Physical dynamics of solitons

M. J. Rice
Xerox Webster Research Center, Webster, New York 14580 and Observatoire de Nice, F-06007 Nice, France
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A collective-coordinate Hamiltonian is derived for a sine-Gordon or ϕ^4 soliton. It describes a material particle whose translational motion is coupled to an internal degree of freedom. The Hamiltonian equations of motion are solved for exactly and show that the "soliton" may exist in a dynamical state of constant translational momentum and constant total energy with an internal vibration which imparts an oscillatory component to the soliton's translational velocity.

In a recent paper[1] on a phenomenological theory of soliton formation in the linearly conjugated polymer *trans*-polyacetylene, a collective-coordinate Hamiltonian was introduced for the soliton. Its construction was based on identifying the soliton's translational position and width as dynamical variables. In a subsequent paper,[2] this Hamiltonian was used as a starting point for a quantum-mechanical theory of the absorption of electromagnetic radiation by a mobile charged soliton (such as that which might occur in polyacetylene).

In this Brief Report we derive the collective-coordinate Hamiltonian specifically for a sine-Gordon (SG) or "ϕ^4" classical field. The Hamiltonian found describes the soliton as a material particle whose translational motion is coupled to an internal (vibrational) degree of freedom. The Hamiltonian is exactly solvable and shows that the "soliton" may exist in a dynamical state of constant translational momentum and constant total energy with an internal vibration which imparts an oscillatory component to the soliton's translational velocity.

We consider the Lagrangian density functional

$$L[\phi]=(\lambda\epsilon/\omega_0^2)[\tfrac{1}{2}\phi_t^2-\tfrac{1}{2}c_0^2\phi_x^2-\omega_0^2V(\phi)] \tag{1}$$

governing a classical field $\phi(x,t)$ in one space dimension x. If we choose $\lambda=\frac{1}{2}$ and $V(\phi)=1-\cos(\phi)$ (1) describes a SG field while if we set $\lambda=8$ and $V(\phi)=8^{-1}(1-\phi^2)^2$ (1) describes a ϕ^4 field.[3] In (1) ϵ, c_0, and ω_0 are constants of the field. The Euler-Lagrange equation of motion for $\phi(x,t)$ is

$$\phi_{tt}-c_0^2\phi_{xx}+\omega_0^2\frac{dV(\phi)}{d\phi}=0 \ . \tag{2}$$

The (uniform) ground-state configurations of (1) are $\phi_0=2\pi n$ $(n=0,\pm1,\ldots)$ for the SG field and $\phi_0=\pm1$ for the ϕ^4 field. If we introduce the dimensionless space variable $y=(x/\beta d)$, where $d=c_0/\omega_0$ and $\beta\equiv1$ for SG and $\beta\equiv2$ for ϕ^4, the well-known static solitary wave solutions of (2), which interpolate between the degenerate ground states, satisfy

$$(2\beta^2)^{-1}\phi_y^2=V(\phi) \ , \tag{3}$$

and are

$$\phi^{(s)}(y)=\pm4\tan^{-1}[\exp(\pm y)] \ , \tag{4}$$

$$\phi^{(s)}(y)=\pm\tanh(y) \ , \tag{5}$$

for SG and ϕ^4, respectively. The creation or rest energies associated with these solutions are

$$E_s^0=\frac{\lambda\epsilon d}{\beta}\int_{-\infty}^{\infty}dy[\phi_y^{(s)}(y)]^2 \ .$$

Our Hamiltonian description is based on introducing the ansatz

$$\phi(x,t)=\phi^{(s)}(\psi(x,t)) \ , \tag{6a}$$

$$\psi(x,t)=[x-x_n(t)][2/l(t)] \ , \tag{6b}$$

for a time-dependent single solitonlike solution of (2). At time t this ansatz describes a SG-like or ϕ^4-like solitary wave of (total) width $l(t)$ centered at the position $x_n(t)$. As discussed in detail in Refs. 1 and 2, the motivation for considering these two dynamical variables is the physical picture of the soliton as an extended, deformable object, having an identifible center $[x_n(t)]$ and an internal structure [characterized most simply by the width parameter, $l(t)$]. We shall refer to x_n as the "translational coordinate" and to l as the "internal coordinate" and, more loosely, to the solitonlike object (6) as the "soliton." Since these collective coordinates are effectively parameters in the structure of the soliton, we call our approach a "parametric collective-coordinate" method and seek equations describing the time dependencies of the collective coordinates $x_n(t)$ and $l(t)$.

The latter equations of motion are obtained from a stationary variation of the classical action $S=\int dt\,L$ where the Lagrangian $L=\int dx\,L[\phi^{(s)}(\psi)]$. Since $L=L(x_n,\dot{x}_n,l,\dot{l})$ where $\dot{x}_n$ and $\dot{l}$ denote the total time differentials of x_n and l, the sought equations of motion are evidently the Lagrange equations

$$\frac{\partial L}{\partial x_n}-\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{x}_n}\right)=0, \quad \frac{\partial L}{\partial l}-\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{l}}\right)=0 \ ,$$

and the task reduces to the evaluation of L. With the use of Eqs. (3) and (6) we find

$$L=\tfrac{1}{2}M_i(l)\dot{l}^2+\tfrac{1}{2}M_s(l)\dot{x}_n^2-V(l) \ , \tag{7}$$

where

$$V(l)=(E_s/2)(l_0l^{-1}+l_0^{-1}l) \ , \tag{8}$$

$$M_s(l)=(l_0E_s/c_0^2)l^{-1}, \quad M_i(l)=\alpha M_s(l) \ , \tag{9}$$

$$\alpha=\begin{cases}\pi^2/48 \ \ (\mathrm{SG}) \ , & (10a)\\ (\pi^2-6)/48 \ \ (\phi^4) \ , & (10b)\end{cases}$$

and $l_0 = 2\beta d$. We shall refer to $V(l)$ as the "internal" potential energy of the soliton and to $M_i(l)$ and $M_s(l)$ as the soliton's internal and translational inertial masses, respectively.

The final step of the derivation is to evaluate the Hamiltonian $H = p_l\dot{l} + p_x\dot{x}_n - L$, in which p_l and p_x denote the canonical momenta $p_l = \partial L/\partial\dot{l}$ and $p_x = \partial L/\partial\dot{x}_n$. We thereby arrive at the Hamiltonian system

$$H = [p_l^2/2M_i(l)] + V(l) + [p_x^2/2M_s(l)] \ , \tag{11}$$

$$\dot{p}_l = -\partial H/\partial l, \quad \dot{l} = \partial H/\partial p_l \ , \tag{12}$$

$$\dot{p}_x = -\partial H/\partial x_n, \quad \dot{x}_n = \partial H/\partial p_x \ . \tag{13}$$

It describes a material particle whose translational motion is coupled to an internal degree of freedom.

In the subsequent discussion of this paper we shall omit the subscript n from the translational coordinate x_n. Since x does not appear explicitly in the Hamiltonian (11) the translational momentum p_x is a constant of motion. Consequently, the Hamiltonian equations of motion are

$$\dot{x} = p_x/M_x(l) = (p_x c_0^2/E_s l_0)\,l \ , \tag{14}$$

$$\frac{d(lM_i(l))}{dt} = -\frac{\partial V(l;p_x)}{\partial l} \ , \tag{15}$$

where $V(l;p_x) = V(l) + p_x^2/2M_s(l)$. The task of arriving at the time dependences of x and l thus reduces to the solution of (15). This equation is the equation of motion for a particle with a position-dependent mass, $M_i(l)$, moving in a potential well $V(l;p_x)$. Despite its apparent highly nonlinear character it may be solved exactly.

We first discuss the special case $\dot{l} = 0$. For this case our ansatz (6) has the form of the exact single solitary wave solution of the original SG or ϕ^4 field Eq. (2). Thus Eqs. (14) and (15) should lead to the standard SG or ϕ^4 relativistic dynamics. The solution of (15) is $l = l_s(p_x)$, where $l_s(p_x) = l_0/[1 + (p_x/M_s c_0)^2]^{1/2}$ is the minimum of the potential $V(l;p_x)$. We have introduced $M_s \equiv M_s(l_0) = E_s/c_0^2$. From (14), $\dot{x} = (p_x/M_s)\,l_0^{-1} l_s(p_x)$. On expressing p_x in terms of $\dot{x}$ we obtain $p_x = M_s\dot{x}/[1 - (\dot{x}/c_0)^2]^{1/2}$ and $l_s(\dot{x}) = l_0(1 - (\dot{x}/c_0)^2)^{1/2}$. The total energy is

$$E = H = (M_s^2 c_0^4 + c_0^2 p_x^2)^{1/2}$$

$$= M_s c_0^2/[1 - (\dot{x}/c_0)^2]^{1/2} \equiv E_s(p_x) \ .$$

These are the standard relativistic results for a soliton translating at a constant velocity x.

The exact time-dependent solution of (15) may be derived by employment of the Hamilton-Jacobi method. The Hamiltonian corresponding to (15) is

$$H = H(l,p_l) = p_l^2/2M_i(l) + V(l;p_x)$$

with dynamical variables l and p_l. We introduce the Hamilton-Jacobi function $S(l,E,t)$ which generates a canonical transformation to a new set of dynamical variables D and E which are time independent. The Hamilton-Jacobi equations are

$$H(l,(\partial S/\partial l)) + \partial S/\partial t = 0 \ , \tag{16}$$

$$p_l = \partial S/\partial l; \quad D = -\partial S/\partial E \ . \tag{17}$$

The solution of Eq. (16) is of the form

$$S(l,E,t) = \int dl\, \{2M_i(l)[E - V(l;p_x)]\}^{1/2} - Et \ ,$$

which with the explicit l dependences given by Eqs. (8) and (9) may be readily evaluated, hence enabling Eq. (17) for D to be explicitly solved for l. We obtain

$$l(t)/l_s(p_x) = E/E_s(p_x) - \{[E/E_s(p_x)]^2 - 1\}^{1/2} \times \sin[\Omega_i(p_x)(t - t_0)] \tag{18}$$

in which

$$\Omega_i(p_x) = (\omega_0/2\beta\alpha^{1/2})[1 + (p_x/M_s c_0)^2]^{1/2} \tag{19}$$

and where E may be identified as the total energy $E = H$ ($E \geq E_s$) and $t_0 = D$ a constant determined by the initial condition of motion.

The solution (18) of the nonlinear equation of motion (15) is somewhat remarkable. For arbitrary $E > E_s$ it describes harmonic motion about a center of oscillation $\langle l\rangle = l_s(p_x)E/E_s(p_x)$; the latter increases with increasing E whereas Ω_i is quite independent of E. In view of Eqs. (19) and (10), the characteristic frequencies Ω_i are, for $p_x = 0$,

$$\Omega_i(0) = \begin{cases} (12/\pi^2)^{1/2}\omega_0 \ \ (\mathrm{SG}) \ , & (20a) \\ [3/(\pi^2 - 6)]^{1/2}\omega_0 \simeq (\tfrac{3}{4})^{1/2}\omega_0 \ \ (\phi^4) \ . & (20b) \end{cases}$$

Since $l(t)$ is oscillatory it follows from Eq. (14) that the soliton's translational velocity $\dot{x}$ possesses an oscillatory component. The latter is superimposed on a mean constant translational velocity:

$$\langle\dot{x}\rangle = (p_x/M_s l_0)[l_s(p_x)E/E_s(p_x)] \ .$$

Thus in a state of constant translational momentum p_x and total constant total energy $E > E_s(p_x)$ the "free" motion of the soliton resembles that of a cross-country skier.

The Hamiltonian system of Eqs. (11)–(13), does not, of course, in general, correspond to an exact solution of the original SG or ϕ^4 field equation. Indeed, inserting the ansatz (6) directly into the field equations (2), one can see that only for uniform translational motion ($\dot{l} = 0$) is it an exact solution. We believe, however, that the picture it gives of the soliton as a deformable material particle whose translational motion is coupled to an internal degree of freedom may be useful in providing physical insight into the dynamical behavior of solitons subject to perturbation. For example, if a soliton is accelerated from rest by the application of an arbitrary external force F it is evident that in general F will excite internal kinetic energy ($\dot{l} \neq 0$). This will lead to a time dependence of the soliton's translational velocity which will not be simply that of a Newtonian particle, i.e., $x \propto t$. Recent numerical studies by Fernandez *et al.*[4] of the SG equation in the presence of an external force have revealed that (at least for certain times during their acceleration) SG solitons do not behave like Newtonian particles.

The internal kinetic energy of a translating soliton may also be excited either by a collision or, if the soliton is charged, by the absorption of electromagnetic energy ("discrete Drude absorption"[2]). Indeed, a resonance structure in ϕ^4 kink-antikink collisions has recently been explained by Campbell, Schoenfeld, and Wingate,[5] in terms of a resonant energy exchange between the translational and internal modes of the individual kinks. Further, as discussed in Ref. 2, for the charged soliton the oscillatory component endows the *mobile* soliton with an oscillatory electric dipole moment which is proportional to its mean translational velocity.

Finally, we note that very recently Segur[6] has shown that in ϕ^4 theory a "wobbling kink" solution, with behavior similar to that of the oscillating soliton found here, can be constructed by asymptotic expansion methods and can be proven to be close to an exact solution of ϕ^4 for reasonably long times. Also, for the SG equation, Segur[6] has shown that standard inverse scattering methods allow the construction of a solution which has the properties of an oscillating kink, although the stability of this solution is unclear.

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[5]D. K. Campbell, J. F. Schoenfeld, and C. A. Wingate, Los Alamos Report No. LA-UR-82 [Physica (in press)], and private communication. These authors use what they term a "linear-eigenfunction collective-coordinate approach "[see, e.g., T. Sugiyama, Prog. Theor. Phys. 61, 1550 (1979)]. This approach is based on the observation that when the ϕ^4 equation is linearized about a kink solution, there are *two* localized modes: one corresponding to the translation of the kink and one to an internal shape oscillation mode directly analgous to our internal degree of freedom. Note that for SG, *only the translation mode exists as a* localized mode in the linear expansion around the kink. Thus, for SG, there is no single *linear mode directly analogous to the internal degree of freedom in our* parametric collective-coordinate approach. The relation between the "linear-eigenfunction" and "parametric" collective-coordinate approach merits further investigation.
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