Unstable periodic orbits and characterization of the spatial chaos in a nonlinear monatomic chain at the $T=0$ first-order phase-transition point

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We consider the problem of characterization of the observed spatial chaos in a nonlinear monatomic chain model. The model is used for describing the systems that show a structural phase transition such as a ferroelectric transition, metal-insulator transition, charge-density-wave transition, etc. The characterization of the spatial chaos in the previously inaccessible chaotic regime of the nonlinear system is made by calculating the unstable periodic orbits associated with the system in the regime using the symbolic dynamic technique. The characteristic quantities such as the Lyapunov exponents are calculated in terms of the periodic points of the unstable periodic orbits so obtained, and the hierarchical framework based on the lengths of the periodic orbits have been used to calculate the topological entropy of the system in the chaotic regime. The usefulness of such unstable periodic orbits so obtained for studying the quantum behavior of the nonlinear system is also discussed.

In recent years, one-dimensional monatomic chain models with harmonic coupling between neighboring sites and an on-site strongly anharmonic potential have been used for describing systems that show a structural phase transition (SPT), such as the ferroelectric phase transition, charge-density-wave transition, metal-insulator transition, etc. The Hamiltonian of such systems can be written as

$$H=\sum_n(\lambda/2)(\phi_n-\phi_{n-1})^2+\gamma V(\phi_n)\ , \tag{1}$$

where ϕ_n denote displacements of the particle at the nth site of the chain and $V(\phi_n)$ is the nonlinear on-site potential. All these models describe two types of SPT, namely, order-disorder and displacive phase transitions. Whereas in the former case the on-site potential is much larger than the intersite interaction, in the latter case the reverse is true. In the case of the displacive phase transition, using an exact nonlinear technique is important, since near the transition temperature the displacement is large and perturbation theory is not valid. It may be noted, however, that these one-dimensional chain models do not show a phase transition at finite temperature. The effect of the nonlinear on-site potential on the dynamics of the system is to create soliton states in the system. The presence of the soliton states in turn gives rise to the observed spatial chaos in the type of systems represented by Eq. (1).

In a recent paper[1] (hereinafter referred to as paper I), we have shown how the occurrence of spatial chaos in the system can be clearly explained in terms of the soliton states present in the system. We considered a model nonlinear on-site potential, which describes a first-order phase transition as

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

The order of nonlinearity in this potential can be adjusted through the parameter m which takes on integer values $m=1,2,3,\ldots$. 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 the parameter m and triply degenerate minima for all even values of m. For $m=2$, this potential describes the well-known $\lambda\phi^6$ theory for the first-order SPT. The $m=1$ case of this potential has been used to study the statistical mechanics of field theories with broken, global, and local SU(3) gauge symmetries, where it has been shown that the presence of the cubic term in the potential restores the symmetry by a first-order phase transition, rather than a second-order transition.[2]

The discrete forms of the equations of motion for this potential have amplitude solitons (kink/antikink) given by (paper I)

$$\phi_n=\begin{cases}2^{-1/m}\phi_0[1\pm\tanh(mna/2\xi_0]^{1/m} & \text{for } m=1,3,5\ldots & \text{(4a)}\\ \pm2^{-1/m}\phi_0[1\pm\tanh(mna/2\xi_0]^{1/m} & \text{for } m=2,4,6\ldots\ , & \text{(4b)}\end{cases}$$

where $\phi_0=[2A/|B|]^{1/m}$, $\delta=2\gamma/\lambda$, $\xi_0^2=\lambda/2A\gamma$, and a is the lattice constant. Note that, because of the chosen form of our potential Eq. (2), we have a two-parameter problem. The parameter m determines the effect of the change in the order of nonlinearity, while the parameter δ describes the effect of the variation in the strength of nonlinearity on the dynamics of the system. We can vary both the parameters m and δ. This is in contrast to the usual one-parameter problem considered in the literature[3–5] where the variation of the parameter involves only a change in the strength of the nonlinearity (δ) while keeping the order of the nonlinearity (m) fixed.

The discrete equation of motion Eq. (3) can be written in the form of a two-dimensional map:

$$\psi_{n+1}=\psi_n+\delta\phi_n[1-\phi_n^m][1-(m+1)\phi_n^m] ,$$
$$\phi_{n+1}=\phi_n+\psi_{n+1} , \qquad (5)$$

where $\psi_n=\phi_n-\phi_{n-1}$. For given arbitrary initial values ϕ_0 and 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. Beside being a two-parameter map, the other advantage in studying this particular map is that it represents a model for the first-order SPT, whereas most of the other models studied in this connection so far have been confined to the study of the second-order SPT.

The iteration of the map in Eq. (5) shows the presence of spatial chaos in the system (paper I),[1] for various values of the parameters m and δ. It is observed that the spatial chaos becomes more pronounced for increasing order of nonlinearity (larger values of the parameter m). Similarly, for a fixed value of the parameter m (order of nonlinearity), the spatial chaos is more pronounced for increasing values of the parameter δ (the strength of the nonlinear on-site potential). In terms of the soliton picture the occurrence of spatial chaos can be described as follows. The soliton gets pinned to the lattice sites due to the lattice commensurability. The pinning energy can be calculated as[1] (paper I)

$$E_{\text{pin}}\sim\exp(-2\pi^2/m\delta\sqrt{A}\,) . \qquad (6a)$$

The pinning of the soliton to the lattice sites is overcome by the soliton (repulsive) interaction energy[1] (paper I)

$$E_{\text{int}}\sim\exp(-lm\delta\sqrt{A}\,/2) , \qquad (6b)$$

where $l=a/c$ (c being the soliton density) is the distance between the solitons. The solitons get pinned to the lattice sites if the soliton interaction energy cannot overcome the pinning energy. If the interaction between the solitons is very weak (for large separation between them), then one expects a random distribution of the soliton states on the lattice. Such a stable random distribution of the soliton states appears as spatial chaos, as is observed[1] (paper I) in the numerical iteration of the map Eq. (5). From Eqs. (6a) and (6b) we see that, in contrast to the soliton interaction energy E_{int}, the soliton pinning energy E_{pin} increases with an increase in the parameters m and δ. This explains why the observed spatial chaos is more pronounced for larger values of the parameters m and δ.

In this paper, we consider the problem of characterization of the observed spatial chaos[1] (paper I) in the nonlinear system represented by a nonlinear on-site potential as in Eq. (2). Chaotic behavior in dynamical systems has been a subject of extensive study in recent years. Many low-dimensional condensed matter systems exhibit a transition from regular to chaotic behavior. More recently, the emphasis has been shifted to the chaotic regime itself[6] and the characterization of the chaos in this regime. There are no systematic methods to get any quantitative information in this regime. For example, in paper I, we have identified the chaotic trajectories by visual inspection of the random distribution of the points in phase space corresponding to that particular trajectory. Characterization of chaos means quantitative measure of the degree of stochasticity for a trajectory in the chaotic regime. Usually, the measure of the degree of stochasticity in the chaotic regime is obtained by calculating, for the nonlinear system concerned, characteristic quantities like the Lyapunov exponents, Kolmogorov entropy, fraction dimension, topological entropy, etc. However, the numerical evaluation of these quantities requires a large number of points in phase space, which are obtained by iterating the map starting from a given initial condition.[7] So the question arises as to how one characterizes chaos for a trajectory which has only a few randomly distributed points in phase space. The present paper is motivated by this question. Here we are faced with the same situation for the chaotic trajectories which have only a few points in phase space as reported in paper I. As has been mentioned above, Eq. (5) represents a two-parameter map; one parameter represents the order of nonlinearity (m) and the other parameter (δ) represents the strength of the nonlinear on-site potential Eq. (2). Now, as we increase the values of either of the two parameters and try to iterate the map Eq. (5), we get a lesser number of points in phase space, as after a few iterations the numbers become very large and cannot be numerically handled any further. For example, in Fig. 6(a) of paper I, the outermost trajectory, which represents the chaotic trajectory, has just 150 points. Further iteration makes the numerical value of ϕ_n very large and it cannot be handled by the computer any more. If we try to increase the values of the parameters m and δ above those considered in Fig. 6(a) of paper I, we get even fewer points to plot in the phase space for a trajectory. Because of this difficulty, it is not possible to characterize chaos for these chaotic trajectories by calculating characteristic quantities like the Lyapunov exponents, etc., as the evaluation of these quantities requires a large number of points in phase space.

To solve this problem, we have used the approach suggested by Auerbach *et al.*[6] that a useful way to get quantitative information in the chaotic regime is to consider the unstable periodic orbits associated with the chaotic dynamics. Such orbits provide a hierarchical framework based on their lengths, which can be used for calculation of the topological entropy, Lyapunov exponents, etc. which characterize the dynamics of chaotic systems. In terms of such unstable periodic orbits, the topological entropy K_0 is defined as the exponential growth rate of the number of periodic orbits and is calculated as

$$K_0=\lim_{p\to\infty} 1/n\,\ln(N_p-1) , \qquad (7)$$

where N_p is the number of points which belong to the periodic orbits of order p and its divisors, i.e., $N_p=\sum_i iN_c(i)$, where $N_c(i)$ is the number of periodic cycles of order i and the summation is over all divisors of p

including 1 and p. For p sufficiently large, we have the approximation to the pth order entropy as $p_0 \simeq 1/p \ln(N_p - 1)$. For such unstable periodic orbits in the chaotic regime, it is now also possible to calculate the Lyapunov exponents which are given by the logarithm of the diagonal elements of the matrix obtained by taking the product of the Jacobian matrices evaluated at each point of the corresponding unstable periodic orbits.[8] Thus, if we can obtain the unstable periodic orbits of the nonlinear system in the chaotic regime, we can also evaluate quantities like the Lyapunov exponents, topological entropy, etc. which characterize chaos in the system.

Cvitanovic, Gunaratne, and Procaccia[9] have given a method for obtaining the periodic orbits of a map by iterating the given map using the symbolic dynamic technique. However, we cannot use this method for our map, because, as has been mentioned above, our problem is with the map iteration itself. As we increase the value of the parameters m and δ and try to iterate the map in Eq. (5), we find that after a few iterations ϕ_n becomes very large and it becomes difficult to handle numerically with the computer. So for our map we have used an alternative method recently suggested by Biham and Wenzel[10] to obtain the unstable periodic orbits and determine the Lyapunov exponents for such orbits. The method involves calculation of the extremal configurations of the Hamiltonian from which the given map can be derived. The extremal configurations are obtained by using the symbolic dynamic technique. From this one can find the unstable periodic orbits to any desired accuracy. The advantage of this method is that it can be used for any range of parameter values. For example, using this method Biham and Wenzel[10] have obtained unstable periodic orbits of the Henon map even in the previously inaccessible region of parameter values. This is exactly what we need for our problem, i.e., to obtain the unstable periodic orbits in the parameter region where map iteration is not possible beyond the first few iterations.

The Hamiltonian Eq. (1) describes an infinite chain of atoms interacting with an on-site potential $V(\phi_n)$ and among themselves. The force on the nth atom in the chain is given by $F_n = -\partial H_n / \partial \phi_n$, which for the potential $V(\phi_n)$ in Eq. (2) becomes

$$F_n = (\phi_{n+1} - 2\phi_n + \phi_{n-1}) - \delta\phi_n(1-\phi_n^m)[1-(m+1)\phi_n^m]$$

with $\delta = 2\gamma/\lambda$. When the chain is in stable or unstable equilibrium (namely, an extremum configuration of the Hamiltonian), then $F_n = 0$ for all n. In this case, $F_n = 0$ corresponds to the static Euler Lagrange equation associated with the Lagrangian corresponding to the Hamiltonian in Eq. (1). Note that this set of equations is equivalent to the map in Eq. (5) in the sense that every trajectory of the map obeys $F_n = 0$ and vice versa. This can easily be seen by taking the map in Eq. (5) and eliminating ψ_n for all n. Now, to find the unstable periodic orbits of the map in Eq. (5), we use the symbolic dynamic technique due to Biham and Wenzel.[10] In the extremum configurations, each atom in the chain can be either at a local minimum or at a local maximum of the potential Eq. (2), there being 2^p configurations of order p. Each of these configurations $x_1, \ldots, x_p$ can be identified by a symbol sequence of the form $S_1, \ldots, S_p$, where the symbol S_n takes the value $+1$ when the atom is at a local minimum and -1 if it is at a local maximum. To find then a specific extremal configuration of order p of the given Hamiltonian, we introduce an artificial dynamics defined by

$$dx_n/dt = S_n F_n \;, \quad n = 1, \ldots, p \;,$$

where $S_n = \pm 1$. Then we solve the above set of coupled equations subject to the periodic boundary condition $x_{p+1} = x_1$ for initial conditions x_n. This drives the system towards the desired extremum associated with the given set $\{S_n\}$. When the forces on all the atoms decrease to zero (to a desired accuracy), the resulting structure x_n, $n = 1, \ldots, p$, is simultaneously an extremum static configuration of the Hamiltonian and an exact periodic orbit of the map in Eq. (5).

We have calculated all the unstable periodic orbits of order p, up to $p = 19$, for the whole allowed set $\{S_p\}$ of the symbol sequence. For example, there are six allowed unstable periodic orbits of order 9, and Table I shows the corresponding symbol sequence, periodic points, and Lyapunov exponents obtained numerically for one of such orbits.

The existence of a positive Lyapunov exponent (λ_1) shows that this particular unstable periodic orbit is a chaotic orbit. The values of the two Lyapunov exponents obtained are equal in magnitude and opposite in sign as is expected for the Hamiltonian system Eq. (1). This result reported here is for the parameter values $m = 6$ and $\delta = 1.0$. As has been mentioned above, the iteration of the map in Eq. (5) is not possible for such values of the parameters and hence it is not possible to characterize chaos for such values of the parameters. However, in terms of the unstable periodic orbits as obtained above, we can now say that there are chaotic orbits present for these particular values of the parameters and such chaotic orbits can also be characterized in terms of the Lyapunov exponents obtained for the corresponding orbits. In Table II we present the number of allowed unstable periodic orbits of order $p = 11-19$ for the values of

TABLE I. Results for one of the six allowed unstable periodic orbits of order 9.

Symbol sequence	$\{S_q\} \equiv \{1,1,-1,-1,1,-1,1,-1,-1\}$		
Points on the unstable periodic orbit	0.8152	0.2074	0.8814
	0.1929	0.7862	0.9873
	0.7862	0.1929	0.2074
Lyapunov exponents	$\lambda_1 = 0.6047$	$\lambda_2 = -0.6047$	

TABLE II. Results for the allowed unstable periodic orbits of order $p=11-19$.

Period	No. of allowed unstable orbits	Topological entropy
11	9	0.6027
12	12	0.5974
13	17	0.5991
14	22	0.5905
15	33	0.5976
16	41	0.5848
17	61	0.5893
18	86	0.5886
19	119	0.5884

the parameters $m=6$ and $\delta=1.0$. The corresponding topological entropy, which is another quantity that characterizes chaos in a system, is also listed for unstable periodic orbits of order p. It can be easily seen that the topological entropy K_0 saturates for orbits of higher order p. The unstable periodic orbits can also be obtained for even higher values of the parameters m and δ.

In conclusion we say that the main aim of the present paper has been to answer the following questions: given a map, how does not get any information about the regular or chaotic behavior of the map in the parameter region where it is not possible to iterate the map (inaccessible parameter region), and, if there is chaotic behavior of the map in the inaccessible parameter region, how does one characterize the chaos? These questions are particularly relevant for the model considered in this paper, because, as has been reported in paper I, it is not possible to iterate the map for all values of the parameters m and δ. The inaccessible parameter region appears in this model, because, as has been said above, this map is different from the similar ones reported in the literature in the sense that this is a two-parameter map, where both parameters m (order of nonlinearity) and δ (strength of nonlinearity) are varied. In the other maps reported in the literature, this problem of map iteration does not arise, because there the parameter m is kept fixed, and for a fixed value of parameter m usually the maps can be iterated for all values of the parameter δ. Moreover, the map considered in this paper represents a model of first-order phase-transition phenomena, whereas most of the systems considered in the literature describe second-order phase transitions. The reason why one is interested in answering this particular question of regular or chaotic behavior of this map is because of the fact that the physical properties of the system, like the metal-to-insulator transition, can be explained in terms of a transition from regular to chaotic behavior of the map, as discussed above in terms of the soliton excitation, soliton interactions, and soliton pinning. It is very important to know the parameter values of the map for which the system admits regular or chaotic behavior. The parameter values once determined can be related (paper I) to physical properties of the system like the soliton concentration (alternatively given by the doped critical impurity concentration, as at each impurity site a soliton is created), which is related to the metal-insulator transition in the system. As the map interaction diverges for this map for parameter values in the inaccessible parameter region, we obviously cannot use the standard procedure of map iteration here to determine the regular or chaotic behavior of the map. We have avoided the problem of map iteration by obtaining quantitative information about the chaotic behavior of the map in the inaccessible chaotic regime in terms of the unstable periodic orbits associated with the chaotic dynamics in this regime. We have also used a different method, the symbolic dynamic procedure, to obtain the unstable periodic orbits, as the usual method of determination of such orbits by the map iteration technique cannot be applied to the map considered here. The advantage of the symbolic dynamic technique used here is that it can be used for any value of the parameters, even for those in the inaccessible parameter region. The periodic points of the unstable periodic orbits so obtained have been used for calculation of the Lyapunov exponents of the corresponding orbits. The hierarchical framework based on the lengths of such orbits has been used to calculate the topological entropy of the system. These quantities characterize chaos in dynamical systems and, from the numerical values of these quantities obtained above, we can now say that there are chaotic orbits present in the previously inaccessible parameter region of the system and also characterize (quantify) the chaos in the orbits. In terms of the soliton picture, the system will be an insulator for such parameter values and these parameter values also give the critical impurity concentration necessary for the metal-insulator transition in the system. This method can be used for other maps which show divergence in the map iteration for some parameter values.

The unstable periodic orbits obtained above are useful for studying the quantum behavior of the system. For example, the eigenstates of quantum systems that are chaotic in the classical limit can be expressed in terms of the periodic orbits of the corresponding classical systems. For some chaotic systems it is found[11] that some eigenstates are strongly peaked near the periodic orbits that are unstable; these peaks are termed "scars." The study of the scar phenomenon in a variety of systems is of current interest.[12] This problem is particularly relevant for the model considered here, because this is a generalized two-parameter model and many other models like the $\lambda\phi^6$ model (corresponding to the parameter value $m=2$), which is a widely used model[13] for first-order phase-transition phenomena like the ferroelectric phase transition, order-disorder transition, charge-density-wave transition, etc., can be obtained from it. Similarly, the model corresponding to the parameter value $m=1$ has been used for studying statistical mechanics of field theories.[2] Neither of these nonlinear theories is quantized so far and thus the quantization of our generalized model will be a step in this direction. In addition, as has been said above, this model is different from other similar models studied in the literature in many aspects and we would like to see how to quantize such systems, which have divergences in the map iteration for some parameter regions. However, this is an independent problem, the result of which will be reported elsewhere.

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