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Discreteness effects in the kink scattering by a mass impurity

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Received 1 June 1990; revised manuscript received 10 July 1990; accepted for publication 10 July 1990
Communicated by A.R. Bishop

We demonstrate analytically that the repulsive character of a mass impurity is stipulated by discreteness effects in the sine-Gordon system. The threshold velocity for the kink reflection by a heavy mass is calculated in the framework of the effective equation of motion for the kink center in the discrete sine-Gordon chain. The result is determined significantly by the lattice spacing, and the effect does not occur in a continuum model since then the Peierls–Nabarro barrier vanishes.

1. Introduction

Recently there has been growing interest in soliton propagation in disordered systems (see, e.g., ref. [1]) to clarify whether or not nonlinearity modifies qualitatively the effects of disorder on transport properties, and vice versa, whether or not disorder modifies the remarkable soliton properties of nonlinear systems. In such a study, the scattering properties of solitons from one impurity play an important role to understand the total behaviour of nonlinear waves in disordered systems (see, e.g., refs. [2–5]).

Most of the previous analytical studies are concerned with the continuum limit. In physical applications, however, there is a natural minimum distance scale, a lattice constant, and discreteness effects can significantly influence the dynamics and thermodynamic properties of the system under consideration [6–18]. Moreover, results of computer simulations demonstrate that the lattice discreteness causes a number of new effects in nonlinear systems [6,10,11,17,18]. The discreteness breaks the continuous symmetry inherent in the nonlinear differential equations associated with soliton solutions, giving rise to a discrete symmetry characteristic of the underlying lattice structure. This in turn leads to the lifting of the spatial degeneracy associated with the kink center and gives rise to a periodic energy potential (the so-called Peierls–Nabarro (PN) potential) with characteristic barriers. The presence of the PN potential provides pinning sites for the kink center, and the kink cannot freely slide but its motion is always accompanied by radiative effects (see, e.g., refs. [11,18]).

To understand a number of features of the discrete sine-Gordon (sG) model, Ishimori and Munakata [8] employed first the perturbation theory (see, e.g., refs. [19,20]) to treat the effect of discreteness on a continuum kink solution as a perturbation. This approach allows us to consider discreteness effects qualitatively, but it does not agree quite well with exact results obtained from numerical simulations (see discussions in refs. [16,18]). A more correct analysis based on the projection operator technique [21] gives rise to an essentially exact agreement between molecular dynamics simulations and theory,

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because it uses the bare ground state of the discrete model [16]. However, in many cases quite good results may be obtained with the help of an effective equation of motion for the kink center using an appropriate ansatz for the kink effective wave form in the discrete system (see, e.g., ref. [17]).

For inhomogeneous models, impurities give rise to effective localized potentials (see, e.g., ref. [20]) which lead to a number of new and important effects together with discreteness ones. As a result, transport properties of a disordered nonlinear system may be strongly modified by the discreteness. The present paper aims to consider analytically one of the effects. As is known, a mass impurity in the continuum nonlinear system cannot reflect a kink, and the kink cannot be trapped by the mass impurity, too. We demonstrate using the discrete sG system as an example, that the repulsive character of the mass impurity is stipulated by the discreteness of the model. We calculate the threshold velocity of the kink allowing the reflection which is determined significantly by the lattice spacing. The kink reflection from a heavy mass impurity has been observed in numerical simulations for the discrete model [22].

2. Effective equation of motion for the kink center

We consider a discrete sG system which can be derived from the following Lagrangian,

$$L=\sum_n \left\{\tfrac{1}{2}m_n\dot{u}_n^2-\tfrac{1}{2}k(u_{n+1}-u_n)^2 - U_0\left[1-\cos\left(\frac{2\pi}{a}u_n\right)\right]\right\}, \tag{1}$$

where u_n is the displacement at the lattice site n, k is the elastic constant, $2U_0$ is the amplitude of the external potential, and a is the lattice spacing. To include a mass impurity in the model, we put

$$m_n=m+(M-m)\delta_{n0}, \tag{2}$$

where m is the mass of particles in the lattice, and M is the mass of the impurity. From the Lagrangian (1) we can deduce the motion equations governing the displacement field dynamics,

$$m\left(1+\frac{M-m}{m}\delta_{n0}\right)\ddot{u}_n-k(u_{n+1}+u_{n-1}-2u_n) + U_0\frac{2\pi}{a}\sin\left(\frac{2\pi}{a}u_n\right)=0\,. \tag{3}$$

Introducing the dimensionless variables

$$\tau=\frac{c}{a}t,\quad \Phi_n=\frac{2\pi}{a}u_n\,, \tag{4a}$$

and setting

$$\mu=\frac{a}{l_0},\quad c^2=\frac{ka^2}{m},\quad \omega_0^2=\frac{4\pi^2}{ma^2}U_0\,,$$

$$l_0^2=\frac{c^2}{\omega_0^2},\quad \delta m=M-m\,, \tag{4b}$$

eq. (3) becomes

$$\frac{d^2\Phi_n}{d\tau^2}=[\Phi_{n+1}+\Phi_{n-1}-2\Phi_n]-\mu^2\sin\Phi_n - \frac{\delta m}{m}\delta_{n0}\left(\frac{d\Phi_n}{d\tau}\right)^2. \tag{5}$$

In the notations (4), the parameter μ has the meaning of the ratio of the lattice spacing a to the kink width l_0 and c is the sound velocity. We now assume that the coupling constant μ^2 between the lattice and the periodic potential is small. With this condition, the distorted kink can reasonably be approximated by the ansatz (see, e.g., refs. [16–18])

$$\Phi_n(\tau)=4\tan^{-1}[\exp(\mu\xi_n)]\,, \tag{6a}$$

where

$$\xi_n=n-Y(\tau)\,. \tag{6b}$$

Ansatz (6) is based on the well-known exact solution to the sG equation in the so-called "non-relativistic" limit (see, e.g., ref. [20]). Our aim is to derive an effective equation of motion for the kink center $Y(\tau)$. We will use the reduced Lagrangian approach [17]. The Lagrangian

$$L=\sum_n\left[\frac{1}{2}\left(\frac{d\Phi_n}{d\tau}\right)^2\left(1+\frac{\delta m}{m}\delta_{n0}\right) - \tfrac{1}{2}(\Phi_{n+1}-\Phi_n)^2-\mu^2(1-\cos\Phi_n)\right] \tag{7}$$

corresponds to the normalized equation (5). Assuming the existence of the function $\Phi_n(\tau)$ of the discrete variable n in the form (6), we can rewrite the Lagrangian in the form

$$L=2\mu^2\left[\left(\frac{dY}{d\tau}\right)^2-2\right]\sum_n\frac{1}{\cosh^2\mu\xi_n}+\frac{2\mu^2}{\cosh^2\mu Y}\frac{\delta m}{m}\left(\frac{dY}{d\tau}\right)^2, \tag{8}$$

where we have used the following results:

$$\frac{d\Phi_n}{d\tau}=-\frac{2\mu}{\cosh\mu\xi_n}\frac{dY}{d\tau},\quad 1-\cos\Phi_n=\frac{2}{\cosh^2\mu\xi_n},$$

$$\Phi_{n+1}-\Phi_n=4\tan^{-1}\frac{\sinh(\frac{1}{2}\mu)}{\cosh(\mu\xi_n+\frac{1}{2}\mu)}\approx\frac{2\mu}{\cosh\mu\xi_n}.$$

Using the Poisson sum formula

$$\sum_{n=-\infty}^{\infty}f(nh)h=\int_{-\infty}^{\infty}dx\,f(x)\left[1+2\sum_{s=1}^{\infty}\cos\left(\frac{2\pi sx}{h}\right)\right], \tag{9}$$

and keeping only the first-order term in eq. (9) (i.e., $s=1$), we can rewrite the effective Lagrangian of the system in the following reduced form,

$$L=4\mu\left[\left(\frac{dY}{d\tau}\right)^2-\frac{4\pi^2}{\mu\sinh(\pi^2/\mu)}\cos(2\pi Y)\right]+\frac{2\mu^2}{\cosh^2(\mu Y)}\frac{\delta m}{m}\left(\frac{dY}{d\tau}\right)^2. \tag{10}$$

As a result, the variational principle associated with the kink center Y leads to the generalized equation of motion:

$$\frac{d^2X}{d\tau^2}=\frac{4\pi^3}{\sinh(\pi^2/\mu)}\sin\left(\frac{2\pi X}{\mu}\right)+\frac{1}{2}\frac{\mu\sinh X}{\cosh^3X}\frac{\delta m}{m}\left(\frac{dX}{d\tau}\right)^2, \tag{11}$$

where

$$X\equiv\mu Y. \tag{12}$$

The value defined by the first term in the r.h.s. of eq. (11),

$$\omega_p^2=\frac{8\pi^4}{\mu\sinh(\pi^2/\mu)}, \tag{13}$$

has the meaning of the frequency of vibrations in the PN potential. Note that the projection operator approach [16] using the bare ground state of the discrete sG lattice yields a similar result with the numerical coefficient 4 instead of $\pi^2/3\approx3.3$. Thus the above approximation is quite good.

3. Kink scattering by a mass impurity

When the discreteness is absent, the kink collective coordinate $X(\tau)$ and the velocity $\dot{X}(\tau)$ are connected by the relation (see eq. (11))

$$\dot{X}(\tau)=\dot{X}(0)\exp[-\tfrac{1}{4}(\delta m/m)\,\mathrm{sech}^2X(\tau)]\approx\dot{X}(0)[1-\tfrac{1}{4}(\delta m/m)\,\mathrm{sech}^2X(\tau)]. \tag{14}$$

In the case of a heavy-mass impurity ($\delta m>0$) the kink decreases its velocity near the impurity. However, it cannot be reflected by it because of $\delta(\dot{X})\sim\dot{X}(0)$. The discreteness allows the kink to be reflected by the impurity. To analyse the kink dynamics and calculate the threshold velocity, let us consider the function

$$y=\dot{X}^2(\tau)=y(X). \tag{15}$$

Substituting (15) into eq. (11) yields

$$\frac{dy}{dX}=2\epsilon_1\sin(\kappa X)+\epsilon_2 y\frac{\sinh X}{\cosh^3X}, \tag{16}$$

where

$$\epsilon_1=\frac{4\pi^3}{\sinh(\pi^2/\mu)}=\frac{\mu\omega_p^2}{2\pi},\quad \epsilon_2=\mu\frac{\delta m}{m},\quad \kappa=\frac{2\pi}{\mu}. \tag{17}$$

Eq. (16) may be simply integrated to yield

$$y(X)=\exp\left(-\frac{\epsilon_2}{2\cosh^2X}\right)\left[C+2\epsilon_1\int_0^X\sin(\kappa x')\times\exp\left(\frac{\epsilon_2}{2\cosh^2x'}\right)dx'\right], \tag{18}$$

C being an arbitrary constant. The dependences $y(X)$ at different C are depicted in fig. 1. The curve at $C=0$

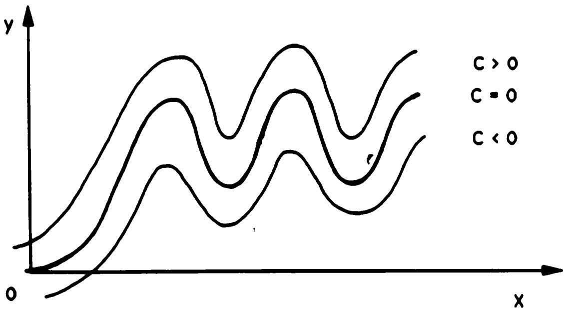

Fig. 1. The function $y=\dot{X}^2$ at different values of C. All curves are symmetric for $x<0$.

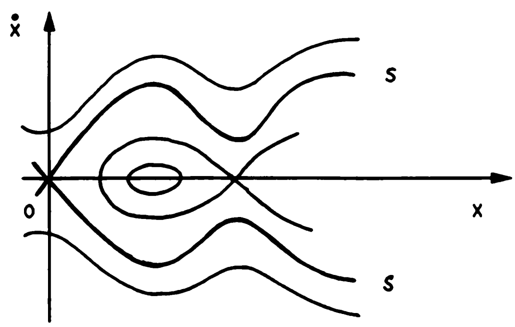

Fig. 2. The phase plane of the dynamical system (15), (16). All curves are symmetric for $x<0$. Curve "s" is the separatrix corresponding to the threshold condition for the kink reflection.

corresponds to the separatrix "s" (fig. 2) on the phase plane which divides two different types of the kink motion, namely, transmission ($C>0$) and reflection ($C<0$) (see fig. 2). To calculate the threshold velocity, we put $C=0$ and consider the asymptote of eq. (18) at $X\to+\infty$,

$$y(X) \xrightarrow[X\to+\infty]{} \frac{2\epsilon_1}{\kappa}(1-\cos\kappa X) + \epsilon_1\epsilon_2 \int_0^\infty \frac{\sin\kappa x'}{\cosh^2 x'}\,dx' . \qquad (19)$$

The last term in eq. (19) describes the shift of the phase curves due to the impurity. The kink reflection is possible for $\epsilon_2>0$ only. Using eqs. (15), (17) we may obtain the threshold value,

$$\left(\frac{dX}{d\tau}\right)^2_{cr} = \frac{\mu^2}{2\pi}\omega_p^2 \frac{\delta m}{m} I(2\pi/\mu) . \qquad (20a)$$

where

$$I(z) = \int_0^\infty \frac{\sin zx}{\cosh^2 x}\,dx . \qquad (20b)$$

Taking account of eqs. (6) and (12b), we may define the threshold velocity of the kink reflection by the mass impurity as follows,

$$V_{cr} = \frac{c}{\mu}\left(\frac{dX}{d\tau}\right)_{cr} = \frac{c\omega_p}{\sqrt{2\pi}}[(\delta m/m) I(2\pi/\mu)]^{1/2} . \qquad (21)$$

When the kink velocity V at infinity is fixed but the impurity mass is a parameter, the kink will be reflected by the impurity provided

$$M > M_{cr} = m[1+g(2\pi/\mu)(v/c)^2] , \qquad (22a)$$

where

$$g(z) = \frac{\sinh(\frac{1}{2}\pi z)}{2\pi^2 z I(z)} . \qquad (22b)$$

As a result, the critical mass depends on the squared kink velocity and it is inversely proportional to the PN potential. In the limit $a\to 0$ the critical mass tends to infinity.

Using the result (22), we can make some estimations of the critical mass calculating the integral (20b). For example, the calculation at $z=2\pi$ yields $I(2\pi)\approx 0.17$ and, as a result, $M_{cr}\approx 42m$ at $V=0.3c$. At $z=8$ we obtain $I(8)\approx 0.13$ which yield at $V=0.2c$ the very large critical mass $M_{cr}\approx 280m$. This strong difference of the critical masses depends on the corresponding (exponential) dependences of the PN potential on the lattice spacing (see eq. (13)).

As a matter of fact, our formulas (21) and (22) are obtained in the framework of the perturbation theory when $\delta m/m$ is not so large. Nevertheless, we believe that the qualitative aspect of the central result is correct while a quantitative agreement with numerical investigations of the same problem may be not so good. In this connection, it is important to note that the kink reflection by a mass impurity has been observed in numerical simulations of the ϕ^4 model performed in ref. [22]. As was observed in this paper, the critical mass M_{cr} for the kink reflection is 40–60 m at $V=0.29c$ which is of the same order as was obtained above. Unfortunately, a more detailed comparison is not possible, because the mentioned paper was devoted to another problem.

4. Conclusions

In this study we have used the effective equation of motion for the kink center in the homogeneous discrete sG model to calculate the threshold velocity for the kink reflection by a heavy mass impurity. The Peierls–Nabarro barrier arising from lattice discreteness plays a dominant role in the reflection. Clearly the effect does not occur in a continuum model since then the Peierls–Nabarro barrier vanishes. Such an effect has been observed in numerical calculations [22] for the ϕ^4 model with a mass impurity because in numerical simulation the discrete version of a continuous model is always used, as a matter of fact. Existence of the Peierls–Nabarro potential in nonlinear inhomogeneous systems may lead to a number of other new and important phenomena and strongly modify transport properties of nonlinear waves in disordered systems. In particular, impurities may strongly modify the kink diffusion coefficient as well as change the probability to create a kink–antikink pair in a thermalized sG chain. The problems are now under consideration and results will be presented elsewhere (see, e.g., ref. [23]).

Acknowledgement

The authors would like to thank Professor C.R. Willis for having sent copies of his papers (refs. [14,16,18,21]). Yuri S. Kivshar acknowledges the hospitality of the Center for Nonlinear Studies at the Los Alamos National Laboratory where the paper was finished; he also thanks A.R. Bishop, D.K. Campbell, P. Lomdahl, St. Pnevmatikos, and M. Peyrard for useful discussions, and R. Scharf for help in numerical calculations.

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