Scattering of the ϕ^4 **kink with an interface**

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We study the scattering of a kink at the interface of two ϕ^4 systems with different substrate potential barriers using collective coordinate method and a direct numerical simulation of the wave equation. During the scattering, it is found that the kink internal mode is excited and the kink emits reflected and transmitted small vibrational waves. For an incoming kink with already excited internal mode, the final velocity after the scattering depends on the amplitude and the phase of the initially existing mode. $[S1063-651X(98)02006-6]$

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I. INTRODUCTION

The study of the motion of topological Klein-Gordon solitons or kinks is one of the interesting problems in the modern theory of nonlinear waves. This is due to the fact that such waves ensure the transport of information in various fields of physics, such as dislocations in crystalline lattices $[1-3]$, atoms adsorbed on metal surfaces [4], domain walls in ferroelectric and ferromagnetic materials $[5-7]$, and fluxons in Josephson transmission lines [8].

During their motion, kinks interact with inhomogeneities of various types: localized impurities, spatial modulated and periodic impurities, localized thermal and stochastic noises, or disorders of several kinds. These inhomogeneities may give some special properties to the physical systems; e.g., the mechanical properties such as plastic deformation of crystals are particularly determined by the concentration of impurities $[3,9]$. It is also known that the nonlinear conductivity and the diffusion coefficient of one dimensional systems are accounted for by the action of impurities $[10,11]$.

In recent years, particular attention has been devoted to the study of the interaction of nonlinear waves with inhomogeneities. In general the kink can be either captured, reflected, or transmitted by the impurity with a distortion of its structure and a change of its dynamical behavior. In some cases the inhomogeneities can generate new degrees of freedom, such as the so-called impurity mode $[12-14]$ and can excite the kink internal mode $[14,15]$. This leads to a resonant interaction due to energy exchange mechanism between the kink, the impurity mode, and eventually the internal mode $[12-15]$. In the case of a spatially periodic parametric perturbation, the sine Gordon kink can propagate steadily and mostly undisturbed and can suffer the phenomenon of length scale competition [16]. For the ϕ^4 model, different types of kink behavior can be distinguished: radiation at high velocity, strong resonant beating and almost periodic behavior for intermediate velocities, and trapping at low velocity $|15|$.

In this paper we consider another type of situation with practical interest. We study the interaction of a ϕ^4 kink with an interface generated by an abrupt change of the substrate potential barrier. A similar problem was considered by Yamamoto for two sine Gordon systems with different dispersion coefficients $[17]$. We also mention the works done by Sakai, Samuelsen, and Olsen for kinks [18] and recently by Kenfack and Kofane^c for breathers [19] in Josephson transmission lines whose inductance is a spatially varying function having asymptotic values. It is worth mentioning that for other types of solitons such as envelope solitons of the nonlinear Schrödinger equation, the scattering with the mass interface has also been considered by several authors (see Ref. $[20]$, and references therein).

Section II of this paper contains the description of the problem and the collective coordinate method analysis. Section III deals with the direct numerical simulation of the scattering. It is found that the kink internal mode is excited by the interface and in the case of transmission (reflection) of the kink at the interface, reflected (transmitted) small vibrational waves are emitted. Some dynamical quantities of kink such as the final velocity after the interface and the critical velocity below which the kink is reflected by a repulsive interface are computed. When the kink internal mode does exist before the scattering, it is found that the final velocity depends on the amplitude of the initially existing mode. We give concluding remarks and discuss some physical applications of the model in Sec. IV.

II. PROBLEM AND THE COLLECTIVE COORDINATE METHOD

We consider an inhomogeneous ϕ^4 system with the Lagrangian

$$
L = \int dx \left[\frac{1}{2} (u_t^2 - u_x^2) - \frac{1}{4} [1 - \epsilon \theta(x)] (u^2 - 1)^2 \right], \quad (1)
$$

where $\theta(x)$ is the Heaviside step function defined by $\theta(x)$ $=0$ for $x < 0$ $\theta(x) = 1$ for $x \ge 0$. The integration in Eq. (1) is over the length (assumed infinite) of the system. The subscripts *t* and *x* denote, respectively, the time and spatial derivatives. ϵ is a small parameter which characterizes the interface. For $x \le 0$, the barrier of the substrate potential is 0.25 while for $x \ge 0$, it is equal to $0.25(1-\epsilon)$. The equation of motion of the spatiotemporal field $u(x,t)$ is

$$
u_{tt} - u_{xx} + [1 - \epsilon \theta(x)](u^3 - u) = 0.
$$
 (2)

When $\epsilon=0$, Eq. (2) supports the propagation of a topological soliton, the so-called kink given by

FIG. 1. (a) Amplitude $A(\tau)$ of the excited internal mode in the case of transmission of kink through the interface (solid line for ϵ = -0.2 and dashed line with squares for ϵ =0.2) with V_i =0.5. (b) $A(\tau)$ in the case of reflection of kink by the interface (ϵ = -0.5 and $V_i = 0.5$).

$$
u_k = \tanh\left[\frac{\gamma[x - X(t)]}{\sqrt{2}}\right],\tag{3}
$$

where $\gamma = (1 - V^2)^{-1/2}$ is the Lorentz contraction factor, *V* being the constant velocity. $X(t) = Vt$ is the kink coordinate. Linearizing Eq. (2) around the kink structure (with $\epsilon=0$), one obtains an eigenvalue problem which has two discrete modes and a continuum spectrum $[5,21]$. The discrete modes correspond to the translation mode with an angular frequency $w=0$ and to localized deformations or internal oscillations of the kink shape. This last mode is defined by

$$
y_2 = A_0 \exp(i\omega_2 \tau) f_2(z), \tag{4a}
$$

with $\omega_2 = \sqrt{3}/2$ and A_0 being a constant. The corresponding eigenfunction is

$$
f_2(z) = \left[\frac{9}{8}\right]^{1/4} \tanh\left[\frac{z}{\sqrt{2}}\right] \sech\left[\frac{z}{\sqrt{2}}\right],\tag{4b}
$$

where τ and *z* are moving coordinates defined by $z = \gamma(x)$ $-vt)$ and $\tau = \gamma(t-vx)$.

When the kink approaches the interface, its motion loses its translational invariance. The kink velocity becomes a time dependent function. Moreover, it is seen, after the numerical simulations, that the interface excites the kink internal mode as in the case of a pointlike impurity $[13,14]$ or a spatially periodic parametric perturbation [15]. Thus, to give a tentative analytical description of the dynamics of kink colliding with the interface, we use the following collective coordinate ansatz:

$$
u(z,\tau) = \tanh[z - Z_0(\tau)] + y_2(\tau),
$$
 (5a)

where

$$
y_2(\tau) = A(\tau) f_2(z - Z_0(\tau)).
$$
 (5b)

 $Z_0(\tau)$ and $A(\tau)$ are two unknown dynamical variables. Their equations of motion are obtained through the effective La-

FIG. 2. Kink final velocity V_f after the interface as a function of ϵ for $V_i=0.5$: Solid line for the principle of conservation of energy without the excitation of the internal mode, dashed line with squares for the collective coordinate equations, and crosses for the direct numerical simulation.

grangian approach which has been recognized to be very useful for studying the kink dynamics [13–15]. Once $Z_0(\tau)$ has been obtained, the coordinate $X(t)$ of the kink center in the original (x,t) reference frame can be obtained by reversing the Lorentz transformation $Z_0(\tau) = \gamma[X(t)-Vt]$. Let us note that one could also tackle the problem by the perturbative method of Fogel *et al.* [22].

Inserting the ansatz (5) in the Lagrangian (1) , we obtain the effective Lagrangian

$$
L = \frac{1}{2} M_k \dot{Z}_0^2 + \frac{1}{2} [\dot{A}^2 - \omega_2^2 A^2] + \frac{\epsilon}{4} [2 + \text{sech}^2 Z_1 \tanh Z_1
$$

+ 2 tanh Z₁] - $\epsilon \sqrt{2} \left[\frac{9}{8} \right]^{1/4} \left[-\frac{1}{4} \text{ sech}^3 Z_1 \tanh Z_1$
+ $\frac{1}{8} \text{ sech } Z_1 \tanh Z_1 - \frac{1}{4} \arctan[\text{exp}(-z_1)] + \frac{\pi}{8} \right] A,$ (6)

where $Z_1 = (Z_0 + V\tau)/\sqrt{2}$ and the dot refers to the derivative with respect to τ . $M_k = 2\sqrt{2}/3$ is the kink mass. The equations of motion for the collective coordinates $Z(\tau)$ and $A(\tau)$ derived from the Lagrangian (6) are

$$
M_k \ddot{Z}_0 = \frac{\epsilon}{4} \operatorname{sech}^4 Z_1 - \epsilon \left[\frac{9}{8} \right]^{1/4} \left(-\operatorname{sech}^5 Z_1 + \operatorname{sech}^3 Z_1 - \frac{1}{4} \operatorname{sech} Z_1 \right) A, \tag{7a}
$$

$$
\ddot{A} + \omega_2^2 A = -\frac{\sqrt{2}}{4} \left[\frac{9}{8} \right]^{1/4} \epsilon \left(-\operatorname{sech}^3 Z_1 \tanh Z_1 + \frac{1}{2} \operatorname{sech} Z_1 \tanh Z_1 - \operatorname{arctan}[\exp(-Z_1)] + \frac{\pi}{2} \right).
$$
\n(7b)

In the course of analyzing Eqs. (7) , let us first assume that the effects of the internal mode are negligible. One can therefore use the principle of conservation of energy to establish that the kink final velocity V_f , far after the interface, is given by the relation

$$
V_f^2 = V_i^2 + \epsilon,\tag{8}
$$

where V_i is the kink initial velocity (far before the interface). Thus for negative ϵ or repulsive interface (positive ϵ or attractive interface) the kink velocity decreases (increases) after it has passed through the interface.

Let us now consider Eq. $(7b)$, which is similar to the equation of a harmonic oscillator with an external pulse force. As the kink moves towards the interface, its internal mode is excited and two possible outcomes can be obtained: reflection and transmission. In the case of reflection, the external pulse force of Eq. $(7b)$ reduces to zero (as $Z_1 \rightarrow -\infty$) but after having set the oscillator *A*(τ) in motion [see Fig. 1(b)]. We may, however, note that depending on the value of ϵ , the soliton needs a sufficient velocity to come close to the interface. Otherwise its reflection occurs at a distance (before the interface) where the value of the pulse force is nearly zero. In this case, the internal mode is not or is slightly excited. When the kink passes through the interface, the external pulse force gradually tends to a constant and the amplitude $A(\tau)$ of the internal mode has the analytical form

$$
A(\tau) = -\frac{\sqrt{2}}{12} \left[\frac{9}{8} \right]^{1/4} \epsilon [1 - \cos(\omega_2 \tau)]. \tag{9}
$$

We have solved numerically the set of equations (7) assuming first that the internal mode does not exist before the scattering. The main aim was to find the kink final velocity after the interaction with the interface, the critical velocity under which the kink is reflected by the interface, and the time evolution of $A(\tau)$. As concerns the above mentioned velocities, the results are reported in Figs. 2, 5, and 6 with the results of a direct numerical simulation (see Sec. III). We report in Fig. 1 the time variations of the amplitude $A(\tau)$ of the excited internal mode in the following cases: transmission with positive ϵ , transmission with negative ϵ , and reflection with negative ϵ . In the case of transmission, $A(\tau)$ varies 1036 P. WOAFO P. WOAFO P. WOAFO P. WOAFO P. WORK ISSNESS

FIG. 3. Excited internal mode y_2 for $V_i = 0.5$ with $\epsilon = 0.2$ (solid line) and $\epsilon = -0.2$ (squares) obtained when the kink is at $X = 12$ after the interface.

around a negative (positive) value for $\epsilon > 0$ ($\epsilon < 0$). In the case of reflection, $A(\tau)$ oscillates around the τ axis.

III. DIRECT NUMERICAL SIMULATION

We have solved the wave equation (2) with the fourth order Runge-Kutta algorithm [23]. The accuracy of the numerical calculation is tested (for the homogeneous system) using the fact that the energy of the system should remain constant during the computation. The length of the system is equal to 70 $[-35$ to 35] with discrete step sizes $\Delta x = 0.1$ and Δt =0.05. Some dissipation is imposed on the last 20 spatial steps at each end of the system to prevent end effects. At the position $x=n \Delta x$ (*n* being an integer) of the system, the displacement field is defined by $u_n(t)$. The initial conditions for the displacement $u(x,t)$ and velocity $u_t(x,t)$ are

$$
u(x,t) = \tanh\left[\frac{\gamma(x - X_0)}{\sqrt{2}}\right],\tag{10a}
$$

$$
u_t(x,t) = -\frac{\gamma V_i}{\sqrt{2}} \operatorname{sech}^2 \left[\frac{\gamma(x - X_0)}{\sqrt{2}} \right],\tag{10b}
$$

where X_0 $(X_0 = -5$ in our study) and V_i are, respectively, the kink initial coordinate and velocity. The interface is located at $x=0$. During the numerical simulation, we compute the kink center by the interpolation

$$
X(t) = \left[\frac{-u_n(t)}{u_{n+1}(t) - u_n(t)} + n \right] \Delta x, \tag{11}
$$

where $u_n(t)$ <0 and $u_{n+1}(t)$ >0. The kink velocity follows the simple differentiation

$$
V(t) = \frac{X(t + \Delta t) - X(t)}{\Delta t}.
$$
 (12)

The results of the numerical simulation are the following. For an attractive interface, the kink velocity increases after the interface and finally attains a final constant value which increases with ϵ and V_i (see Fig. 2). As it appears in this figure, the values of V_f obtained from the collective coordinate equations (7) and from the direct numerical simulation are lower than that predicted by the principle of conservation of energy (without including the excitation of internal mode). This is due to the excitation of the kink internal mode, but also to the reflection of small vibrational waves at the interface. The excited internal mode obtained from the numerical simulation of the wave equation (2) is reported in Fig. 3 for two values of ϵ and for a kink at the distance $X \approx 12$ after the interface. The shape and the amplitude of the internal mode

FIG. 4. Time dependent behavior of the displacement at the lattice point $n=-20$ for V_i = 0.5 with ϵ = 0.3 (solid line) and ϵ = 0.6 (dashed with squares).

FIG. 5. Critical velocity V_C below which the kink is reflected by the interface as a function of ϵ : collective coordinate method (dashed with crosses), numerical simulation (dashed with squares).

are consistent with the results of the collective coordinate method (showing the effects of the type of the interface; note also that the amplitude of the internal mode increases with the strength ϵ of the interface).

In Fig. 2 a divergence also appears between the results of the collective coordinate method and that of the direct numerical simulation when ϵ increases (V_f from the numerical simulation being lower than that of the collective coordinate method). Besides the fact that the collective coordinate method is limited in its capacity to account quantitatively for the results of the numerical simulation when ϵ increases, an explanation of the divergence is due to the fact that during the collision, the kink loses a part of its energy to generate reflected waves. Indeed, after the incident kink collides with the interface, it emits small vibrational reflected waves (see Fig. 4). With an increase of ϵ or of the initial velocity, the amplitude of the reflected waves increases and the corresponding energy also increases.

For a repulsive interface, we have been particularly interested by the evaluation of the critical velocity V_C below which the kink is reflected by the interface. The results are reported in Fig. 5. As can be expected, V_C increases with $|\epsilon|$. We have found here that after the reflection of the kink, small vibrational waves are transmitted through the interface and with a sufficient initial velocity, the kink goes back with its internal mode excited.

We have also considered the case where the kink internal mode is excited prior to the scattering [this is done in the collective coordinate equations by setting $A_0 = A(0)$ different from zero and for the direct numerical simulation by adding to the initial conditions (10) term $y_2(t)$ $=$ *A*₀cos($\omega_2 t$) $f(\gamma(x - X_0)/\sqrt{2})$ and the corresponding time derivative. The simulation shows that the kink final velocity decreases as A_0 moves from negative to positive values (Fig. 6!. Another interesting point is the role that the phase of the internal mode plays during the scattering. By adding a phase θ in the cosine factor of the above expression of y_2 , the direct numerical simulation indicates that the kink final velocity is a function of θ . Although the form of the function

FIG. 6. Kink final velocity after the interface as a function of the amplitude of the initially excited internal mode for $\epsilon = 0.5$ and V_i $=0.20$: collective coordinate method (dash with crosses), direct numerical simulation (dashed with squares).

 $V_f(\theta)$ depends on the value of A_0 , it is found that for each A_0 , $V_f(\theta)$ varies around $V_f(0)$ as θ sweeps the range 0 to 2π .

IV. CONCLUDING REMARKS AND SOME PHYSICAL IMPLICATIONS

We have studied analytically and numerically the collision of the ϕ^4 kink with an interface. The analytic treatment uses the collective coordinate method which takes into account the kink coordinate and the amplitude of the internal mode of the ϕ^4 kink. The results obtained show the excitation of the kink internal mode and the emission of reflected or transmitted small vibrational waves. The interaction between these generated excitations and the kink explains the energy lost during the scattering. The kink final velocity after the interface and the critical velocity below which the kink is reflected by the interface have been computed as functions ϵ . The study also shows that the final velocity depends on the initial amplitude and the initial phase of the kink internal mode (when we consider an excited kink before the scattering).

We have limited ourselves to the interface with different strengths of substrate potential barriers. However, one can extend the study to the case of two ϕ^4 systems with different masses or different dispersion coefficients.

We think it will be possible to apply the results obtained here in general to various mesoscopic condensed matter systems in which kink solitons play an important role $[24]$. In particular, our results can be applied to devices made by a junction of two ferroelectric materials such as lead germanate and antimony sulphoiodide whose technological properties are well known $[25,26]$. Moreover, our work can shed some light on the study of the dynamics of domain walls separating two coexisting phases in symmetric binary systems or in ferroelectric materials (see Ref. $[27]$ for symmetric binary systems). Indeed, for such systems, the substrate potential has the general form $V(u) = (A^2/4B)[1]$ $-(B/A)u^2$ ² where *A* > 0 is a temperature dependent coefficient [e.g., $A(T) = \alpha(T - T_c)$ where T_c is the Curie temperature] and *B* is a constant. If we assume the ratio B/A to be constant (this assumption is always consistent in the above quoted ferroelectric materials), then our study is comparable to the physical situation where, as a result of a temperature gradient, the value of *A* is changed from a certain point of the physical system. We must note, however, that in various ferroelectric materials, we should take into account the discreteness effects $[26]$.

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