A Collective Coordinate Method for Classical Dynamics of Nonlinear Klein-Gordon Kinks

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Abstract A collective coordinate method is used to study the motion of a nonlinear Klein-Gordon (NKG) kink [1] in the presence of a weak, localized perturbation. An equation of motion is derived for the kink "center of mass" position which includes the effects of phonons. A perturbation expansion of these equations shows that through second order, no extended phonons are generated by the "collision" of the kink with a static perturbation. As a consequence, the kink recovers its initial velocity after passing through the perturbation region.

The study of kink dynamics in NKG models has been greatly facilitated by the introduction of a collective coordinate describing the "center of mass" (CM) motion of the kink [2-5]. As the kink is a coherent, extended object, it seems natural to assign a coordinate which describes the motion of its center. Separating out this degree of freedom also removes secular terms caused by the zero-frequency Goldstone mode (translation mode) [6].

Although many times introduced purely as an ansatz, a canonical transformation which utilizes a collective coordinate has been discovered for the NKG class of field theories [7]. This canonical structure allows us to easily derive the equations of motion and leads to a well-defined quantization procedure [2,3,7,8]. We extend this canonical formalism to include the effects of a spatially localized perturbation $\lambda v(x,t)$ which couples linearly to the field $\Phi(x,t)$. With λ as a small parameter measuring the strength of the perturbation, we consider Lagrangians of the form:

$$L = \int_{-\infty}^{\infty} dx \left\{ \frac{1}{2}\partial_\mu \Phi \, \partial^\mu \Phi - U(\Phi) + \lambda v(x,t)\Phi \right\} \quad . \tag{1}$$

The equation of motion for the Lagrangian in (1) is:

$$\Phi_{tt} - \Phi_{xx} + U'(\Phi) - \lambda v(x,t) = 0 \quad . \tag{2}$$

The unperturbed equation (λ=0) is assumed to have a static (classical) kink solution $\phi_c(x)$. Solutions to (2) are further studied via the canonical transformation:

$$\Phi(x,t) = \phi_c(x-X) + \psi(x-X,t) + \chi_0(x,t) \quad , \tag{3a}$$

$$\Pi_0(x,t) = \pi(x-X,t) - (M_0+\xi)^{-1} \left\{ p + \int_{-\infty}^{\infty} dx \, \pi(x,t)\,\psi'(x,t) \right\} \phi_c'(x-X) - \dot{\chi}_0(x,t) \quad , \tag{3b}$$

$$\xi = \int_{-\infty}^{\infty} dx \, \phi_c'(x)\,\psi'(x,t) \;,\; M_0 = \int_{-\infty}^{\infty} dx \, \phi_c'(x)\,\phi_c'(x) \;,\; \int_{-\infty}^{\infty} dx \, \phi_c'(x)\,\psi(x,t) = 0 \;,\; \int_{-\infty}^{\infty} dx \, \phi_c'(x)\,\pi(x,t) = 0 \quad . \tag{3c}$$

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The first term on the right-hand side of (3a) represents a kink whose CM moves according to the dynamical variable $X(t)$. The ψ field will account for the interaction of the kink with the perturbation. The major contribution to ψ will be localized about the kink center and will have an appreciable amplitude only when the kink is in the region of the perturbation. In addition, $\psi(x,t)$ must account for any extended phonons radiated in the "collision", however, as will be shown later, for static perturbations, such phonons first appear in the third order terms of a perturbation series for ψ in powers of the strength parameter λ. The final contribution to the field is the "background" response χ_0, that is, the response of the system in the absence of the kink. The equation which determines χ_0 is (2) with Φ replaced by χ_0. We approximate $\chi_0(x,t)$ by linearizing (2) to obtain

$$\chi_{0_{tt}} - \chi_{0_{xx}} + \chi_0 - \lambda v(x,t) = 0 \qquad . \tag{4}$$

We explicitly account for this background or vacuum response of the field because unless the perturbation is turned on adiabatically, this response will be present long before and after the kink interacts with the perturbation (a situation often realized in physical systems [6]). When the kink is far from the impurity, ψ is zero and the ansatz of a translating kink ϕ_c plus the background χ_0 is a solution to the perturbed equation of motion to lowest order in χ_0. As the kink approaches the perturbation, this ansatz breaks down and the ψ field begins to contribute.

The momentum, Π_0, conjugate to the field Φ, is expressed in terms of the new canonically conjugate pairs (X,p) and (ψ,π) in (3b). The transformation,

$$\{\Phi(x,t), \Pi_0(x,t)\} \longrightarrow \{X(t), p(t), \psi(x,t), \pi(x,t)\} \qquad , \tag{5}$$

does not conserve the number of degrees of freedom, hence the last two equations in (3c) are introduced as constraints. The first of these constraints has the interpretation that the ψ field may not account for any translation of the kink since ϕ_c' is the translation mode. Using the Dirac formalism for constrained systems [9], (3) may be shown to form a canonical transformation [10]. With a canonical transformation in hand, we may derive the equations of motion using the standard rules of Hamilton-Jacobi theory. Details of this will be presented elsewhere [10] and here we simply state the equation of motion for the CM collective coordinate $X(t)$:

$$M_0 \ddot{X} = \frac{1}{1+\frac{\xi}{M_0}} \left\{ \int_{-\infty}^{\infty} dx\, \phi_c'(x-X) \left[U'[\Phi(x,t)] - U'[\chi_0(x,t)] \right] + (1+\dot{X}^2) \int_{-\infty}^{\infty} dx\, \psi'(x,t)\, \phi_c''(x) \right.$$
$$\left. - 2\dot{X} \int_{-\infty}^{\infty} dx\, \phi_c'(x) \left[\pi'(x,t) - \dot{\chi}_0'(x+X,t) \right] \right\} \qquad . \tag{6}$$

The right-hand side of (6) has what appear to be dissipative terms. However, in a system such as ours in which there is no coupling to other degrees of freedom such as a heat bath, these "dissipative" terms can only represent a transfer of energy between the degrees of freedom. In our case, the energy transfer is from the kink CM motion to the "phonon field" $\psi(x,t)$. Below we carry out a perturbation expansion in which we show that to lowest order, no energy transfer occurs, and in second order, the energy given to the phonon field during the collision is ultimately given back to the kink's translational motion.

Carrying out this expansion, we have for the first-order equation of motion for the CM variable:

$$M_0 \ddot{X} = -\frac{\partial V(X,t)}{\partial X} \qquad , \qquad V(X,t) \equiv \int_{-\infty}^{\infty} dx\, \chi_0(x+X,t) \left[\phi_c''(x) - \phi_c(x) \right] \qquad . \tag{7}$$

Equation (7) simply states that to first order the kink behaves as a Newtonian particle of mass M_0 (see (3c)) moving in the effective potential $V(X,t)$. Proceeding to second order we have,

$$M_0 \ddot{X} = - \left[1 - \frac{\xi}{M_0}\right] \frac{\partial V(X,t)}{\partial X} + \frac{1}{2}\int_{-\infty}^{\infty} dx\, U'''[\phi_c(x)] \left[\psi(x,t) + \chi_0[x+X,t]\right]^2$$

$$- \frac{1}{2}\int_{-\infty}^{\infty} dx\, U'''(0)\, \chi_0^2(x+X,t) - 2\dot{X}\int_{-\infty}^{\infty} dx\, \phi_c'(x)\, \dot{\psi}'(x,t) \quad . \qquad (8)$$

From (8), we see that to obtain $X(t)$ through second order, we need ψ to first order. The first order equation for ψ may be written as [10]:

$$\ddot{\psi}(x,t) - \psi''(x,t) + U''[\phi_c(x)]\psi(x,t) = \chi_0(x+X,t)\ \{1 - U''[\phi_c(x)]\}$$

$$- \frac{\phi_c'(x)}{M_0}\int_{-\infty}^{\infty} dx\, \phi_c'(x)\, \chi_0(x+X,t)\ \{1 - U''[\phi_c(x)]\} \quad . \qquad (9)$$

Denoting the (inhomogeneous) terms on the right-hand side by $I(x,t)$, we have the following integral expression for $\psi(x,t)$:

$$\psi(x,t) = \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dt'\ G(x,x',t,t')\, I(x',t') \quad , \qquad (10)$$

where $G(x,x',t,t')$ is the appropriate Green function [10,11]. Analytic expressions for $G(x,x',t,t')$ are available in terms of modified Lommel functions of two variables for the sine-Gordon, ϕ^4, and double-quadratic potentials [11].

Using the localized nature of χ_0 and the assumption that $U(\phi_c)$ is scaled so that $U''[\phi_c(x)] \to 1$ as $x \to \pm\infty$, one can show [10] that $\psi(x,t)$ is localized in both space and time. Since all second order terms in (8) are proportional to ψ, ψ^2, or spatial derivatives of ψ, all second order terms in (8) are localized in time, therefore as $t \to \pm\infty$, we have $M_0\ddot{X} \to -\partial V(X,t)/\partial X$. Furthermore, for static perturbations or perturbations which are turned on and off adiabatically we have $V(X,t) \to 0$ as $|X| \to \infty$. Thus we see that through second order, the kink behaves as a free particle as $t \to \pm\infty$ (recall that in zeroth order, $X(t)=X_0 + V_0 t$). Since energy is conserved, all energy is returned to the translational motion of the kink.

To illustrate the methods outlined, we present an example in which a sine-Gordon kink, initially traveling to the right, encounters the time-independent perturbation

$$v(x) = e^{-(x-x_0)^2} - e^{-(x+x_0)^2} \quad . \qquad (11)$$

In our simulation, the following initial conditions and parameters were used:

$$X(t{=}0) \equiv X_0 = -20 \quad , \quad \dot{X}(t{=}0) \equiv \dot{X}_0 = .3 \quad , \quad \lambda = .04 \quad , \quad x_0 = 5 \quad . \qquad (12)$$

Plots of $v(x)$ along with the linear response χ_0 it generates are given in Fig. 1. The background $\chi_0(x)$ is localized as it should be for localized $v(x)$. Figure 2 shows the effective potential $V(X)$ experienced by the kink CM in first order. As expected, the effective potential is localized in X. Since to first order the kink behaves as a Newtonian particle moving in the potential well $V(X)$, we expect the kink's velocity to increase upon entering the region of the perturbation, then return to its original value when leaving. The first-order motion for the kink CM is shown in Fig. 3 and confirms this potential energy analysis.

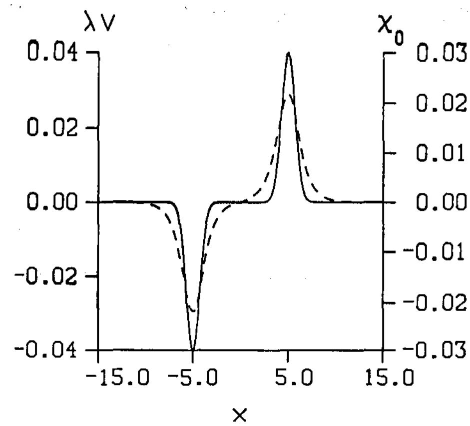

Fig. 1 The perturbation $\lambda v(x)$ and the linear response $\chi_0(x)$ (dashed curve) it generates

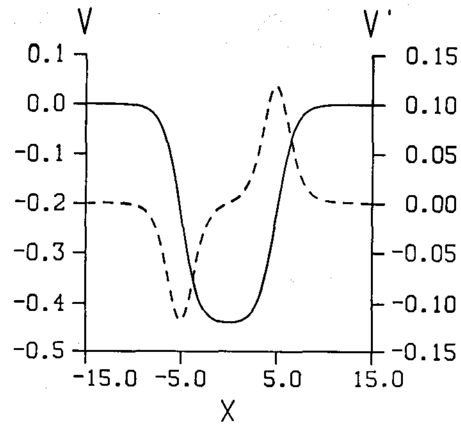

Fig. 2 The effective potential V(X) and its derivative (dashed curve)

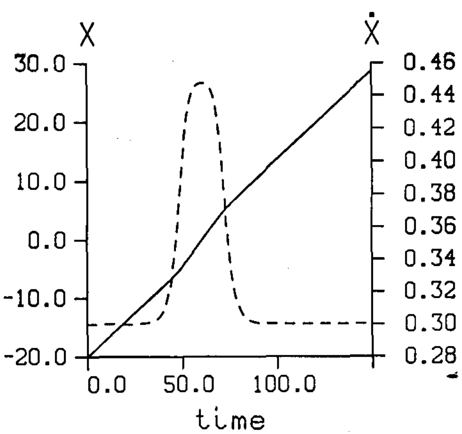

Fig. 3 The first-order kink position and velocity (dashed curve) as a function of time

The second-order motion for the CM variable X(t) deviates from the first order motion only in that the maximum velocity (see Fig. 3) attained by the kink is slightly smaller since some energy is given to the phonon field $\psi(x,t)$. However, since the final kink velocity equals the initial velocity, this energy is given back to the kink when it leaves the perturbation region. Since the phonon field ψ remains localized (through second order) about the kink CM, it can be regarded as a (temporary) shape change of the kink during the collision. It is possible that in third and higher orders, in addition to a phase shift, the kink will be accompanied by extended phonons and the kink's final velocity will not equal its initial velocity. However, before proceeding to higher order, one must examine the approximations made to see if they are still valid in higher order. One point of concern is the approximation of the response of the field to the perturbation by the background χ_0, which is obtained by linearization. These questions along with applications of this method to different classes of perturbations shall be addressed in further publications.

REFERENCES

1. A. R. Bishop, J. A. Krumhansl, and S. E. Trullinger, Physica 1D, 1 (1980)
2. J. L. Gervais, A. Jevicki, and B. Sakita, Phys. Rev. D12,1038 (1975), Physics Reports, 23C, 281 (1976)
3. J. L. Gervais and A. Jevicki, Nuclear Phys. B110, 93 (1976)
4. M. J. Rice and E. J. Mele, Solid St. Commun. 35, 487 (1980); T. Holstein, Proc. Int. Conf. Low-Dim. Cond., Boulder, Col., August 1981 (Gordon and Breach, Science Publishers, Inc. 1981)
5. D. K. Campbell, J. F. Schonfeld, and C. A. Wingate, Physica 9D, 1 (1983)
6. M. B. Fogel, S. E. Trullinger, A. R. Bishop, and J. A. Krumhansl, Phys. Rev. Lett. 36,1411 (1976); Phys. Rev. B15, 1578 (1977)
7. E. Tomboulis, Phys. Rev. D12, 1678 (1975)
8. S. E. Trullinger, Solid St. Commun. 29, 27 (1979)
9. P. A. M. Dirac, Lectures on Quantum Mechanics (Academic, New York, 1964)
10. B. Horovitz, R. J. Flesch, and S. E. Trullinger, to be published
11. R. J. Flesch and S. E. Trullinger, to be published