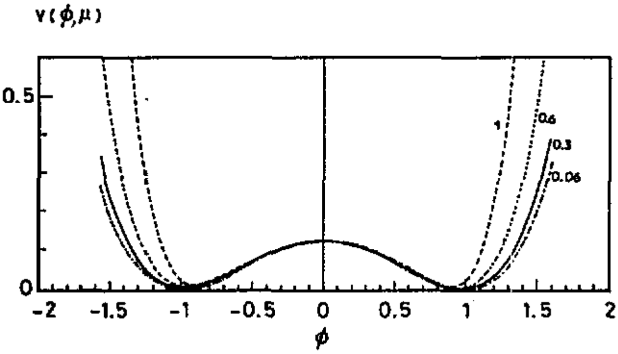

Figure 1. Plot of parametric double-well one-site potential for different values of μ. The double-well shape is preserved for any value of μ.

parameter μ. In this model, the anharmonic one-site potential is a double-well potential of the form

$$V(\varphi, \mu) = (a/8)(\sinh^2(\mu\varphi)/\mu^2 - 1)^2 \qquad \mu \neq 0 \tag{8}$$

with two degenerate minima ($V = 0$) at

$$\varphi_{1,2} = \mp(1/\mu)\sinh^{-1}(\mu). \tag{9}$$

In our potential, the quantity $a/8$ is the barrier height. On figure 1, $V(\varphi, \mu)$ is plotted as a function of φ for different values of μ. The double-well form is preserved even for large values of the parameter μ. The small-values limit corresponds approximatively to the well known φ^4 field which is explained in the form

$$V(\varphi, \mu \to 0) = (a/8)(\varphi^2 - 1)^2 \tag{10}$$

from equations (7) and (8) using equation (9); we obtain the family of exact kink solutions

$$\varphi(S, \mu) = \mp(1/\mu)\tanh^{-1}\{(\mu/\sqrt{1+\mu^2})\tanh[\sqrt{1+\mu^2}\sqrt{a}(\gamma/2d_0)S]\}. \tag{11}$$

In the limit of $S \to \pm\infty$, equation (11) gives

$$\varphi(S = \pm\infty, \mu) = \mp(1/\mu)\sinh^{-1}\mu \tag{12}$$

which are the values of φ corresponding to the degenerate minima.

The small-limit values of the parameter μ gives approximatively

$$\varphi(S) = \mp(1/\sqrt{1+\mu^2})\tanh[\sqrt{1+\mu^2}\sqrt{a}(\gamma/2d_0)S] \tag{13}$$

and $\varphi_{1,2} = \mp 1$, which correspond to the φ^4 case.

Figure 2 shows the kink solution dependence of the parameter μ. The kink form is preserved and only the wave amplitude is varied as a function of μ.

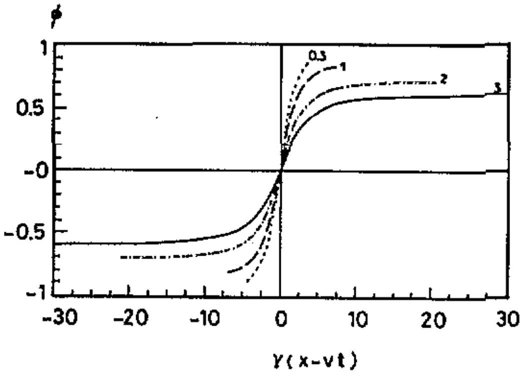

Figure 2. Waveform of a travelling kink viewed in its rest frame, plotted for three values of μ. The anti-kink is obtained by reflection through the horizontal axis.

We now turn our attention to the particle properties of the kink moving with velocity v ($|v| \ll C_0$). Its energy is uniquely determined and can be expressed in the relativistic form (Currie *et al* 1980)

$$E^{(v)} = \gamma E^{(0)} \tag{14}$$

where $E^{(0)} = M_k C_0^2$ is the rest energy of the kink and M_k is its rest mass:

$$M_k = \frac{\sqrt{2}A}{d_0} \int_{\varphi_1}^{\varphi_2} (V(\varphi, \mu))^{1/2}\, \mathrm{d}\varphi. \tag{15}$$

Substituting the expression (8) for $V(\varphi, \mu)$ in equation (15) and integrating, we obtain

$$M_k = (A\sqrt{a}/2d_0)(1/\mu^3)[\mu\sqrt{1+\mu^2} - (1+2\mu^2)\sinh^{-1}\mu]. \tag{16}$$

In summary, we have introduced a potential that has the advantage that its shape can be varied continuously leading simply to a change of the associated kink wave form. An appropriate choice of the parameter μ enables us to employ a form of the potential that is closer to the situation in a particular physical system. Moreover, our model admits the φ^4 potential as a particular case for small values of μ. The dipolar character and bi-stability of the hydrogen bond can be conveniently described in our model when discussing high protonic mobility in filamentary crystals, or non-linear collective phenomena in biological macromolecules, in ice, or the transport of energy across biological cellular membrane. Finally, the statistical mechanics of this model are left for treatment in future work.

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