PHYSICAL REVIEW LETTERS

VOLUME 72 | 21 MARCH 1994 | NUMBER 12

Movability of Localized Excitations in Nonlinear Discrete Systems: A Separatrix Problem

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(Received 19 November 1993)

We analyze the effect of internal degrees of freedom on the movability properties of localized excitations on nonlinear Hamiltonian lattices by means of properties of a local phase space which is at least of dimension six. We formulate generic properties of a movability separatrix in this local phase space. We prove that due to the presence of internal degrees of freedom of the localized excitation it is generically impossible to define a Peierls-Nabarro potential in order to describe the motion of the excitation through the lattice. The results are verified analytically and numerically for Fermi-Pasta-Ulam chains.

PACS numbers: 03.20.+i, 63.20.Pw, 63.20.Ry

Recently localized breatherlike excitations were discovered to exist in several different Hamiltonian lattices in one and two dimensions [1–6]. They are self-localized (no disorder) and appear in nonlinear lattices—thus we name them nonlinear localized excitations (NLEs). For certain systems it was possible to create moving NLEs [7,8]. Consequently, the idea arose to describe their motion in a Peierls-Nabarro potential (PNP) [9–12] related to the PNP of kinks [13,14]. Numerical simulations strongly support the existence of a PNP-related phenomenon in Fermi-Pasta-Ulam systems [15] and Klein-Gordon systems [16]. However, as we show below it is generically impossible to define a PNP for NLEs.

The NLE solutions are nontopological, i.e., no special structure of the underlying many-particle potential is required. The only condition is to have nonlinear terms in the potential. One can perform stability analysis and show that if the NLE is localized enough (in practice it will contain only a few particles which are involved in the motion) then generically all Hamiltonian lattices will exhibit families of stable time-periodic NLE solutions [6,17,18]. Hereafter we will call these stable periodic NLEs elliptic NLEs to emphasize their stability property (in a Poincaré mapping they would appear as stable elliptic fixed points [6]). One can view the NLE as a solution of a reduced problem where only M particles are involved in the motion; the rest of the lattice members are held at their ground-state positions. We showed that many frequency NLEs can be excited by perturbing the elliptic NLEs and that thus NLE solutions are motions on M-dimensional tori in the phase space of the reduced problem and in the corresponding local subspace of the phase space of the full system [6,17]. Besides these stable NLE solutions unstable periodic NLEs exist. Their feature is that certain local perturbations destroy the unstable NLE or cause it to move [9,15,19]. Hereafter we will call them hyperbolic NLEs. If one calculates the energy density distribution e_l for the NLE solutions, one can define the position of the energy center of the distribution by $X_E = \sum_l l e_l / \sum_l e_l$. For a given system the elliptic NLE solution yields $X_E = l_0$ (i.e., centered on a lattice site l_0) and the hyperbolic NLE solution $X_E = l_1 + 0.5$ (i.e., centered between lattice sites l_1 and $l_1 + 1$) or vice versa [9,15,19]. Here l, l_0, l_1 denote lattice sites and the lattice spacing is 1. Both elliptic and hyperbolic NLEs as well as certain stable subclasses of their perturbations obey a symmetry during their whole evolution, namely, that the evolution of the NLE part for $x < X_E$ is symmetric (or antisymmetric) to the evolution of the NLE part for $x > X_E$. This symmetry is just the manifestation of Hamiltonian character of motion combined with the discrete translational symmetry of the lattice.

The writing down of a certain PNP for the collective coordinate which describes the motion of the NLE is

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conceptually equivalent to the problem of a pendulum. The PNP barrier $\Delta_{\rm PN}$ is then intimately connected with the energy that is required to overcome the separatrix of the pendulum. This separatrix separates oscillating pendulum solutions from rotating ones [20]. The PNP frequency $\omega_{\rm PN}$ is essentially the pendulum frequency for infinitely small amplitudes.

To describe a periodic elliptic NLE we need to introduce one degree of freedom. We will work in the action-angle phase (J,θ) space and name this degree of freedom J_1. Its corresponding frequency will be $\omega_1 = \dot{\theta}_1 = \partial H/\partial J_1$. Here H denotes the full Hamiltonian of the lattice. We assume that there exists a certain transformation between the original variables (positions, momenta) and the actions and angles. This does not imply integrability of the system as well as it does not imply the inverse. Since our NLE solutions are regular solutions (at least on moderate time scales), there is no need to introduce stochasticity (cf. [17] for details). Because of the symmetry of the elliptic NLE, the NLE will be stationary (nonmoving) for any value of J_1 in the whole range of its existence. To excite a moving NLE we have to excite an additional degree of freedom J_3. Exciting J_3 we destroy the symmetry of the elliptic NLE. But since it is always possible to perturb the NLE conserving the symmetry, we have to include an additional symmetry conserving degree of freedom J_2 into the consideration. Thus we end up with the simplest generic case of a Hamiltonian problem with three degrees of freedom:

$$H = H(J_1; J_2; J_3), \quad \omega_i = \dot{\theta}_i = \frac{\partial H}{\partial J_i}, \quad i = 1,2,3. \tag{1}$$

According to our notation $i = 3$ labels the symmetry-breaking degree of freedom. If it is excited strongly enough, we expect to hit a separatrix which separates stationary NLEs from moving ones. We will name this separatrix movability separatrix. All three degrees of freedom are of local character; they especially can be well defined in the reduced problem for the NLE. Since we can consider the NLE excitation at (or between) any lattice site(s), we thus study the local character of a movability separatrix which is also defined for the infinite system. The movability separatrix for the full system is just a periodic continuation of the local movability separatrix.

Let us state the general condition for the movability separatrix we are looking for. Since on the movability separatrix a trajectory will for infinite times asymptotically reach a hyperbolic state (which is nothing but the hyperbolic NLE and its symmetric perturbations), the corresponding frequency of the 3D degrees of freedom

$$\omega_3 = \frac{\partial H}{\partial J_3} = f(J_1; J_2; J_3) \tag{2}$$

has to vanish on the movability separatrix, i.e.,

$$f(J_1; J_2; J_3) = 0, \tag{3}$$

which implies an equation for a surface in the three-dimensional subspace of the actions $(J_1; J_2; J_3)$. We can always eliminate J_2 using the expression for the energy $E = H(J_1; J_2; J_3)$, so that (3) yields

$$f(J_1; J_2; J_3) = \tilde{f}(E; J_1; J_3) = 0. \tag{4}$$

From (4) it follows that there exists a critical value for J_3 on the movability separatrix:

$$J_3^s = g(J_1; J_2) = \tilde{g}(E; J_1). \tag{5}$$

The only possibility of introducing the PNP would be to use the relation between the potential of a pendulum and its critical value for the action as well as the frequency of small amplitude oscillations:

$$\omega_{\rm PN} = f(J_1; J_2; J_3 = 0) = \tilde{f}(E; J_1; J_3 = 0). \tag{6}$$

It is very important to note that if f from (2) or $\tilde{f}$ from (4) depends on $(J_1; J_2)$ or $(E; J_1)$, respectively, then the same fact holds for $\omega_{\rm PN}$ in (6) as well as for J_3^s in (5). As we immediately recognize a PNP would be different for different $(E; J_1)$ because of the generic dependence of the PNP parameters on the values of E and J_1 in (5) and (6). It is not only that we would obtain different PNPs by varying the energy. Even for a fixed energy different PNPs occur because of the dependence of the right-hand sides in (5) and (6) on J_1.

Let us discuss special nongeneric cases: (i) The Hamiltonian separates in the actions in the following way:

$$H(J_1; J_2; J_3) = H_{12}(J_1; J_2) + H_3(J_3). \tag{7}$$

Then according to its definition ω_3 depends only on J_3. Thus the value of J_3^s becomes independent on $(J_1; J_2)$ or $(E; J_1)$ and a unique PNP can be immediately associated with the term $H_3(J_3)$ in (7). (ii) A more subtle nongeneric case appears if no separation holds but the frequency ω_3 is only a function of energy E. In this case a PNP can be introduced which would depend on the energy of the NLE.

Let us apply the results from above to a class of systems where moving NLEs were detected [7,8,15]:

$$H = \sum_l \left(\frac{1}{2} \dot{P}_l^2 + V(X_l - X_{l-1}) \right) , \tag{8}$$

$$V(x) = \frac{1}{2} C x^2 + \frac{1}{4} x^4 . \tag{9}$$

These systems belong to the class of Fermi-Pasta-Ulam systems [21]. P_l and X_l are the momentum and position of the lth particle, respectively. The parameter C regulates the strength of the quadratic terms. For $C \to \infty$, $E =$ const, Eq. (8) becomes the well-known linear atomic chain, which is integrable and has no NLE solutions. For $C \to 0$, $E =$ const, Eq. (8) becomes a highly nonlinear nonintegrable atomic chain. All properties of (8) can be obtained by fixing the energy, e.g., at $E = 1$ and varying C. All solutions for other energies can be obtained by proper scaling of the times, displacements, and the parameter C: If $\{X_l(t; E = 1; C)\}$ is a solution of (8), then $\{\tilde{X}_l(\tilde{t}; \tilde{E}; \tilde{C}\}$ is a solution for the energy $\tilde{E} = \lambda^{-4}$, parameter $\tilde{C} = C/\lambda^2$, and $\tilde{X}_l(\tilde{t}) = \lambda^{-1}X(\lambda^{-1}t)$. Let us first discuss the case $C = 0$. Then an even simpler scaling holds—it is enough to study the system at one given energy, e.g., $E = 1$, and through the above described scaling all solutions for other energies are obtained. The elliptic NLE solution is the well-known even parity mode [2,15]. It is centered between two particle sites ($X_E = l + 0.5$) and four particles are essentially involved in the motion. Its amplitude distribution can be qualitatively indicated by $(\cdot\cdot\uparrow\ \Downarrow\ \Uparrow\ \downarrow\cdot\cdot)$. More precisely the scaled absolute values of the amplitudes in decreasing order read: 1, 0.165 79, 0.000 48,.... No exact compacton structure is observed as was wrongly claimed in [11] because of a calculation error in Eq. (13) of [11]. The frequency of the elliptic NLE for $E = 1$ is $\omega_1(E = 1) = 1.760 \pm 0.0018$. The hyperbolic NLE solution is known as the odd parity mode [15,19]. It is centered on a particle ($X_E = l$) and essentially three particles are involved in the motion. Its amplitude distribution is roughly $(\cdot\cdot\downarrow\ \Uparrow\ \downarrow\cdot\cdot)$. More precisely the scaled absolute values in decreasing order read: 1, 0.523 04, 0.023 05,.... The frequency of the hyperbolic NLE is found to be $\omega_h(E = 1) = 1.751 \pm 0.0018$.

Let us mention an important property of (8). Besides the energy conservation law this system conserves the total mechanical momentum: $\sum_l P_l = \text{const}$. It is sufficient to study the system in the center of mass frame, so that the total momentum vanishes and the center of mass does not move. All other cases can be obtained by a Galilean boost in (8). Since the NLE solution is localized, the total mechanical momentum outside the NLE is zero. Thus it has to be zero inside too, i.e., our NLE solutions have to obey mechanical momentum conservation, at least approximately. The consequence is that the elliptic NLE (four particles) is described by $4 - 1 = 3$ degrees of freedom. That is exactly our simplest generic problem as described above.

The properties of the perturbed elliptic NLE can be studied with Poincaré mappings for symmetry-preserving perturbations, i.e., for $J_3 = 0$. Then we can consider a reduced problem where the particles outside the NLE are fixed at position zero. This fixed boundary does not break the momentum conservation because of the antisymmetry of the perturbed NLE. The result for the Poincaré map is shown in Fig. 1. The point in the middle of the map corresponds to the elliptic fixed point solution. All torus intersections inside the diamondlike structured torus correspond to stable two-frequency NLEs in the full system (1000 particles). Every torus in Fig. 1 corresponds to a certain triple of $(J_1; J_2; J_3 = 0)$. The fixed point (elliptic NLE) is defined by $(J_1; J_2 = 0; J_3 = 0)$. Thus we first arrive at the unambiguous result that a perturbation of the elliptic NLE preserving the symmetry leads to two-frequency NLE solutions $(J_1; J_2; J_3 = 0)$. This is similar to NLE properties in Klein-Gordon lattices [6,17].

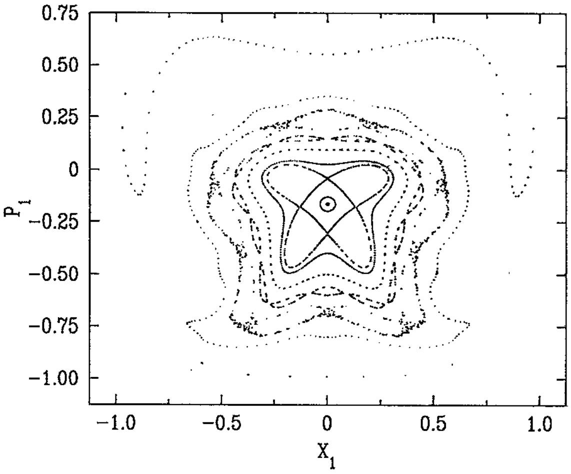

FIG. 1. Poincaré intersection between the trajectory of system 89 for a reduced problem with fixed boundaries: $C = 0$, $E = 1$, $P_1 = -P_0$, $X_1 = -X_0$, $P_2 = -P_{-1}$, $X_2 = -X_{-1}$; all other lattice members are fixed at position zero.

Now we excite the third degree of freedom $J_3 \neq 0$ which destroys the symmetry of the elliptic NLE. We choose a path in phase space where $P_1(t = 0) = -P_0(t = 0)$, $P_2(t = 0) = -P_{-1}(t = 0) = s$, $X_1(t = 0) = -X_{-1}(t = 0) = a$, and all other displacements or momenta are equal to zero at $t = 0$. The total energy is still $E = 1$. We work with 1000 particles. Here the elliptic NLE is chosen to be centered between the lattice sites $l = 0$ and $l = 1$, respectively. The actions are some functions of the chosen path: $J_1 = J_1(E; s; a)$ and $J_3 = J_3(E; s; a)$. We especially know that $J_3(E, s, a = 0) = 0$. By increasing a we measure the time dependence of the energy center $X_E(t)$. The energy density is defined by

$$e_l = \frac{1}{2}P_l^2 + \frac{1}{2}[V(X_l - X_{l-1}) + V(X_{l+1} - X_l)]. \quad (10)$$

Since $X_E(t)$ is independent of time for $a = 0$, we can hope that the energy center will essentially couple only to $(J_3; \theta_3)$ so that we can measure the frequency ω_3. Indeed for $a \neq 0$, $X_E(t)$ oscillates around its mean value of 0.5. There are modulations of this oscillation with the frequency ω_1, but their amplitude is small and we clearly observe the frequency $\omega_3 = \tilde{f}(E; J_1(E; s; a); J_3(E; s; a))$. For small values of a ($< 10^{-4}$) the value of ω_3 becomes independent of a, thus we can measure $\tilde{f}(E; J_1(E; s; a = 0); J_3 = 0)$ which is nothing else than $\omega_{\rm PN}$ [cf. (6)]. Especially for the elliptic NLE solution we find $\omega_3 = 0.343 \pm 0.006$. For two other tori within the diamondlike torus in Fig. 1 ($s = 0.1$, $s = 0.2$) we find $\omega_3 = 0.391 \pm 0.005$ and $\omega_3 = 0.322 \pm 0.005$. Thus we find variations of $\omega_3 = \tilde{f}(E; J_1; J_3 = 0)$ for a fixed value of the energy (by varying J_1) of at least 21%. Now let us increase a for a given value of s and monitor the time evolution of $X_E(t)$.

It is shown in Fig. 2. In agreement with our expectations we find that with increasing a the frequency ω_3 decreases and the amplitude of the oscillations of $X_E(t)$ increases. At a threshold value of $a = a_s$ we clearly observe the crossing of the movability separatrix—the NLE escapes from its mean position.

The properties of the movability separatrix are easily constructed. Because of the scaling property of the Hamiltonian for $C = 0$ we find all solutions at other energies by proper scaling. Since the frequencies scale too, we immediately find that $\tilde{f}(E; J_1; J_3 = 0)$ depends on the energy. Because we found strong (20%) variation of this frequency on the energy hypersurface (for constant energy), the J_1 dependence is also significant. Having $\tilde{f}(E; J_1; J_3 = 0)$ to be strongly dependent on E and J_1 we find using (2)–(6) that the same holds for the critical value of J_3^s on the movability separatrix. Thus we see that our example is a generic case, and a PNP cannot be constructed.

If one considers $C \neq 0$ (here $C = 0.3$), one rediscovers all the above statements. There are only quantitative changes—the dependence of ω_3 on E and J_1 becomes weaker. For large enough values of C (fixing the total energy) the frequencies ω_2 and ω_3 can become resonant with the phonon band (which still does not prevent us from studying the movability separatrix on short time scales). For too large values of C the frequency ω_1 becomes resonant with the phonon band and the whole NLE solution then quickly disappears [6,17,22,23].

Let us make some final comments. First our results demonstrate a clear way of studying and characterizing the movability properties of NLEs in terms of a movability separatrix in phase space. Second we find that generically no simple PNP can be introduced. The reason is the intimate connection between the "translational" degree of freedom (J_3) and the "internal" degrees of freedom (J_1, J_2) through the Hamilton function. Consequently, the necessary energy supply to an elliptic NLE in order to cross the movability separatrix at a certain orbit can be positive, zero, or negative depending on the chosen orbit on the movability separatrix. That is the reason why intuitive approaches to derive PNPs are sometimes even self-contradictory: in [12] under assumption of separability property [our Eq. (7)] of a discrete nonlinear Schrödinger equation a PNP is derived which is energy dependent, but that implies the nonseparability of the Hamiltonian. The results in the present paper disprove the conjecture in [11], where it is predicted that for our equations (8) and (9) and $C = 0$ freely moving NLEs exist, i.e., no PNP (no separatrix) should exist. Our Fig. 2 shows that the separatrix exists. A very interesting perturbation analysis was carried out in [10,12] for a weakly perturbed integrable Ablowitz-Ladik lattice. The authors were able to show analytically that the NLE solution is described by the evolution of three internal degrees of freedom, so that the movability separatrix can be analyzed analytically in their case. Finally we mention the treatment of a discrete sine-Gordon breather with a collective coordinate method [24]. There it was shown how to treat unambiguously a NLE with 2 degrees of freedom. Already there it is clear that no unique PNP exists, i.e., the amplitude of the PNP is a function of E and the NLE amplitude.

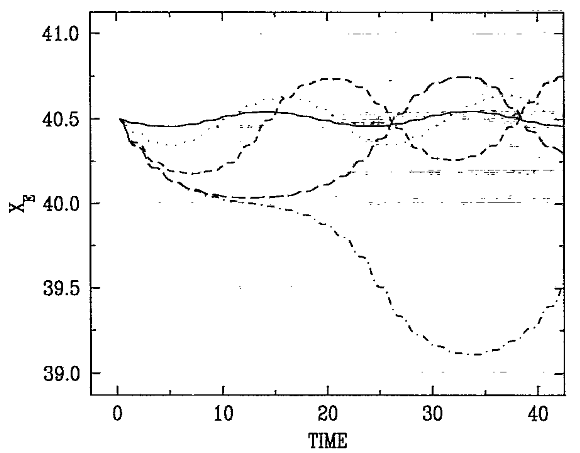

FIG. 2. Time dependence of the center of energy of an NLE for different asymmetric perturbations a (see text): solid line, $a = 0.02$; dotted line, $a = 0.06$; dashed line, $a = 0.1$; long dashed line, $a = 0.112$; dash-dotted line, $a = 0.113$.

This work was supported in part (S.F.) by the Deutsche Forschungsgemeinschaft (Fl200/1-1).

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