Resonant kink-impurity interactions in the sine-Gordon model

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We present results concerning kink-impurity interactions in the sine-Gordon (SG) model. In particular, we demonstrate that the SG kink may be totally reflected by an *attractive* impurity if its initial velocity is in some resonance windows. This effect can be predicted by a suitable collective-coordinate method, and the resonance structures can be explained with an energy exchange between the kink translational mode and the impurity mode. We also study the scattering of the kink by an excited impurity and show that such a scattering strongly depends on the amplitude and phase of the impurity mode. In particular, resonance phenomena are also observed in the scattering. In addition, we consider the interactions of the kink with an isotopic (heavy-mass) impurity. We demonstrate that if the impurity mass is not too large in comparison with the standard mass in the SG model, the kink can pass the impurity almost freely at any initial velocity. However, if the impurity mass is large enough, a higher-velocity kink will be reflected while a lower-velocity kink will pass. We explain this effect analytically and show that the impurity mode plays an important role in the scattering. In all the cases considered we find good agreements between the collective-coordinate analysis and the direct numerical simulations.

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I. INTRODUCTION

In recent years, wave propagation through inhomogeneous and disordered media has attracted increasing attention [1–4]. One central issue is how nonlinearity can qualitatively modify the effects of disorder on transport properties, and conversely, how disorder may change the steady-state motion of solitons in nonlinear systems. Now it is generally recognized that nonlinearity can significantly improve the transport properties when it contributes to create soliton pulses. Being more robust than linear waves or wave packets, solitons can give a nonzero contribution to the transmission coefficient of a disordered medium. In particular, it has been demonstrated that the transmission coefficient in the case of dynamical solitons decays according to a power law (see Refs. [4, 5], and references therein) instead of an exponential law, as the Anderson localization shows in *linear* disordered systems. Moreover, an envelope soliton described by the nonlinear Schrödinger equation can propagate almost freely (with very little radiation) if its amplitude reaches over a certain threshold value [4, 6]. Recently, the kink dynamics in the stochastically perturbed sine-Gordon and ϕ^4 models has also been studied extensively (see, e.g., Refs. [7–11]).

To gain a deeper understanding of the behavior of nonlinear excitations in disordered systems, one has to investigate the interactions of solitons with separate localized inhomogeneities (impurities). Such impurities break the translational invariance of the original unperturbed system, so the solitons can no longer propagate with a constant velocity and/or a constant amplitude because a general effect in the soliton scattering by local impurities is energy loss through radiation (see, e.g., [12–26]). Furthermore, the impurity may frequently give rise to an effective potential (attractive or repulsive) to a soliton; thus the soliton can be either captured or reflected by the impurity (see, e.g., Ref. [18]).

In some cases a pointlike impurity can allow the system to support a localized excitation even in the framework of the linear theory, the so-called *impurity mode* (see, e.g., [12, 13, 16, 19, 20]). The impurity mode may be easily excited during the soliton scattering and has a long lifetime [19, 23–25]. Most importantly, due to the energy exchange between a soliton and an impurity mode, the soliton can be totally reflected by an *attractive* impurity [23]. As was mentioned in our previous paper [23], this effect is quite similar to the resonance phenomena previously observed in the kink-antikink collisions in some nonlinear Klein-Gordon equations [27–31].

There are a number of papers discussing the kink-impurity interactions in the framework of the sine-Gordon model (see, e.g., Refs. [14, 15, 17, 18, 20, 23, 24, 26], and references therein). Most of the earlier studies are related to the fluxon dynamics in the presence of local inhomogeneities (microshunts and microresistors) in long Josephson junctions, where the inhomogeneities are installed into the junction during fabrication (see, e.g., Ref. [32]). Recently, Braun and Kivshar [20] have considered the Frenkel-Kontorova (FK) model, including different types of impurities, where the continuum limit of the FK model is nothing more than the sine-Gordon (SG) equation.

In this paper we present our results concerning the kink-impurity interactions in the SG model and describe the complete "two-bounce" resonance structures in the interactions. Our main goal is to study the resonance effects from *different perspectives*. First, we investigate the mass impurity in addition to the substrate impurity. We show that the both types of impurities can support local-

ized modes in the system, which are found to be responsible for resonances. Second, we analyze the kink-impurity interactions by the collective-coordinate method, taking into account two dynamical variables: the kink coordinate and the amplitude of the impurity-mode oscillation. This approach allows us to calculate the threshold velocity of the kink capture analytically, and, in particular, it can help to understand *why* and *how* the resonance phenomena may occur in the kink-impurity interactions. Third, we report our direct simulation results of the kink-impurity interactions and demonstrate that the ϵ, V_i plane (V_i being the kink initial velocity, and ϵ the impurity strength) can be divided into three different regions: the region of kink pass, the region of kink capture, and the region of coexistence of capture and resonant reflection. Fourth, we study, for the first time, the scattering of a kink by an *excited* impurity. Such a scattering naturally depends not only on the initial velocity of the kink but also on the initial amplitude and phase of the impurity mode. In particular, we demonstrate that the resonance effects still exist in such a type of scattering. Finally, we study analytically and numerically the kink scattering by a mass impurity in the SG model. We find that, if the mass ratio is less than a certain value, then the kink with any velocity can pass; however, for a given heavy-mass impurity with a larger ratio, a lower-velocity kink can pass the impurity, but a high-velocity kink will be *reflected* by the impurity. We point out that this effect may be easily explained with the help of a suitable collective-coordinate method that takes into account excitations of the impurity mode. A similar problem was considered by Fraggis, Pnevmatikos, and Economou [19] for the ϕ^4 chain but they did not provide an analytical explanation of the effects observed numerically.

The paper is organized as follows. In Sec. II we present the model and describe the properties of the impurity mode that is a localized excitation at the impurity site. In Sec. III we analyze the interactions of the kink with the substrate impurity by the collective-coordinate approach and calculate the threshold velocity for the kink capture. We show how to predict resonance phenomena in the framework of the collective-coordinate dynamical system. In Sec. IV we report our direct numerical simulation results and demonstrate that below the threshold velocity a SG kink is not necessarily going to be captured by the impurity, instead it still may escape from the impurity *if* its initial velocity lies in certain resonance windows. In Sec. V we discuss the scattering of the kink by an excited impurity. Section VI is devoted to a detailed study of the kink scattering by an isotopic (heavy-mass) impurity. Using the collective-coordinate analysis we explain why a higher-velocity kink can be reflected by the mass impurity, while a lower-velocity kink may pass it almost freely. Finally, in Sec. VII we conclude our paper with some remarks.

II. MODEL AND IMPURITY MODES

We consider the SG model including a localized inhomogeneity (impurity), which is given by the equation

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

When the perturbation is absent ($\epsilon = 0$), the SG model supports a topological soliton, the so-called kink,

$$u_k(x,t) = u_k(z) = 4\tan^{-1}\exp(\sigma z), \tag{2}$$

where $z = (x - X)/\sqrt{1 - V^2}$, $X = Vt + X_0$ is the kink coordinate, V is its velocity, and $\sigma = \pm 1$ is the kink polarity (without loss of generality we assume that $\sigma = +1$ below).

Now let us consider the SG model (1) with a substrate impurity, i.e., $P(u) = \sin u$. For $\epsilon > 0$, the system supports a localized impurity mode (see, e.g., Ref. [23]). To show this, we linearize Eq. (1) around its ground state $u = 0$, and obtain the equation

$$u_{tt} - u_{xx} + [1 - \epsilon\delta(x)]u = 0, \tag{3}$$

which has a localized oscillating mode

$$u_{im}(x,t) = a(t)e^{-\epsilon|x|/2}, \tag{4}$$

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

$$\Omega = \sqrt{1 - \epsilon^2/4}, \tag{5}$$

and θ_0 an initial phase. Note that the impurity mode [Eqs. (4) and (5)] exists if and only if $\epsilon > 0$ (the so-called *attractive* impurity). As follows from Eq. (4), the impurity mode is periodic in time and localized in space (it falls off exponentially). In nonlinear systems the impurity mode also exists and it may be described as a small-amplitude breather captured by the impurity (see, e.g., Refs. [20, 33]). The energy stored in the impurity mode (4) may be easily calculated as

$$E_{im} = \frac{1}{2}\int_{-\infty}^{\infty} dx\left[\left(\frac{\partial u_{im}}{\partial t}\right)^2 + \left(\frac{\partial u_{im}}{\partial x}\right)^2 + [1 - \epsilon\delta(x)]u_{im}^2\right]$$

$$= \Omega^2 a_0^2/\epsilon. \tag{6}$$

To introduce an isotopic impurity into the SG model, we will take in Eq. (1) the perturbation in the form $\epsilon P(u) = -\gamma u_{tt}$, where the parameter $\gamma \equiv (M - m)/m$ describes the relative ratio of the impurity mass M and the standard mass $m(< M)$ in the SG chain. In this case the linearized SG equation takes the form

$$u_{tt} - u_{xx} + u = -\gamma\delta(x)u_{tt}, \tag{7}$$

and it also supports an impurity-mode oscillation,

$$u_{im} = A(t)e^{-q|x|}, \tag{8}$$

where $A(t) = A_0\cos(\omega t + \theta_0)$, $q = (\gamma/2)\omega^2$, and the frequency ω is given by

$$\omega^2 = \frac{2}{\gamma^2}(\sqrt{1 + \gamma^2} - 1). \tag{9}$$

It is easy to see that the frequency of the impurity mode

(9) lies in the gap of the phonon spectrum, $0 < \omega^2 < 1$. In the case of a heavy-mass impurity, i.e., when $\gamma \gg 1$, the frequency ω goes to zero as $2/\gamma$, and $q \approx 1$.

III. COLLECTIVE-COORDINATE ANALYSIS

A. Effective equations of motion

To describe the motion of the kink (2) in the presence of a localized inhomogeneity in the substrate, the so-called adiabatic approximation is usually used [14, 15, 18]. In the framework of this perturbative approach, the kink coordinate X is considered as a collective variable, and its evolution is described by a simple motion equation for a classical particle with mass $m_{\rm eff} = 8$ placed in the effective potential (see, e.g., Ref. [15])

$$U(X) = -2\epsilon/\cosh^2 X. \tag{10}$$

As a result, if $\epsilon > 0$ the impurity in Eq. (1) creates an attractive potential to the kink. Since the particle (kink) conserves its energy, it cannot be trapped by the potential well if it has a nonzero velocity at infinity. However, the kink may be trapped by the attractive impurity due to radiative losses and there exists a radiation-induced critical velocity $V_c(\epsilon)$, such that if the kink initial velocity is larger than $V_c(\epsilon)$ it will pass through the impurity and escape to infinity; otherwise it will be trapped by the impurity. The critical velocity was firstly discussed by Malomed with the help of the perturbation theory based on the inverse scattering technique (since the unperturbed SG model is integrable) [17]:

$$V_c = 2^{21/8}\pi^{1/4}\epsilon^{3/8}\exp(-\sqrt{2/\epsilon}). \tag{11}$$

However, the perturbation theory used in Ref. [17] totally ignored the possibility of exciting an impurity mode during the scattering, so, as we recently proved, the result (11) is valid only for very small ϵ [24], because, as a matter of fact, the impurity mode may be easily excited because of the kink scattering (see Fig. 1). Therefore, when calculating the critical velocity of the kink capture, we should take into account the energy transfer to the impurity mode.

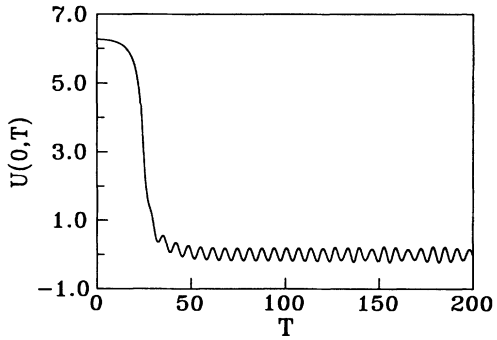

FIG. 1. Impurity displacement $u(0,t)$ calculated by numerical simulation of Eq. (1) with a substrate impurity ($\epsilon = 0.5$). It shows that, above the critical velocity, the kink passes the impurity, inelastically losing part of its energy to excite the impurity mode that is a long-lived oscillating state.

Now we will analyze the kink-impurity interactions by the modified collective-coordinate approach, taking into account *two* dynamical variables, namely the kink coordinate $X(t)$ [see Eq. (2)] and the amplitude of the impurity-mode oscillation $a(t)$ [see Eq. (4)]. Substituting the ansatz

$$u = u_k + u_{im} = 4\tan^{-1}\exp[x - X(t)] + a(t)e^{-\epsilon|x|/2} \tag{12}$$

into the Lagrangian of the system,

$$L = \int_{-\infty}^{\infty}\{\tfrac{1}{2}u_t^2 - \tfrac{1}{2}u_x^2 - [1 - \epsilon\delta(x)](1 - \cos u)\}, \tag{13}$$

and assuming that a and ϵ are small enough so that the higher-order terms can be neglected, we may derive the following (reduced) effective Lagrangian:

$$L_{\rm eff} = 4\dot{X}^2 + \frac{1}{\epsilon}(\dot{a}^2 - \Omega^2 a^2) - U(X) - aF(X), \tag{14}$$

where $U(X)$ is given by Eq. (10), and

$$F(X) = -2\epsilon\frac{\tanh X}{\cosh X}. \tag{15}$$

The equations of motion for the two dynamical variables X and a are

$$\begin{aligned} &8\ddot{X} + U'(X) + aF'(X) = 0, \\ &\ddot{a} + \Omega^2 a + (\epsilon/2)F(X) = 0. \end{aligned} \tag{16}$$

The system (16) describes a particle (kink) with coordinate $X(t)$ and mass 8 placed in the attractive potential $U(X)$ (for $\epsilon > 0$), and "weakly" coupled with the harmonic oscillator $a(t)$ (the impurity mode). Here we say "weakly" because the coupling term $aF(X)$ is of the order of ϵ and falls off exponentially. The system (16) is a generalization of the well-known equation $8\ddot{X} = -U'(X)$ describing the kink-impurity interactions in the adiabatic approximation.

B. Critical velocity

We find that the dynamical system (16) can describe all features of the kink-impurity interactions (for $\epsilon > 0$). First of all, it may be used to calculate properly the critical velocity of kink capture. The main idea is to use an energy transfer argument. Let us consider a kink with an initial velocity $V > 0$, coming from $-\infty$. Then in the zeroth-order approximation the equation of motion for the kink coordinate $X(t)$ takes the form $8\ddot{X} + U'(X) = 0$, which has an exact solution

$$X(t) = \sinh^{-1}[A\sinh(Vt)], \tag{17}$$

where $A = \sqrt{V^2 + \epsilon/2}/V$. Now we insert the result (17) into $F(X)$ of the second equation of (16) and consider the function

$$f(t) \equiv -(\epsilon/2)F(X(t)) = \frac{\epsilon^2 A\sinh(Vt)}{1 + A^2\sinh^2(Vt)} \tag{18}$$

as a pulse force acting on the harmonic oscillator. Introducing the complex variable $\xi(t) = \dot{a} + i\Omega a$, Eq. (16) may be reduced to $\dot{\xi} - i\Omega\xi = f(t)$, which has the solution

$$\xi(t) = e^{i\Omega t} \int_{-\infty}^{t} f(\tau) e^{-i\Omega\tau} d\tau, \tag{19}$$

with the initial conditions $a(-\infty) = \dot{a}(-\infty) = 0$, i.e., the oscillator (impurity mode) is not excited prior to the interaction. The total energy transferred from the particle (kink) to the oscillator (impurity mode) may be calculated as

$$\begin{aligned} E_{\rm osc} &= \frac{1}{\epsilon}(\dot{a} + \Omega^2 a^2) \\ &\equiv \frac{1}{\epsilon}|\xi(+\infty)|^2 \\ &= \frac{1}{\epsilon}\left|\int_{-\infty}^{\infty} f(t) e^{-i\Omega t} dt\right|^2 = 2\pi^2\epsilon^2 \frac{\sinh^2[\Omega Z(V)/2V]}{\cosh^2(\Omega\pi/2V)}, \end{aligned} \tag{20}$$

where

$$Z(V) \equiv \cos^{-1}\left(\frac{2V^2 - \epsilon}{2V^2 + \epsilon}\right). \tag{21}$$

At the critical velocity $V = V_c$, the particle must transfer all of its kinetic energy, $E_k = 4V^2$, to the oscillator. Thus the critical velocity of the kink capture should be determined by

$$V_c = \frac{\pi\epsilon}{\sqrt{2}} \frac{\sinh[\Omega Z(V_c)/2V_c]}{\cosh(\Omega\pi/2V_c)}. \tag{22}$$

For a given $\epsilon > 0$, this equation can be solved numerically to obtain the critical velocity $V_c(\epsilon)$. In Fig. 2 we have plotted the critical velocity determined by Eq. (22) (solid line) as well as by Eq. (11) (dashed line). Comparing the analytical results with the direct numerical simulations (the stars in Fig. 2), we find that the perturbation theory used in Ref. [17] is valid only for very small ϵ (in fact, for $\epsilon \leq 0.05$), while the formula (22) gives good estimations of $V_c(\epsilon)$ for ϵ over the region (0.2, 0.7).

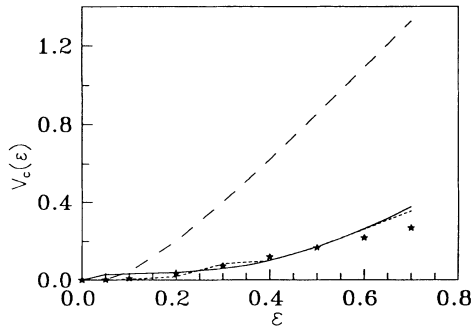

FIG. 2. Critical velocity of the kink capture as a function of ϵ determined by Eq. (22) (solid line) as well as by Eq. (11) (dashed line). Dotted line is obtained numerically for the collective-coordinate equations (16). The stars are the results of numerical simulations of Eq. (1).

C. Prediction of resonance structures

The best result we can obtain by using the collective-coordinate dynamical system (16) is to predict a possible resonance phenomenon in the kink-impurity interactions. As is pointed in Sec. III B, the system (16) describes a particle moving in a potential well and locally coupled with a harmonic oscillator (see the schematic picture in Fig. 3). There exists a critical velocity V_c, below which the particle cannot pass the potential well to escape to infinity (asymptotically) after the first interaction. Instead, the particle will be bounded by the potential and comes back to interact with the oscillator again. Since the system is conservative, in the second interaction it is possible for the particle to restore enough kinetic energy from the oscillator (provided the phase is right) and escape to infinity in the opposite direction. This energetic analysis clearly shows that some resonance phenomena may occur in the kink-impurity interactions.

In order to see the resonance phenomena in the model system (16), we simulate the equations with the initial conditions $X(0) = -6, \dot{X}(0) = V_i > 0, a(0) = 0$, and $\dot{a}(0) = 0$. First, we find that, for a given $\epsilon > 0$, there does exist a critical velocity $V_c(\epsilon)$ such that, if the initial velocity of the particle is larger than $V_c(\epsilon)$, then the particle will pass the attractive potential well $U(X)$ and escape to $+\infty$, with a final velocity $V_f < V_i$, because part of its kinetic energy is lost to excite the oscillator. In particular, at $\epsilon = 0.5$, we find numerically that the critical velocity is $V_c \approx 0.1697$.

Below the critical velocity, resonance phenomena are indeed observed. More precisely, if the initial velocity of the particle is smaller than $V_c(\epsilon)$, the particle cannot escape to $+\infty$ after the first interaction with the oscillator, but will return to interact with the oscillator again. The time between the first and the second interactions can be estimated as

$$T_{12}(V_i) = \frac{3.05855}{\sqrt{V_c^2 - V_i^2}} + 4.848\,72. \tag{23}$$

For some special initial velocities, the second interaction may cause the particle to escape to $-\infty$ with final velocity $V_f < 0$ (see Figs. 4 and 5). This resonance

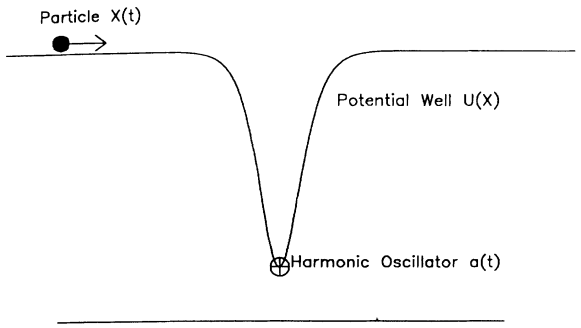

FIG. 3. A particle moving in a potential well and weakly coupled with a harmonic oscillator: a schematic drawing of the dynamical system (16) raised in the collective-coordinate approach.

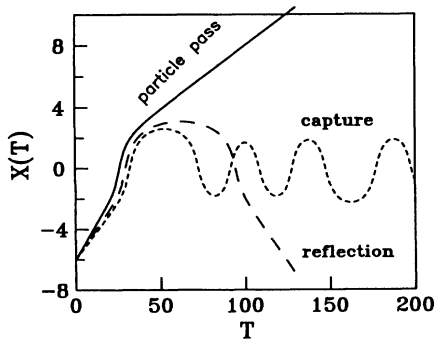

FIG. 4. Particle coordinate $X(t)$ vs time, showing the pass, trap, and reflection in the framework of Eqs. (16).

phenomenon can be easily explained by the energy exchange mechanism between the particle and the oscillator. In this case a resonance condition must be satisfied: $T_{12}(V_n) = nT_{\rm im} + \tau$, $T_{\rm im} = 2\pi/\sqrt{1-\epsilon^2/4} = 6.4892$ being the period of the impurity mode and $\tau = 0.0$ being a constant. Combining this resonance condition with Eq. (23) we can obtain the formula to predict the resonance windows,

$$V_n^2 = V_c^2 - \frac{(3.058\,55)^2}{(6.4892n - 4.848\,72)^2}, \tag{24}$$

where $V_c = 0.1697$ is the critical velocity and n is an integer. We have checked the formula (24) and find that it can predict the resonance windows *exactly*, at least for $6 \leq n \leq 22$. For example, at $n = 10$, the formula gives $V_{10} = 0.161\,87$, while in numerical simulation the particle will indeed be reflected after the second interaction if its initial velocity is taken to be exactly the *same* value.

As a matter of fact, the resonance structures of such kinds of systems (a particle coupled with *one* harmonic oscillator, see Fig. 3) have been more extensively studied in Ref. [31] for the kink-antikink collisions in the ϕ^4 model. The main results are that below the critical velocity there exist infinite "two-bounce" resonance windows (of reflection), and, also, near the two-bounce resonance windows there exist "n-bounce" resonance windows ($n > 3$ is an arbitrary integer), which means that the particle can escape to infinity (either $+\infty$ or $-\infty$) after interacting with the oscillator for n times. Indeed, we have observed all these resonance phenomena in the simulation of the system (16).

The reflection of the particle in the system (16) means that a kink can be reflected by an attractive impurity through a resonant energy exchange process. In the next section we are going to report our direct numerical simulation results; we will demonstrate that a SG kink can indeed be reflected by an attractive impurity if its initial velocity lies in some well-defined resonance windows.

IV. DIRECT NUMERICAL SIMULATIONS

To study the kink scattering by a pointlike substrate impurity, we use a conservative numerical scheme to discretize Eq. (1), and carry out simulations in the spatial interval $(-80, 80)$ with discrete step sizes $\Delta x = 2\Delta t = 0.04$. When handling the δ function we take its value equal to $1/\Delta x$ at $x = 0$ and zero otherwise. The initial conditions are taken as a kink centered at $X_0 = -6$ moving toward the impurity with an arbitrary given velocity $V_i > 0$.

First, we take the impurity amplitude $\epsilon = 0.5$. In the numerical simulations, we find that there are three different regions of kink initial velocity, namely, the regions of pass, of capture, and of reflection (see Fig. 6). The region of pass is the velocity interval $(V_c, 1)$, $V_c \approx 0.165\,85$ being the critical velocity, such that if the kink initial velocity is larger than V_c, the kink will pass the impurity and escape to the positive infinity (see Fig. 6). Such an interaction is inelastic in the sense that the kink loses part of its kinetic energy to excite the impurity mode (see Fig. 1) in a manner similar to the excitation of the oscillator in the collective-coordinate model (16), but here the radiation effect is also naturally presented. Roughly speaking, in this case a linear relationship between the squares of the kink initial velocity V_i and its final velocity V_f is held:

$$V_f^2 = \alpha(V_i^2 - V_c^2), \tag{25}$$

where the constant parameter $\alpha \approx 0.987$ (at $\epsilon = 0.5$) is determined empirically from numerical data.

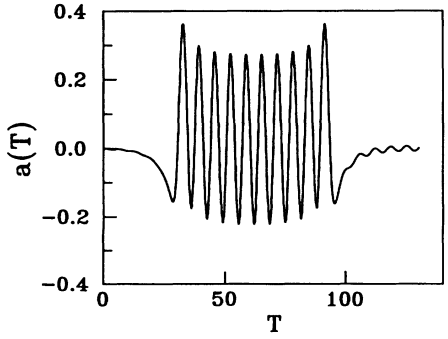

FIG. 5. Excitation and deexcitation of the harmonic oscillator $a(t)$, showing a resonance energy exchange between the particle and the oscillator in the model (16).

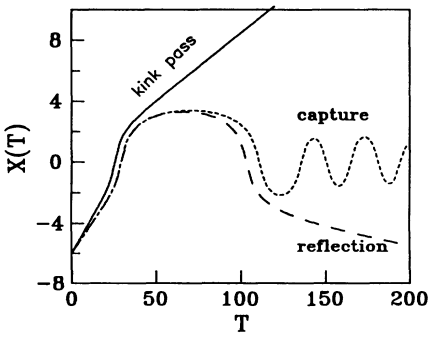

FIG. 6. Kink coordinate X vs time at $\epsilon = 0.5$. The kink initial velocity V_i is taken from the three different regions: the region of pass (solid line, $V_i = 0.19$), of capture (dotted line, $V_i = 0.1611$), and of reflection (dashed line, $V_i = 0.1600$).

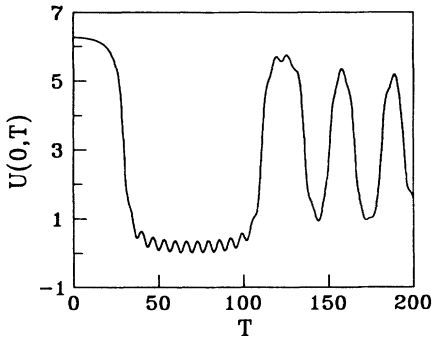

FIG. 7. Impurity displacement $u(0,t)$ vs time in the case of the kink capture. The kink initial velocity is $V_i = 0.1611$ and $\epsilon = 0.5$.

Below the critical velocity V_c, the final results of the kink-impurity interactions are very sensitive to the initial kink velocity. More precisely, if the incoming velocity of the kink is smaller than V_c, the kink cannot escape from the impurity after the first interaction, but will stop and then return to interact with the impurity again. For most of the initial velocities, the kink will lose its energy again in the second interaction and finally become trapped by the impurity (see Figs. 6 and 7). However, for some special initial velocities, the kink may escape to negative infinity after the second interaction, i.e., the kink may be *totally reflected by the attractive impurity* (see, e.g., Figs. 6 and 8).

Here we would like to point out two salient features in the resonant kink-impurity interactions. First, the reflection of the kink is realized by two steps: the first interaction removes kinetic energy from the kink and causes the kink to be trapped by the impurity, while the second interaction retransfers enough energy back to the kink and allows it to escape from the attractive impurity. To explain this trapping-escaping behavior one clearly needs an energy exchange mechanism. Secondly, below the critical velocity, the regions of the kink capture alternate with the regions of kink reflection (see Fig. 9). These two features make this effect similar to the resonant kink-antikink collisions in some nonlinear Klein-Gordon equations [27–31].

In order to analyze the kink-impurity interactions quantitatively, we define the center of the kink $X(t)$ as the spatial point x at which the field function $u(x,t)$ is equal to π. Let us also introduce the time between the first and the second interaction, $T_{12}(V_i)$, V_i being the kink initial velocity. More precisely, $T_{12}(V_i)$ is the time difference between the first two instants at which the center of the kink is just at the impurity. Since the attractive potential created by the impurity falls off exponentially [cf. Eq. (10)], based on the classical mechanics we can obtain an approximate formula to estimate $T_{12}(V_i)$ [see Eq. (23)],

$$T_{12}(V_i) = \frac{a}{\sqrt{V_c^2 - V_i^2}} + b, \tag{26}$$

where the parameters a and b are empirically determined

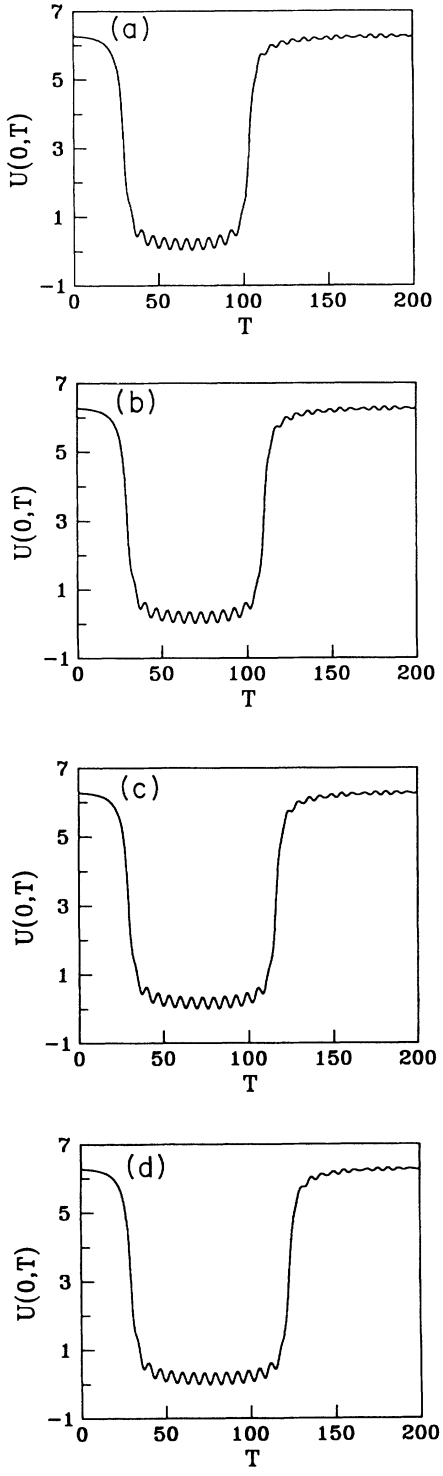

FIG. 8. Impurity displacement $u(0,t)$ vs time in the case of reflection. The kink initial velocities are taken from the first four resonance windows: (a) $V_i = 0.1600$, (b) $V_i = 0.160\,94$, (c) $V_i = 0.161\,67$, and (d) $V_i = 162\,25$. Note that after the first interaction the impurity mode is excited, but after the second interaction the energy in the excited impurity mode is transferred back to the kink. The number of impurity oscillations between the two interactions is increased one by one for the adjacent resonance windows, which agrees with the resonance condition.

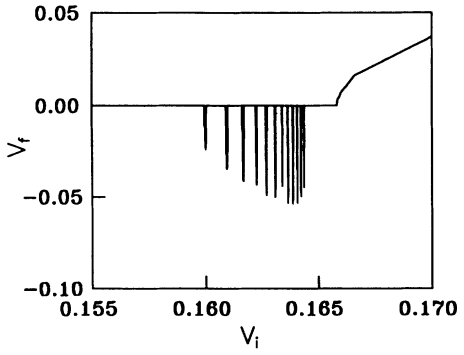

FIG. 9. Final kink velocity as a function of the initial kink velocity ($\epsilon = 0.5$). Zero final velocity means that the kink is captured by the impurity. In the case of resonances, we simulate until the kink is reflected far away from the impurity [$X(t) \geq 10$], and then the final velocity is calculated by averaging over 20 time units.

by numerical data. At $\epsilon = 0.5$, we have $a \approx 3.153\,786$, $b \approx 1.608\,516$. We have verified this formula and found that it is valid, at least in the interval $(0.10, 0.165)$, where the resonance windows are situated (see Table I).

We also observe that the first interaction always results in exciting the impurity mode (see Figs. 1 and 8), and the resonant reflection of the kink after the second interaction is just a *reverse* process, i.e., to extinguish the impurity mode [see Figs. 8(a)—8(d)] when the timing is right, in order to restore enough of the lost kinetic energy and to escape from the impurity with a nonzero final velocity (see Fig. 9). 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 characteristics 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

$$T_{12}(V) = nT + \tau, \tag{27}$$

where $T = 2\pi/\Omega \approx 6.4892$ (at $\epsilon = 0.5$) is the period of the impurity-mode oscillation, n is an integer, and τ is an offset phase, which is found, for our case, to be about 2.6512.

Combining Eqs. (26) and (27), we may obtain the general formula to predict the centers of the resonance windows,

$$V_n^2 = V_c^2 - \beta/(nT + \delta)^2, \tag{28}$$

where $\beta = a^2$ and $\delta = \tau - b$. In particular, at $\epsilon = 0.5$, we have determined the parameters: $V_c = 0.165\,85$, $\beta = 9.946\,366$, $\delta = 1.0427$, and $T = 6.4892$.

It is natural that the formulas (26) and (28) are quite similar to those obtained in Sec. III C, where the resonance structures of the collective-coordinate dynamical system (16) are analyzed. From Table I we can see that formulas (26)–(28) are very accurate in comparison with the direct numerical simulation results.

The resonance windows corresponding to the integers $5 < n < 11$ were found to be absent. Instead, we observed quasiresonances at the velocities predicted by the formula (28) for $n < 11$, i.e., the second interaction may cause the kink to be reflected further away from the impurity but yet not able to escape to infinity. Vanishing of these lower-order resonance windows can be explained by taking into account the strong radiation generated during the scattering. If the initial kink velocity is too small, the kink will not be able to restore enough kinetic energy at the second interaction because the radiative losses have extracted a sufficient part of the energy from the kink translational mode and impurity mode.

Furthermore, there are no reasons why higher-order resonances ($n > 22$) do not exist. But according to Table I, the windows become narrower and narrower when n

TABLE I. Two-bounce resonance windows in the kink-impurity interactions in the SG model (1) with the substrate impurity at $\epsilon = 0.5$. The value $T_{12}(V_n)$ is defined as the time between the first and second interactions. The data in the last two columns are obtained by the formulas (26) and (28), respectively. Note that the resonance windows determined by the numerical simulations are in very good agreement with the theoretical predictions.

n	Resonance windows	Window centers V_n	$T_{12}(V_n)$ Numerical	$T_{12}(V_n)$ Theoretical	Predicted centers
11	(0.15996, 0.16003)	0.1600	73.9	73.8	0.16003
12	(0.16090, 0.16097)	0.16093	80.2	80.2	0.16095
13	(0.16164, 0.161704)	0.16167	86.8	86.8	0.16167
14	(0.16222, 0.16227)	0.16224	93.3	93.2	0.16226
15	(0.16268, 0.16273)	0.16271	99.8	99.8	0.16272
16	(0.16309, 0.16311)	0.16310	106.5	106.4	0.16310
17	(0.16340, 0.16342)	0.16341	113.0	113.1	0.16341
18	(0.16365, 0.163677)	0.163663	119.3	119.0	0.16367
19	(0.16387, 0.16389)	0.16388	125.6	125.4	0.16390
20	(0.16406, 0.16408)	0.16407	132.5	131.8	0.16409
21	(0.16423, 0.16424)	0.164235	138.7	137.7	0.16425
22	(0.16437, 0.16438)	0.164375	145.2	144.5	0.16439

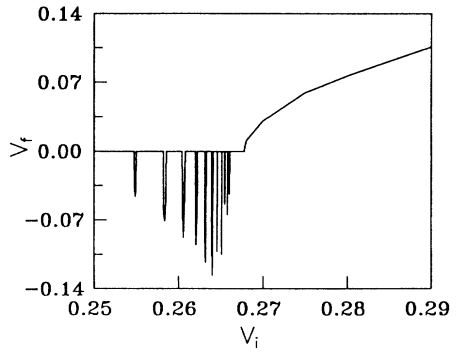

FIG. 10. The same as in Fig. 9 but at $\epsilon = 0.7$.

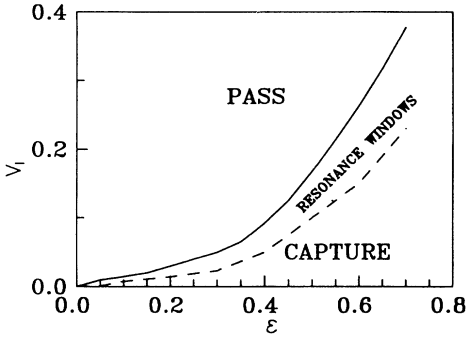

FIG. 11. Three different regions in the ϵ, V_i plane for the kink interactions with a substrate impurity. It is shown that above the critical velocity the kink can always pass the impurity and escape to infinity, but that below the critical velocity (solid) curve the kink can be either captured or resonantly reflected.

increases, so it would be very difficult to detect the high-order resonance windows even if they did exist. From formula (26) we see that $T_{12}(V_i)$ becomes very large when V_i is close to V_c; thus one has to take a long time at numerical simulations to find the higher-order resonance windows. On the other hand, since the impurity mode is an exact solution in the linear theory, it can oscillate for a long time without any appreciable decay in its amplitude (this has been verified by our direct numerical simulations). Therefore, it is more sensible to consider the kink scattering by an *excited* impurity (see the next section).

We have demonstrated that a kink can be reflected after colliding with an attractive impurity for *two* times; henceafter, these resonances will be called *two-bounce* resonances. Such resonance effects have also been observed for other values of ϵ (see, e.g., Fig. 10 for the case of $\epsilon = 0.7$; the corresponding tables can be found in Ref. [23]). Thus, from our numerical simulations and theoretical analysis, we can make a general conclusion about the kink-impurity interactions in the SG model. In Fig. 11 we show that in the ϵ, V_i plane (V_i being the kink initial velocity) there are *three* regions that correspond to kink pass, capture, and coexistence of capture and reflection (resonance windows), respectively.

Finally, another interesting question is whether it is possible to observe *three-bounce* (or higher-bounce) resonances, i.e., when the kink escapes from the impurity after colliding with the impurity for three times. Our numerical simulations show that if the kink cannot escape after the second interaction, which means that there is no resonance between the kink translational motion and the impurity oscillation, then the *radiative losses* will take away more energy from the two modes (impurity mode and kink translational mode) during this process, and as a result, the kink will never be able to restore enough energy to escape. On the other hand, even if the three-bounce windows existed, they would be extremely narrow (see Refs. [27–31]), and the numerical detection of these windows would consume a large amount of computer time. Nevertheless, recently it has happened that we have observed a three-bounce resonance window in the kink-impurity interactions in the ϕ^4 model [25], but for the ϕ^4 model we have found that the kink *internal* mode also plays a very important role in the resonant energy exchange process, and the resonance effects in this model are explained by the energy exchange between the kink translational mode and *two* effective oscillators (the impurity mode and the kink internal mode).

V. KINK INTERACTION WITH AN EXCITED IMPURITY

In the preceding section we have considered the interactions of the SG kink with an initially *unexcited* impurity. It has been observed that the first interaction always results in exciting the impurity mode, so that the second interaction looks like the kink scattering by an *excited* impurity, but with the kink being trapped in the potential well. Our purpose now is to study the scattering of a kink by an excited impurity, where the kink is initially separated *far away* from the impurity and has a *nonzero* initial velocity. As far as we know, such a problem has not been considered previously.

As a matter of fact, the problem can be also analyzed by the collective-coordinate method described in Sec. III B. The equations of motion for the collective coordinates $X(t)$ (kink center) and $a(t)$ (impurity-mode amplitude) are the same as Eq. (16), but the initial conditions for $a(t)$ should be changed. We may use the same arguments as before to calculate the energy stored in the impurity mode after the first scattering.

$$E_{\rm imp}(V_i, a_0, \theta) = \frac{1}{\epsilon}[G^2(V_i) + \Omega^2 a_0^2 + 2G(V_i)\Omega a_0 \cos\theta], \tag{29}$$

where, V_i is the kink initial velocity, a_0 is the initial amplitude of the impurity mode, θ is the phase of the impurity oscillations at the instant of the collision, and

$$G(V_i) = -\sqrt{2}\pi\epsilon^{3/2}\frac{\sinh[\Omega Z(V_i)/2V_i]}{\cosh(\Omega\pi/2V_i)}, \tag{30}$$

$Z(V_i)$ being given by Eq. (21). Note that if $a_0 = 0$, then

$E_{\rm imp}$ will be the same as $E_{\rm osc}$ given by Eq. (20).

Equation (29) shows that for a given initial kink velocity the energy transferred to the impurity mode after the first scattering depends 2π-periodically on the phase of the impurity mode. Due to this phase effect, the results of the kink-impurity interactions will be more complicated. We will analyze the problem in two cases. Let us first consider the case $V_i > V_c(\epsilon)$, $V_c(\epsilon)$ being the critical velocity determined by Eq. (22). By a simple energy-balance argument, it can be shown that the kink may get trapped by the impurity if the following condition is fulfilled:

$$4V_i^2 + \Omega^2 a_0^2/\epsilon \leq \sup_\theta E_{\rm imp}(V_i, a_0, \theta), \tag{31}$$

which yields the condition for the initial amplitude of the impurity mode,

$$a_0 \geq \frac{G^2(V_i) - 4\epsilon V_i^2}{2\Omega G(V_i)}. \tag{32}$$

It is easy to prove that the right-hand side (rhs) of Eq. (32) is always positive, provided $V_i > V_c$. Similarly, in the case of $V_i < V_c$, the kink can still pass through the impurity if the initial amplitude of the impurity mode is not small,

$$a_0 \geq \frac{4\epsilon V_i^2 - G^2(V_i)}{2\Omega G(V_i)}. \tag{33}$$

For a given initial amplitude of the impurity mode, there exists a critical velocity $V_c(\epsilon, a_0) > V_c(\epsilon)$ above which the kink can escape from the impurity just after the first interaction. By an energy transfer argument as used in Sec. III B, it is easy to prove that the critical velocity should be determined by the relation

$$4V_c^2(\epsilon, a_0) = G^2(V_c(\epsilon, a_0)) - 2\Omega a_0 G(V_c(\epsilon, a_0)). \tag{34}$$

Below the critical velocity $V_c(\epsilon, a_0)$ there are *three* possibilities: pass, capture, and reflection, because the scattering will depend on the *phase* of the impurity mode.

To verify the above theoretical predictions by direct numerical simulations of the SG model, we take the initial conditions (at $\epsilon = 0.5$) with an excited impurity mode whose shape is given by Eq. (4), where the amplitude $a_0 = 0.1$. First of all, we find that for larger initial velocities (> 0.2) the kink can always pass and then escape from the impurity (for any initial phase of the impurity mode). However, for smaller velocities there are three possibilities, as is pointed out in the above theoretical analysis. In particular, we take the kink initial velocity $V_i = 0.18$, which is lager than the critical velocity $V_c = 0.16585$ at $a_0 = 0.0$, and then change the initial phase θ of the impurity mode in the interval $(0, 2\pi)$. In the numerical simulations we observe that, for θ in the intervals $(0.0, 0.8\pi)$ and $(1.2\pi, 2\pi)$ the kink may pass through the impurity (inelastically) and escape to infinity after the first interaction; but for θ in the interval $(0.9\pi, 1.1\pi)$ the kink will get trapped by the impurity after the first interaction. In this region, a two-bounce resonance window is observed, i.e., the kink can escape from the impurity after the *second* interaction (see Fig. 12).

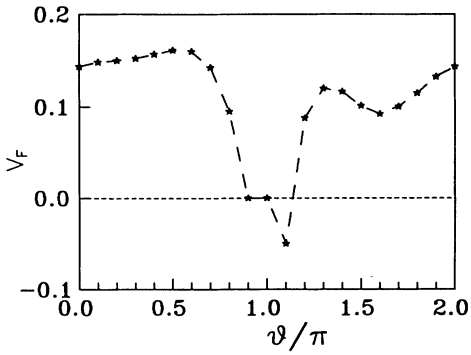

FIG. 12. Final kink velocity V_f vs the impurity phase θ when the impurity is excited prior to the collision. The kink initial velocity V_i is taken as 0.18. The pass, trapping, and reflection are observed at different values of the phase.

We have also made simulations for other kink initial velocities ranging from 0.15 to 0.19. The results agree well with our theoretical predictions; that is, the scattering of the kink strongly depends on the initial phase of the impurity mode, and the kink may pass, be trapped, or be reflected by the excited impurity due to the energy exchange between the kink translational mode and the oscillating impurity mode.

VI. MASS IMPURITY

Now we will consider the interaction of a kink with an istopic (heavy-mass) impurity in the SG model (1) when $\epsilon P(u) = -\gamma u_{tt}$. Since the heavy-mass impurity may also support a localized impurity mode (8), it is natural to employ the collective-coordinate technique, taking into account the impurity-mode amplitude as an additional variable. Inserting the ansatz

$$u_a = 4\tan^{-1}\exp[x - X(t)] + A(t)e^{-q|x|} \tag{35}$$

into the system Lagrangian,

$$L = \int_{-\infty}^{\infty} dx\{\tfrac{1}{2}[1 + \gamma\delta(x)]u_t^2 - \tfrac{1}{2}u_x^2 - (1 - \cos u)\}, \tag{36}$$

we may obtain, in the lowest approximation, the effective Lagrangian,

$$L_{\rm eff} = 4\left(1 + \frac{\gamma}{2\cosh^2 X}\right)\dot{X}^2 + \frac{1}{2}G(\gamma)(\dot{A}^2 - \omega^2 A^2) - \frac{2\gamma}{\cosh X}\dot{X}\dot{A} \tag{37}$$

where ω is the frequency of the isotopic impurity mode given in Eq. (9), and

$$G(\gamma) = \sqrt{1+\gamma^2}(\sqrt{1+\gamma^2} + 1)/\gamma. \tag{38}$$

The equations of motion for $X(t)$ and $A(t)$ are

$$8\left(1+\frac{\gamma}{2\cosh^2 X}\right)\ddot{X}-\frac{2\gamma}{\cosh X}\ddot{A}-\frac{4\gamma\sinh X}{\cosh^3 X}\dot{X}^2=0, \tag{39}$$

$$G(\gamma)(\ddot{A}+\omega^2 A)-\frac{2\gamma}{\cosh X}\ddot{X}+\frac{2\gamma\sinh X}{\cosh^2 X}\dot{X}^2=0. \tag{40}$$

First, let us consider the case $\gamma \ll 1$, i.e., where the isotopic impurity is small enough. Then, in the effective Lagrangian (37) we may neglect the impurity mode and obtain the energy-conservation relation in the form

$$\dot{X}^2\left(1+\frac{\gamma}{2\cosh^2 X}\right)=V_i^2, \tag{41}$$

where V_i is the kink velocity at infinity. Equation (41) has an approximate solution

$$X(t)+(\gamma/4)\tanh X(t)=V_i t, \quad \gamma \ll 1 \tag{42}$$

from which we can see that the effect of the kink scattering in this case is nothing but a phase shift of $\gamma/2$.

Taking the approximation $X(t)\approx V_i t$ in Eq. (40) and using an approach similar to that in Sec. III, we can calculate the energy transferred to the isotopic impurity after the kink scattering, assuming that the impurity is not excited prior to the interaction.

$$E_{\rm imp}=\frac{1}{2}G(\gamma)\left|\int_{-\infty}^{\infty}\frac{2\gamma V_i^2\sinh(V_i t)}{G(\gamma)\cosh^2(V_i t)}e^{-i\omega t}dt\right|^2$$
$$=\frac{4\gamma^3\pi^2}{\sqrt{1+\gamma^2}(1+\sqrt{1+\gamma^2})^2\cosh^2(\pi/2V_i)}. \tag{43}$$

If $\gamma \ll 1$, then the energy transferred to the impurity, $E_{\rm imp}$, is of the order of $\gamma^3 e^{-\pi/|V_i|}$. Therefore, if the impurity intensity γ is small, then the kink cannot lose enough of its kinetic energy, $4V_i^2$, to the impurity, and can pass the isotopic impurity almost freely at any initial velocity. However, if the heavy-mass impurity is large enough ($\gamma \gg 1$) there exists a critical velocity $V_{\rm cr}(\gamma)$ such that, if the initial kink velocity V_i is *larger* than $V_{\rm cr}(\gamma)$, then $E_{\rm imp}(V_i)$ may exceed the kinetic energy $4V_i^2$, and that means that in this case the kink cannot pass the impurity. By using the energy conservation we find that the critical velocity $V_{\rm cr}$ is determined by the relation

$$\frac{\gamma^3\pi^2}{\sqrt{1+\gamma^2}(1+\sqrt{1+\gamma^2})^2\cosh^2(\pi/2V_{\rm cr})}=V_{\rm cr}^2. \tag{44}$$

With the help of the computer we have solved Eq. (44) and obtained $V_{\rm cr}(\gamma)$ at some values of γ. In particular, we have found that for $\gamma \le 5.0$ there is no solution, which means that the kink can pass the impurity and escape to infinity if γ is not big enough. However, for larger heavy-mass impurities, there indeed exists a critical velocity $V_{\rm cr}(\gamma)$, which is a decreasing function of γ. In particular, at $\gamma = 30$ the critical velocity is about 0.76.

We have verified the above analysis by direct numerical simulations of the SG model. First, we observe that, if γ is smaller than 6.0, then the kink with any velocity in the region $0 < V < 0.99$ can pass the impurity and escape to infinity. This is in agreement with our theoretical prediction that the kink cannot be reflected by an impurity with small mass ratio γ. Second, for $\gamma \ge 6$ there indeed exists a critical (initial) velocity *above which the kink will be reflected*; otherwise the kink may pass the impurity. In particular, at $\gamma = 30$ we find that the critical velocity is about 0.415. The latter results differ from the predicted $V_{\rm cr}$ given by the collective-coordinate model; however, for such a large value of γ the perturbation theory is not valid anymore, and we expect to have only qualitative agreements with direct simulations because radiative effects are very strong.

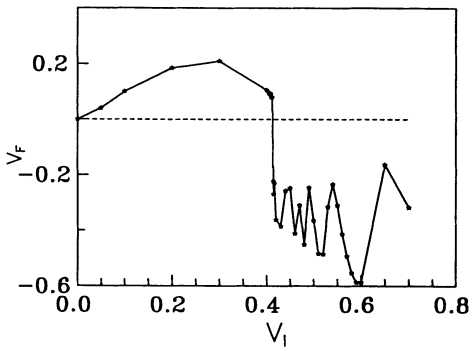

FIG. 13. Final kink velocity vs its initial velocity for the isotopic (heavy-mass) impurity at $\gamma = 30$. Higher-velocity kinks are reflected, while the lower-velocity kinks may pass.

We have made a detailed investigation for the case $\gamma = 30$, taking different initial kink velocities. In Fig. 13 we plot the kink final velocity V_f as a function of its initial velocity V_i. It is seen that for small initial velocities ($V_i \le 0.3$) the kink can pass the impurity almost freely ($V_f \approx V_i$) and it loses very little kinetic energy. However, above the critical velocity the kink final velocity is negative, which means that the kink is reflected. Moreover, in the case of reflection the final kink velocity is not proportional to its initial velocity; instead there are some oscillations in the dependence. This effect can also be explained by the *energy exchange* between the kink and the impurity mode: if the kink final velocity is smaller, then the amplitude of the impurity mode will be larger; inversely, if the kink final velocity is larger, then the impurity-amplitude will be smaller. As an example, in Fig. 14 we plot the impurity-mode oscillation after the kink scattering for the three initial velocities $V_1 = 0.46$, $V_2 = 0.54$, and $V_3 = 0.58$, whose corresponding final velocities V_f are -0.41, -0.23, and -0.55, respectively.

Therefore, the collective-coordinate approach may demonstrate the main features of the kink scattering by an isotopic (heavy-mass) impurity. In particular, it has been shown that if the mass ratio is large enough, a higher-velocity kink will be reflected, while a lower-velocity kink will pass; such a behavior is explained by the inelastic interactions of the kink with the impurity-mode oscillation. At last, we would like to point out that the similar features were observed numerically by Fraggis, Pnevmatikos, and Economou [19] for the kink scat-

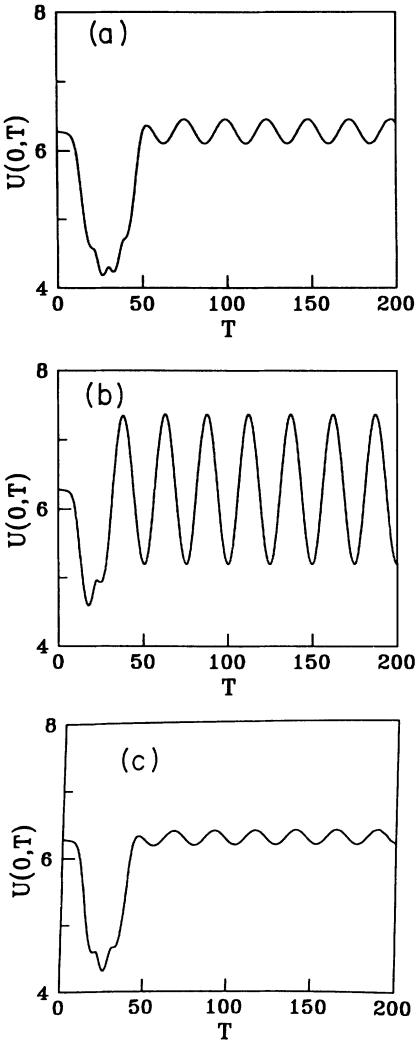

FIG. 14. Excitation of the impurity mode oscillations at the different initial velocities: (a) $V_i = 0.46$, (b) $V_i = 0.54$, (c) $V_i = 0.58$, which result in the different final velocities $V_f = -0.41, -0.234$, and -0.55, respectively. Note that at $V_i = 0.54$ the impurity amplitude is the largest, while the kink reflected velocity is the smallest.

tering by an isotopic impurity in the ϕ^4 chain, although they did not explain the origin of this phenomenon.

VII. CONCLUDING REMARKS

In conclusion, we have studied the kink scattering by an attractive impurity in the SG model and demonstrated that all the effects observed numerically may be explained even in the framework of the collective-coordinate approach, taking into account a concept of the impurity mode. In particular, we have explained the resonance structures in the kink-impurity interactions by an energy exchange between the kink translational mode and the impurity mode that is excited at the first collision. Although the radiative effects were not included into our analytical consideration, the collective-coordinate approach allows us to understand qualitatively and even quantitatively why and how the resonances may occur. We would like to point out again that the general features of the resonances observed in the kink-impurity interactions are similar to the resonance phenomena in the kink-antikink collisions in some nonlinear Klein-Gordon models that support kinks with internal degrees of freedoms, the so-called internal modes, which play the role of the effective oscillators [27–31].

For the isotopic (heavy-mass) impurity the appropriate collective-coordinate method also gives a general understanding of an interesting effect in the kink dynamics, namely, the reflection of the kink by the heavy-mass impurity at higher kink velocities.

Since the attractive impurity may support a localized impurity mode in the other nonlinear systems, we can predict, by a collective-coordinate analysis, that resonance phenomena may be observed in soliton-impurity interactions in the other nonlinear systems, such as a generalized Klein-Gordon model, e.g., the modified SG model [28], the double SG model [30], etc. We expect that the resonance structures will be similar to those described in the present paper for the SG model, or to those reported in our recent work [25] for the ϕ^4 model. However, we would also like to mention more interesting expansions of the resonant effects involving other types of solitons. Indeed, as was shown recently [33], the dynamics of the so-called intrinsic localized modes in the chain with nonlinear interatomic interactions may be described by the effective nonlinear Schrödinger (NLS) equation. Moreover, an isotopic impurity in this nonlinear system produces a potential inhomogeneity in the NLS equation for the wave envelope. According to Ref. [34], the interaction of the NLS soliton with such an impurity is described in the framework of the collective-coordinate approach by a motion equation similar to the classical particle equation arising for the kink scattering. Therefore, for this problem we may obtain the system of the collective-coordinate equations that is similar to those described in the present paper. So, we can expect to observe some kind of resonant interactions for the envelope solitons, too.

Another large class of soliton problems where the resonant kink-impurity interactions may be observed is the hydrogen-bonded chains (see, e.g., Ref. [35], and references therein), where the kink-type excitations are composed of two coupled fields that are nothing but oxygen and hydrogen displacements. Some preliminary results on the kink-impurity interactions were obtained in Ref. [21] without the concept of the impurity mode, and subsequent direct simulations would be needed.

The most relevant systems in which the kink-impurity interactions may be observed experimently are the long Josephson junctions, with inhomogeneities installed during fabrication (see, e.g., [32], and references therein). In these systems kinks describe quanta of the magnetic flux (fluxons). Recently, a method of creating fluxons in an annular Josephsen junction by a low-intensity electron beam was reported by Ustinov *et al.* [36,37]. As a matter of fact, the electron beam acting on the junction plays the role of an effective magnetic impurity whose properties for the kink scattering are known [38,39]. So, we may expect the same kind of resonant interactions

between the fluxon and the magnetic impurity. However, in real physical systems such as Josephson junctions strong dissipative losses will likely destroy fine resonance structures such as those described in the present paper, because the impurity-mode oscillations will fade after their excitation. To save the oscillations, we have to consider a forced impurity dynamics, e.g., assuming that the electron beam creating the magnetic impurity may move transversely to the junction coordinate, changing periodically the impurity intensity. As a result, a fine structure of phase-locked steps due to the resonant interactions has to be observed on a zero-field step. We would like to point out that phase-locked steps produced by a coupling with an external magnetic field through a junction edge, have been recently analyzed by Salerno and Samuelsen [40]. Therefore, the effect analyzed in Ref. [40] is analogous (and, roughly speaking, it has a common physical origin) to the resonant kink-impurity scattering described in the present paper.

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