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Resonant Soliton-Impurity Interactions

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We describe a new type of soliton-impurity interaction and demonstrate that the soliton can be totally *reflected by an attractive impurity* if its initial velocity lies in certain resonance "windows." This effect has an analogy with the resonance phenomena in kink-antikink collisions [Campbell, Schonfeld, and Wingate, Physica (Amsterdam) **9D**, 1 (1983)], and it can be explained by a resonant energy exchange between the soliton and the impurity mode. Taking the sine-Gordon and ϕ^4 models as examples, we find a number of resonance windows by numerical simulations and develop a collective-coordinate approach to describe the effect analytically.

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Wave propagation in nonlinear disordered media has become an extensively studied subject in recent years [1]. It is known that nonlinearity may drastically change transport properties of disordered systems when it contributes to create solitons (see e.g., Refs. [2] and [3], and references therein). As a first step to understand soliton transmission through disordered media, one has to study soliton scattering by a single impurity. The properties of such a process depend on the type of soliton [2], but generally, they can be explained by a simple model in which a soliton moving in an inhomogeneous medium is considered as an effective particle, the soliton position being the particle coordinate [4-6]. In this approach, the only effect of the impurity is to give rise to an effective potential on the particle. In particular, a soliton may be trapped by an attractive impurity due to loss of its kinetic energy through radiation [6]. However, the impurity is not a "hard" object, and it may support a localized oscillating state, the so-called impurity mode (see, e.g., Refs. [7] and [8], and references therein). As a consequence, a soliton may excite the impurity mode, transferring part of its kinetic energy to the impurity, and the interaction will be inelastic [7]. The purpose of this Letter is to describe numerically and analytically a *new type* of interaction between a soliton and an impurity when the impurity supports a localized impurity mode. We demonstrate that the soliton can be totally *reflected* by an *attractive* impurity if its initial velocity lies in certain resonance "windows." This effect is quite similar to the resonance phenomena in kink-antikink interactions [9-12], and it can also be explained by the resonant energy exchange mechanism proposed by Campbell, Schonfeld, and Wingate [9]. In the framework of the sine-Gordon and ϕ^4 models, we find a number of resonance windows and develop a collective-coordinate approach to describe the resonant interactions. We believe that the resonant effects studied in this Letter may be observed in other nonlinear systems which support soliton excitations, e.g., in hydrogen-bonded chains when ionic or bonded defects interact with localized inhomogeneities (see, e.g., Ref. [13]).

To analyze an example of such a resonant interaction, let us consider the well-known sine-Gordon (SG) model including a local impurity,

$$u_{tt} - u_{xx} + \sin u = \epsilon\delta(x)\sin u\,, \tag{1}$$

where $\delta(x)$ is the Dirac δ function. When the perturbation is absent ($\epsilon=0$) the SG model supports undistorted propagation of a topological soliton, the so-called kink, which is given by

$$u_k = 4\tan^{-1}\exp\{[x - X(t)]/(1-V^2)^{1/2}\}\,, \tag{2}$$

where $X = Vt$ is the kink coordinate and $V = \dot{X}$ is its velocity. For $\epsilon > 0$, the impurity in Eq. (1) creates an effective attractive potential well for the kink. Previous analytical considerations of this problem, taking into account only

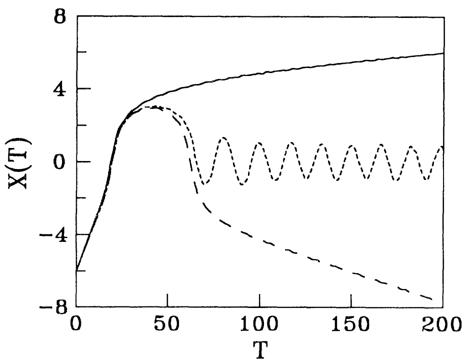

FIG. 1. The kink coordinate $X(t)$ vs time for initial velocities V_i situated in three different regions: the region of pass (solid line, $V_i=0.268$), of capture (dotted line, $V_i=0.257$), and of reflection (dashed line, $V_i=0.255$).

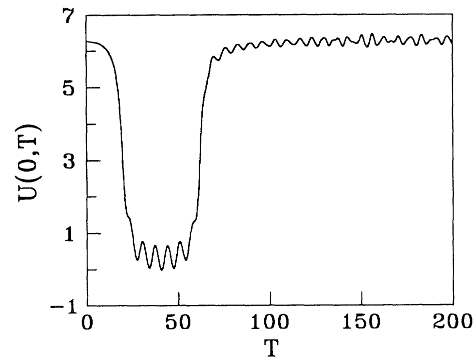

FIG. 2. $u(0,t)$ vs time in the case of resonance ($V_i=0.255$). Note that between the two interactions there are four small bumps which show the impurity mode oscillation, and after the second interaction the energy of the impurity mode is resonantly transferred back to the kink.

radiation losses (see Ref. [6], p. 841), demonstrate that the threshold velocity for the kink capture is exponentially small in ϵ, and that the scattering may be described by a simple model of a particle moving in an attractive potential $U(X)=-2\epsilon/\cosh^2 X$. Such a consideration suggests that the kink will either pass the impurity or be captured, and that reflection of the kink is impossible.

We have studied the kink scattering by a pointlike impurity numerically, using a conservative numerical scheme to integrate Eq. (1) [14]. The simulations are performed in the spatial interval $(-40,40)$ with discrete step sizes $\Delta x=2\Delta t=0.04$. When handling the Dirac δ function, we take its value to be equal to $1/\Delta x$ at $x=0$, and zero otherwise. The initial conditions are always taken as a kink centered at $X=-6$, moving toward the impurity with a given velocity $V_i>0$. Fixed boundary conditions are used: $u(-40)=0$ and $u(40)=2\pi$. Here we are only interested in the attractive impurity, i.e., $\epsilon>0$, because in the opposite case the possible resonance phenomena are not likely to exist. We have made intensive numerical simulations of the problem, and here we will describe the results for the case $\epsilon=0.7$ in detail.

In the numerical simulations, we find that there are three different regions of initial kink incoming velocity, namely, pass, capture, and reflection (see Fig. 1), and a critical velocity $V_c\approx 0.2678$ (for $\epsilon=0.7$) exists, such that if the incoming velocity of the kink is larger than V_c, the kink will pass the impurity inelastically and escape to the positive direction, losing part of its kinetic energy through radiation and excitation of an impurity mode. In this case, there is a linear relationship between the squares of the incoming velocity V_i and the final velocity V_f: $V_f^2=\alpha(V_i^2-V_c^2)$, α being constant ($\alpha\approx 0.887$ for $\epsilon=0.7$).

If the incoming velocity of the kink is smaller than V_c, the kink cannot escape to infinity from the impurity after the first interaction, but will stop at a certain distance and return back, due to the attracting force of the impurity, to interact with the impurity again. For most of the velocities, the kink will lose energy again in the second interaction and finally get trapped by the impurity (see Fig. 1). However, for some special incoming velocities, the kink may escape to *negative* infinity after the second interaction, i.e., the kink may be totally *reflected* by the impurity (see Figs. 1 and 2). This effect is quite similar to the so-called resonance phenomena in kink-antikink collisions [9–12]. The reflection of the kink is possible only if the initial kink velocity is situated in some resonance windows. By numerical simulation, we have found *eleven* such windows. The detailed results are presented in Table I and Fig. 3.

In order to understand the resonance structure, we define the center of the kink, $X(t)$, as the point at which the field function $u(x,t)$ is equal to π. The final velocity

TABLE I. Centers of the resonance windows predicted by Eq. (5), where $T=2\pi/\Omega\approx 6.707$ is determined by Eq. (7) for $\epsilon=0.7$. Numerical $T_{12}(V_N)$ is defined as the time between the first and the second interactions. Note that $T_{12}(V_{n+1})-T_{12}(V_n)\approx 6.7$ is just another expression of the resonance condition (4). The resonance windows determined by numerical simulations are in very good agreement with the theoretical predictions.

n	V_n predicted by Eq. (5)	Numerical $T_{12}(V_n)$	Resonance windows
6	0.25498	42.5	(0.2548, 0.25505)
7	0.25842	49.2	(0.25825, 0.2585)
8	0.26064	56.2	(0.2605, 0.2607)
9	0.26215	62.8	(0.26205, 0.26222)
10	0.26323	69.5	(0.26315, 0.26327)
11	0.26403	75.9	(0.26395, 0.26408)
12	0.26463	82.8	(0.26461, 0.264635)
13	0.26510	89.6	(0.26510, 0.26512)
14	0.26547	97.1	(0.26546, 0.26547)
15	0.26577	103.3	(0.26577, 0.26579)
16	0.26602	109.9	(0.26600, 0.26602)

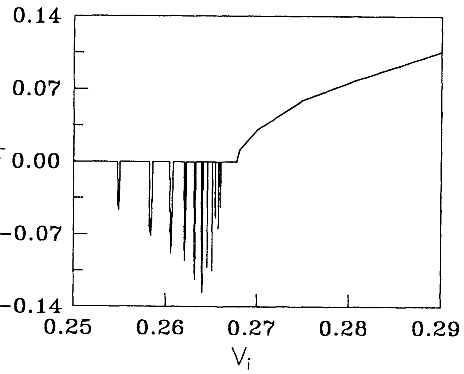

FIG. 3. Final kink velocity as a function of the initial kink velocity ($\epsilon=0.7$). Zero final velocity means that the kink is captured by the impurity.

is averaged over a period of 20 time units. We define T_{12} as the time between the first and the second interaction; more precisely, T_{12} is the time difference between the first two instants at which the center of the kink is just at the impurity. It is clear that the attractive potential caused by the impurity falls off exponentially, so that using the same arguments as in Ref. [9] [see Eq. (3.6)], we obtain an approximate formula to estimate $T_{12}(V)$,

$$T_{12}(V)=\frac{a}{(V_c^2-V^2)^{1/2}}+b\,, \tag{3}$$

where V is the kink initial velocity, a and b are two constants. For $\epsilon=0.7$, the parameters are empirically determined by numerical data: $a\approx 3.31893$, $b\approx 1.93$. We have found that the formula (3) is very accurate for the velocities over the interval (0.12,0.267).

On the other hand, we have observed that the first kink-impurity interaction always results in exciting the impurity mode, and the resonant reflection of the kink after the second interaction is just the reverse process, i.e., to extinguish the impurity mode (see Fig. 2), when the timing is right, to restore enough of the lost kinetic energy, and to escape from the impurity to infinity. Favorable timing in this case means that the occasion of the second interaction coincides with the passage of the impurity oscillation through some phase angle characteristic of the impurity mode extinction. Thus the condition for restoration of the kink kinetic energy after the second interaction ought to be of the form

$$T_{12}(V)=nT+\tau\,, \tag{4}$$

where T_{12} is the time between the first and the second interaction, T is the period of the impurity mode oscillation, τ is an offset phase, and n is an integer. By numerical simulation we find that $\tau\approx 2.3$ for the case $\epsilon=0.7$.

Combining Eqs. (3) and (4), we may obtain a formula to predict the centers of the resonance windows,

$$V_n^2=V_c^2-\frac{11.0153}{(nT+0.3)^2},\quad n=2,3,\ldots. \tag{5}$$

Similar formulas have been derived for kink-antikink collisions [9–11]. From Table I, we see that this formula can give a very good estimation of the resonance windows.

However, we have not found resonance windows corresponding to the index $n=2,3,4,5$; instead, quasiresonances have been observed when the initial kink velocity is close to one of those predicted velocities: The second interaction causes the kink to move even further away from the impurity. Disappearance of these lower-order resonance windows may be explained by radiation effects during the interactions, because if the initial kink velocity is small, it cannot restore enough energy for escape from the attractive impurity. Higher-order resonances ($n>16$) are also possible, but they are very narrow, so we have not tried to detect them.

To describe the resonant effects theoretically, first of all we note that the attractive impurity ($\epsilon>0$) supports a localized oscillating state, the impurity mode

$$u_{\rm im}(x,t)=a(t)e^{-\epsilon|x|/2} \tag{6}$$

where $a(t)=a_0\cos(\Omega t+\theta_0)$, Ω is the frequency of the impurity mode,

$$\Omega=(1-\epsilon^2/4)^{1/2}\,, \tag{7}$$

and θ_0 is a constant phase.

We shall analyze the kink-impurity interaction by the so-called collective-coordinate approach taking into account two dynamical variables: the kink center $X(t)$ and the amplitude of the impurity mode oscillation $a(t)$. Substituting the ansatz $u=u_k+u_{\rm im}$ into the Lagrangian

$$L=\int_{-\infty}^{\infty}dx\{\tfrac{1}{2}u_t^2-\tfrac{1}{2}u_x^2-[1-\epsilon\delta(x)](1-\cos u)\}\,, \tag{8}$$

in the lowest-order approximation, when the kink may be considered as nonrelativistic ($V^2\ll 1$), and it is assuming that $a\ll\epsilon$ and $a\ll 1$, we derive the following effective Lagrangian:

$$L_{\rm eff}=4\dot{X}^2+\epsilon^{-1}(\dot{a}^2-\Omega^2a^2)-U(X)-aF(X)\,, \tag{9}$$

where $U(X)=-2\epsilon/\cosh^2X$, $F(X)=-2\epsilon\sinh X/\cosh^2X$, and Ω is defined in Eq. (7). The corresponding equations of motion for the two dynamical variables are

$$\begin{aligned}&8\ddot{X}+U'(X)+aF'(X)=0\,,\\&\ddot{a}+\Omega^2a+(\epsilon/2)F(X)=0\,.\end{aligned} \tag{10}$$

The system (10) describes a particle with the coordinate $X(t)$ and mass 8 placed in the attractive potential $U(X)$, and coupled with the harmonic oscillator $a(t)$. We have solved Eqs. (10) numerically with initial conditions $X(0)=-6$, $\dot{X}(0)=V_i$; $a(0)=0$, $\dot{a}(0)=0$, and indeed we have observed similar resonance phenomena. In particular, for $\epsilon=0.7$, we find that there exists a critical velocity $V_c=0.3546$ above which the particle (kink) will pass the potential well and escape to $+\infty$, transferring part of its kinetic energy to the harmonic oscillator (the impurity mode). Below the critical velocity the particle cannot escape after the first interaction and will return back to interact with the oscillator again. The particle may be resonantly reflected to $-\infty$ after the second interaction if its initial velocity lies in certain resonance windows. In fact, we find that system (10) possesses a very rich resonance structure, and it is quite similar to the dynamical system that arises in the phenomenological collective-coordinate analysis of kink-antikink collisions in some nonlinear Klein-Gordon equations [12].

Finally, we would like to point out that we have observed similar resonance phenomena for the kink-impurity interactions in the ϕ^4 model, $\phi_{tt} - \phi_{xx} - [1 - \epsilon\delta(x)](\phi - \phi^3) = 0$. The inelastic interaction of kink with an impurity was first discussed by Belova and Kudryavtsev [15]. However, they totally ignored the impurity mode, and tried to explain the resonance effects by energy exchange between the kink translational mode and its internal mode. We have studied the ϕ^4 kink-impurity interactions by intensive numerical simulation and found that both the internal mode and the impurity mode take part in the resonant interactions [16]. For example, at $\epsilon = 0.5$ we have found *six* resonance windows below the critical velocity $V_c \approx 0.185$. We have observed that the resonance structure in the ϕ^4 kink-impurity interactions is more complicated than in the SG model because the ϕ^4 kink has an internal mode which also can be considered as an effective oscillator. We have developed a collective-coordinate approach taking into account *three* dynamical variables, and the detailed results will be reported elsewhere [16].

In conclusion, we have described a new type of soliton-impurity interaction when the impurity supports a localized mode. In particular, we have demonstrated that the soliton can be totally reflected by an attractive impurity if its initial velocity is situated in certain resonance windows. These resonance phenomena can be explained by the mechanism of resonant energy exchange between the kink translational mode and the impurity mode. We believe that the similar resonance phenomena might be observed in other nonlinear systems supporting soliton excitations.

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