Spatial chaos in a nonlinear monatomic chain

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We derive an area-preserving map from the microscopic model of a nonlinear monatomic chain at a $T=0$ first-order phase-transition point. The model is useful for describing first-order structural phase transitions and the metal-insulator transition in various condensed-matter systems. We numerically study the nature of the trajectories of this two-parameter map associated with the lattice displacement pattern. The map displays spatial chaotic behavior for various values of the parameters m and δ. The result is interpreted in terms of soliton interaction, soliton pinning, and the metal-insulator transition in these systems.

In recent years nonlinear monatomic-chain models have been extensively used in condensed-matter physics, because they provide a nonperturbative approach to strongly anharmonic systems. These models have been found particularly useful for systems that show structural phase transitions like the ferroelectric phase transition, charge-density-wave transition, metal-insulator transition, etc. They usually consist of a one-dimensional lattice with harmonic coupling between neighboring lattice points and a nonlinear on-site potential.[1] The nonlinear on-site potential gives rise to soliton states in the system. A typical example is the discrete $\lambda\phi^4$ theory in which the amplitude at the nth site is given by[2]

$$\phi_n=(-1)^n\phi_0\tanh(na/l_0)\ , \tag{1}$$

where a is the lattice constant, l_0 represents the width of the amplitude soliton, and ϕ_0 denotes distortion in the dimerized state. Because of the existence of the modulated structure (lattice distortion) in the system, there occurs a competition between the modulated period (P) and the lattice period (Q). The wave number of a commensurate state of the system is $q=P/Q$. As is well known, such types of competition between the spatial periods usually lead to spatial chaos. In fact, spatial chaos has been seen in the discrete area-preserving iterative maps of this particular system[2,9] and also in other systems.[4,5]

In terms of the soliton picture, the occurrence of spatial chaos can be understood more clearly. The soliton gets pinned to the lattice due to lattice commensurability. The pinning of the soliton to the lattice is overcome by the soliton interaction energy $E_{\text{int}}\sim\exp(-al)$, where l is the distance between solitons. So when the distance between the solitons becomes large, the soliton interaction cannot overcome the pinning energy, and the soliton remains pinned to the lattice. When the pinned soliton states are regularly spaced, we get high-order commensurate states. If the interaction between the solitons is very weak (for large separation between them) one expects a random distribution of the soliton states in the lattice. Such stable random distribution of the soliton states appears as a "chaotic" solution of the discrete map of the given system.

However, these studies so far have been confined mostly to systems which show a second-order phase transition.[2,5]

Recently we have considered a model[6] of a nonlinear monatomic chain with higher-order nonlinearity that describes a first-order structural phase transition at zero temperature. The generalized nonlinear on-site potential considered is

$$V(\phi)=C\phi^{2m+2}+B\phi^{m+2}+A\phi^2+D \tag{2}$$

with an adjustable order of nonlinearity for $m=1,2,3,\ldots$. At the transition point

$$B^2=4AC,\quad A,C>0 \text{ and } B<0\ . \tag{3}$$

The potential has doubly degenerate minima for all odd values of m and triply degenerate minima for all even values of m. For $m=2$, this potential [Eq. (2)] describes the well-known $\lambda\phi^6$ theory.

The energy E of the system can be written in the continuum approximation as

$$E=\int_{-\infty}^{\infty}[\tfrac{1}{2}\lambda(d\phi/dx)^2+\gamma V(\phi)]dx\ , \tag{4}$$

and the equation of motion (static) in the displacive regime is given by

$$\lambda(d^2\phi/dx^2)-\gamma(dV(\phi)/d\phi)=0\ . \tag{5}$$

We have obtained the exact solutions (kinks and antikinks) of Eq. (5) as[6]

$$\phi(x)=\begin{cases}2^{-1/m}\phi_0[1\pm\tanh(mx/2\xi_0)]^{1/m} & \text{for } m=1,3,5,\ldots \quad (6a)\\ \pm 2^{-1/m}\phi_0[1\pm\tanh(mx/2\xi_0)]^{1/m} & \text{for } m=2,4,6,\ldots, \quad (6b)\end{cases}$$

where $\phi_0=(2A/|B|)^{1/m}$, $\xi_0^2=\lambda/2A\gamma$. We have also shown that these solutions are stable and have finite energy. In general, the solution to Eq. (5) is a soliton lattice with distance $l=a/c$ (c being soliton density) between the solitons. As mentioned above, the solitons interact with each other through an exponential repulsive potential.[7] In the continuum limit, we obtain[2] the energy of interaction between the solitons separated by a distance l as

$$E_{\text{int}}=k\exp(-lm/2\xi_0)\sim\exp(-1m\sqrt{A\delta}/2)\ , \qquad (7)$$

where k is a constant that depends[2] on the soliton energy E_s [Eq. (4)] and $\delta=2\gamma/\lambda$. The soliton energy can be easily evaluated, which in our case is given by

$$E_s=A\gamma\xi_0(2A/|B|)^{2/m}[1/(1+2/m)]\ .$$

Thus we see that E_{int} decreases with increase of parameters m (order of nonlinearity) and δ (strength of nonlinearity).

The solution has translational symmetry, and the lattice can be shifted along the x axis without any cost of energy. Since the solitons are charged ($\pm e$), the soliton lattice can conduct.[2] However, as mentioned above, the solitons also experience a pinning potential (attractive) due to the periodic nature of the lattice. Using the Poisson summation method[8] we can estimate the pinning energy of soliton as

$$E_{\text{pin}}=\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty}dx\,E_s(x)\exp(2\pi imx)\ . \qquad (8)$$

We estimate the term with $m=1$ only, since the term with $m=0$ gives the continuum energy E_s [Eq. (4)] and the remaining terms are small. Now from Eq. (5) we get

$$\tfrac{1}{2}\lambda(d\phi/dx)^2=\gamma V(\phi)\ ,$$

which gives $E_s(x)=2\gamma V(\phi)$. Substituting this in Eq. (8) and using Eq. (6) we can write the pinning energy of the soliton as

$$\begin{aligned}E_{\text{pin}}&=4\gamma\int_{-\infty}^{\infty}dx[(1+\tanh mx/2\xi_0)^{(2/m)-2}\text{sech}^4 mx/2\xi_0\cos2\pi x]\\&=2^{2+m/2}(\xi_0/m)\text{Re}\int_{-\infty}^{\infty}dk\left\{\frac{\exp[-2(1+i\xi_0\pi/m)k]}{[1+\exp(-k)]^{2+2/m}}\right\}.\end{aligned}$$

This integration can be evaluated exactly for arbitrary values of m, and we obtain[9]

$$E_{\text{pin}}=2^{2+2/m}(\xi_0/m)\times\text{Re}[B(2-2i\xi_0\pi/m,2/m+2i\xi_0\pi/m)]\ ,$$

where $B(x,y)$ denotes a β function. Using the relation between the β and γ functions and the Gauss multiplication formula for the γ function,[9] it can be shown that, for $\xi_0\gg1$,

$$E_{\text{pin}}=k(m)\exp(-2\xi_0\pi^2/m)\sim\exp(-2\pi^2/m\sqrt{A\delta})\ , \qquad (9)$$

where $k(m)$ is a constant that depends on the value of m. For $m=1$, $k(1)=64/3(\xi_0\pi)^4$. Similarly, it can be obtained for other values of parameter m. Thus we see that, in contrast to the soliton interaction energy E_{int}, the soliton pinning energy increases with an increase in the parameters m and δ.

As has been mentioned above, the soliton gets pinned to the lattice if the soliton interaction energy cannot overcome the pinning energy. The translational invariance is lost and the lattice cannot have Frölich conductivity. A depinning transition takes place when $E_{\text{int}}=E_{\text{pin}}$, which determines the critical concentration (density) of the solitons[2] as

$$c_{\text{cr}}=(m^2a)/4\pi^2\xi_0^2=m^2aA\delta/(4\pi^2)\ . \qquad (10)$$

A metal-insulator transition takes place at soliton concentration (density) $c>c_{\text{cr}}$. This can be very easily seen from the numerical study of Eq. (5).

The energy of the system can be written in the discrete form as

$$E=\sum_{n=-\infty}^{n=\infty}\lambda/2(\phi_n-\phi_{n-1})^2+\gamma V(\phi_n)\ . \qquad (11)$$

The discrete form of the equation of motion [Eq. (5)] can be written as infinity of coupled difference equations,

$$(\phi_{n+1}-\phi_n)-(\phi_n-\phi_{n-1})=(2\gamma/\lambda)\phi_n[1-\phi_n^m][1-(m+1)\phi_n^m]\ , \qquad (12)$$

where ϕ_n denotes displacements of the particle at the nth site on the chain. Introducing $\psi_n=\phi_n-\phi_{n-1}$, we get a two-dimensional discrete map,

$$\begin{aligned}\psi_{n+1}&=\psi_n+\delta\phi_n[1-\phi_n^m][1-(m+1)\phi_n^m]\ ,\\ \phi_{n+1}&=\phi_n+\psi_{n+1}\ .\end{aligned} \qquad (13)$$

For a given arbitrary initial value (ϕ_0,ψ_0) the above map determines the displacement field ϕ_n at all subsequent sites along the chain for different choices of the parameters m and δ.

Now we present the results of the numerical study of this discrete map. The advantage of studying this map is that it has two parameters, namely, δ and m. By varying δ in the corresponding discrete map [Eq. (13)] we can study the effect of variation in the strength of nonlinearity, whereas by varying m we can study the effect of varying order of nonlinearity, on the lattice displacement pattern. So far other studies have been confined to variation only in parameter δ with fixed order (m) of nonlinearity.[2,4] Jensen and Lomdahl[5] have studied a two-dimensional area-preserving map that depends on two parameters. However, in their case the parameters depend only on the strength of the coupling constants (the strength of the interaction between the ions on the chain and that of interchain interaction), and hence by varying the parameters they could study the effect of variation of strength of nonlinearity of the soliton states. In their model it is not possible to check the effect of higher-order nonlinearity on the soliton states. The other advantage of studying this map is that it represents a model for first-order phase transitions, while other similar studies so far have been confined only to models of second-order phase transitions.[2-4] It should be noted that for odd values of m, the nonlinear on-site potential [Eq. (2)] is asymmetric (in $\phi \to -\phi$), whereas it is symmetric for even values of m.

The map [Eq. (13)] is area preserving. From the stability analysis[10] it can be easily checked that this map has three fixed points (ϕ,ψ) at (0,0), (1,0), and $([1/(m+1)]^{1/m},0)$ for odd values of m $(=1,3,5,\ldots)$. Out of these three fixed points the first two are hyperbolic fixed points and the last one is an elliptic fixed point. Similarly, for even values of m $(=2,4,6,\ldots)$, there are five fixed points, of which the three points at (0,0) and $(\pm 1,0)$ are hyperbolic fixed points, and the two others at $(\pm[1/(m+1)]^{1/m},0)$ are elliptic fixed points. The iterates of the discrete map given by Eq. (13) are shown in Figs. 1–3 and are obtained for different values of the parameters m and δ with some chosen sets of initial conditions (ϕ_0,ψ_0). To be specific we have chosen the initial conditions on the $\psi_n=0$ axis. For our study we have chosen two values of δ (one low value, $\delta=0.15$ and a high value, $\delta=0.41$) and vary the order of nonlinearity (m).

Let us first consider the case in which the values of m are odd. The ψ_n versus ϕ_n plot for $\delta=0.15$ and $m=1$ displays periodic incommensurate states for different chosen initial conditions. When the value of δ is increased to 0.41, we get the regular orbits again. Thus for $m=1$ and for these values of δ we do not find any chaotic trajectory. As the order of nonlinearity is increased to 3, for $\delta=0.15$ we get regular orbits and chain of islands (high-order commensurate states) but chaotic orbits are still absent in this case [Fig. 1(a)]. The system is still conducting. However, when the strength of nonlinear coupling is increased to $\delta=0.41$, the plot for $m=3$ [Fig. 1(b)] displays well-pronounced chaotic states along with the regular orbits and chains of islands. This is expected because, as shown above (analytically), the pinning energy increases with an increase in m and δ, and the soliton gets pinned. When the pinned solitons are regularly placed, we get a high-order commensurate state (islands), whereas the chaotic regime is formed by the random distribution of pinned solitons.[2] Figures 2(a) and 2(b) show the plots for $m=5$ with $\delta=0.15$ and $\delta=0.41$, respectively. Thus, when $m=5$, the nonlinearity is already increased to such an extent that, even for a low value of $\delta=0.15$, well-pronounced chaotic states are seen as shown in Fig. 2(a). Similar lattice displacement patterns are also seen for even values of m, in which case there are five fixed points. For $m=4$ and $\delta=0.15$ and 0.41 the plots are shown in Figs. 3(a) and 3(b), respectively. Here again the chaotic states are very pronounced for $\delta=0.41$. Similar plots are also obtained for $m=6$. For higher values of m (>7), the lattice displacement patterns show chaotic behavior for almost all the initial conditions.

In conclusion, we say that we have yet another exam-

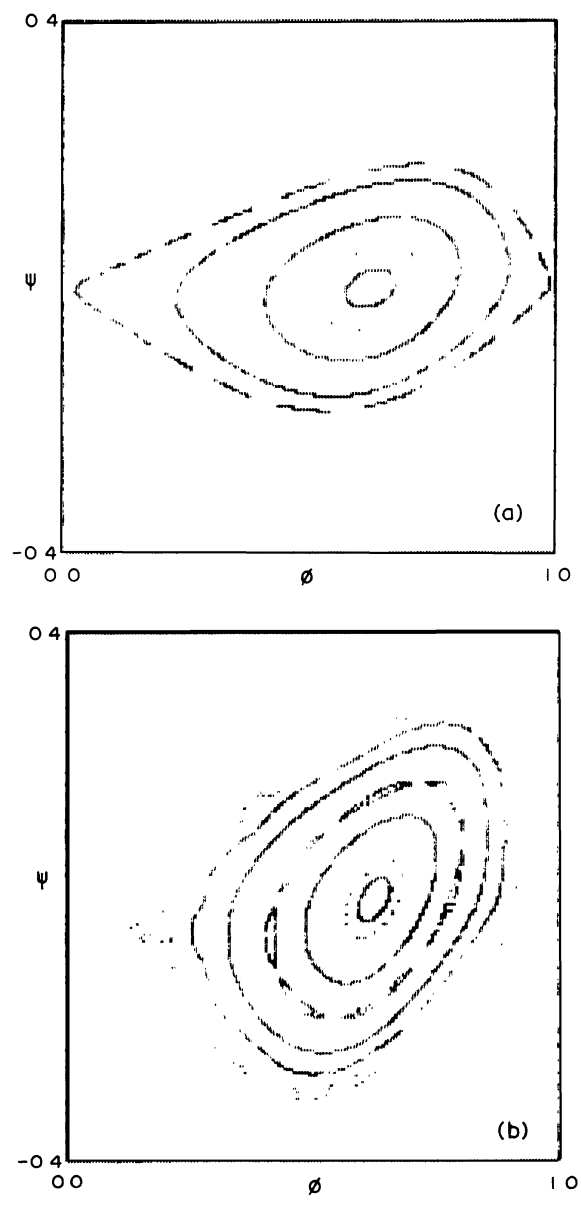

FIG. 1. ψ_n vs ϕ_n plots of Eq. (13) for (a) $m=3$, $\delta=0.15$ and (b) $m=3$, $\delta=0.41$.

ple of the discrete area-preserving map, which is derived from a microscopic model. The advantage of this map is that it is a kind of generalized map such that we can vary two parameters, m and δ, to see the effect of higher-order nonlinearity and strength of nonlinearity on the lattice displacement patterns. As compared to a discrete $\lambda\phi^4$ map,[2] the numerical iterations of this map display a greater number of high-order commensurate states (chains of islands). It is seen from the plots that as the order (m) and strength (δ) of nonlinearity is increased, the chaotic regime becomes more pronounced. This agrees with the analytical calculation that shows that the pinning energy increases and the interaction energy decreases with an increase in m and δ, thereby creating soliton states. The chaotic regime is formed by random distribution of the pinned solitons. Also it is seen from the plots that, as the order of nonlinearity is increased the chaotic solutions occur even for lower values of δ. The plot also shows a very sensitive dependence of the trajectories on the initial conditions for higher values of m.

Recently we have shown that[11] a diatomic chain with this nonlinear on-site potential [Eq. (2)] also supports soliton solutions apart from the nonlinear phonon and periodic solutions. It would be interesting to see the

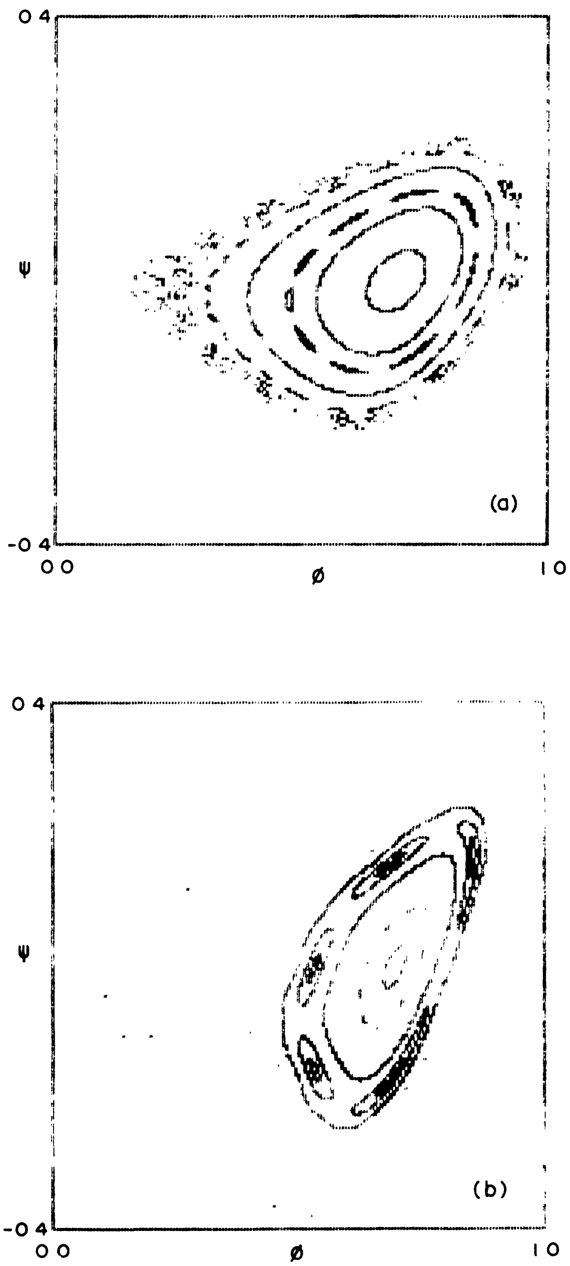

FIG. 2. ψ_n vs ϕ_n for (a) $m=5$, $\delta=0.15$ and (b) $m=5$, $\delta=0.41$.

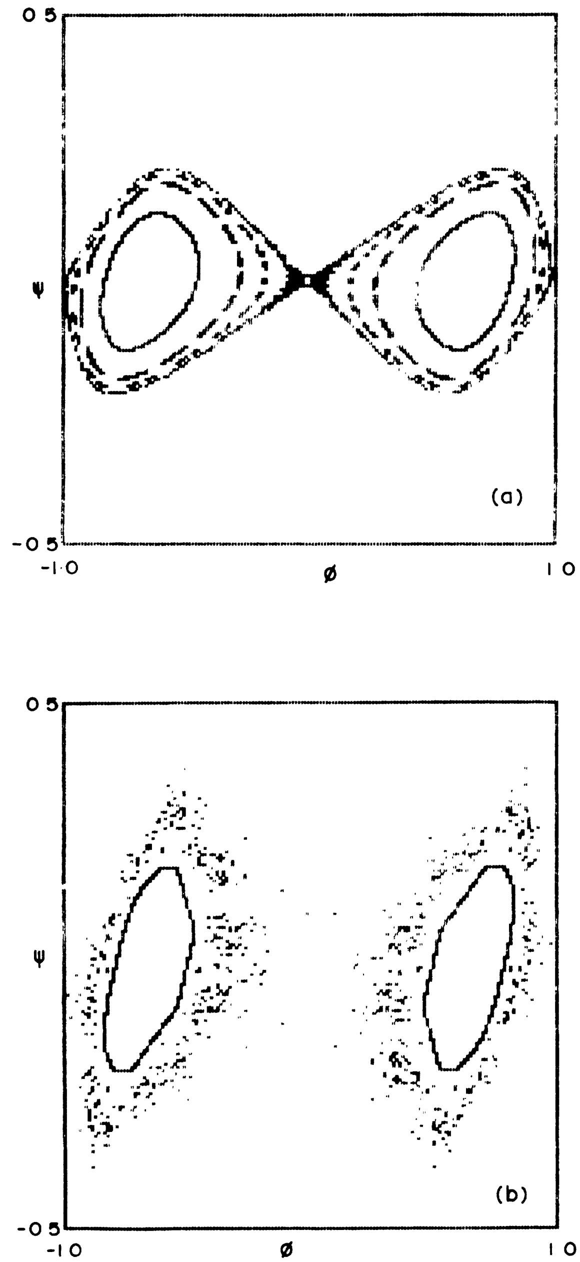

FIG. 3. ψ_n vs ϕ_n for (a) $m=4$, $\delta=0.15$ and (b) $m=4$, $\delta=0.41$.

effect of an m and δ variation on the lattice displacement pattern in this system.

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