From a unstable periodic orbit to Lyapunov exponent and macroscopic variable in a Hamiltonian lattice: Periodic orbit dependencies

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Abstract

We study which and how a periodic orbit in phase space links to both the largest Lyapunov exponent and the expectation values of macroscopic variables in a Hamiltonian system with many degrees of freedom. The model which we use in this paper is the discrete nonlinear Schrödinger equation. Using a method based on the modulational estimate of a periodic orbit, we predict the largest Lyapunov exponent and the expectation value of a macroscopic variable. We show that (i) the predicted largest Lyapunov exponent generally depends on the periodic orbit which we employ, and (ii) the predicted expectation value of the macroscopic variable does not depend on the periodic orbit at least in a high energy regime. In addition, the physical meanings of these dependencies are considered.

§1. INTRODUCTION

We are interested in characterizing chaotic Hamiltonian systems. One of the most basic indicators to characterize chaos for physicists is the largest Lyapunov exponent, and then there have been attempts to estimate the largest Lyapunov exponents for several systems. For low-dimensional Hamiltonian systems, Chirikov has found that the largest Lyapunov exponent is close to an averaged eigenvalue in a strong chaotic regime for the standard map. For high-dimensional Hamiltonian systems, an analytical method to estimate the largest Lyapunov exponents has been developed and applied. The method is based on a random approximation and Riemannian geometry. For the Hamiltonian mean field model, which shows a second-order transition, the largest Lyapunov exponent has analytically been calculated. This study has shown that the relation between the largest Lyapunov exponent and the second-order phase transition. There are similar studies for the $\alpha$-XY model, which is one of the extended models to study how non-additivity affects the statistics and dynamics. For the $\alpha$-XY model, it has been shown that the largest Lyapunov exponent is a function of the interaction length.

It is important to estimate the expectation value of a macroscopic variable for a system with many degrees of freedom. Note here, the term “a macroscopic variables” refers to a quantity obtained by taking the average over many degrees of freedom. For instance, well-known macroscopic variables are the temperature and magnetization. In the equilibrium state, the expectation values of macroscopic variables can be estimated using tools of equilibrium statistical mechanics with some basic assumptions. These assumptions, such as ergodicity, the principle of equal weight, and so on, are not usually proved. Then estimating the expectation value of a macroscopic without such classical tools sheds light on basics of statistical mechanics.

In dynamical systems theory, not only for Hamiltonian systems but for dissipative systems, utilizing and searching for periodic orbits are one of the most fundamental issues. When a periodic orbit is found in a system, we can see a part of the skeleton of phase space because the periodic orbit forms an invariant subset in the phase space. (see Ref. for the Fermi-Pasta-Ulam-β model as an example).

There is the question whether a periodic orbit is related to the largest Lyapunov exponent and the expectation values of macroscopic variables. For the Navier-Stokes equation, it has
recently been shown that values of some macroscopic quantities can be estimated using only one unstable periodic orbit.\textsuperscript{10–12} In order to clarify the meanings of these numerical studies, it has theoretically been studied that only one unstable periodic orbit is enough to derive relevant statistical property in a hyperbolic chaotic system with many degrees of freedom.\textsuperscript{13} Independently of such studies, it has been shown that a method with only one periodic orbit can predict the largest Lyapunov exponent in a class of models including the Fermi-Pasta-Ulam-\(\beta\) model.\textsuperscript{15} In Ref.,\textsuperscript{15} they have proposed the method predicting the largest Lyapunov exponent in a system with \(N\) degrees of freedom. The estimate consists of the following three steps:

1. Find one periodic orbit \((q^{PO}(t), p^{PO}(t))\).
2. Estimate the linear growth rate along the periodic orbit, \(\tau_j\) \((j = 1, \ldots, 2N)\), and define the instability entropy \(S_{IE} := \sum_{j(\tau_j > 0)} \tau_j\).
3. Predict \(\lambda_1 = 2S_{IE}/N\), based on the assumption \(S_{IE} = S_{KS} \approx \lambda_1 N/2\), where \(S_{KS}\) is the Kolmogorov-Sinai entropy.

On the other hand, for a macroscopic variable \(O(q, p)\), we could predict the expectation value in the equilibrium state. The method is given by the following procedure:

\[
\langle O \rangle_{PO} := \int_0^{T_0} O(q^{PO}(t), p^{PO}(t)) dt / T_0, \text{ where } T_0 \text{ is the period of } (q^{PO}(t), p^{PO}(t)).
\]

This kind of substitution has also been used for the Fermi-Pasta-Ulam-\(\beta\) model in Ref.,\textsuperscript{16} where they have analytically shown that the largest Lyapunov exponent can also be obtained using an Riemannian geometric approach with this kind of substitution.

If the above two estimates depend on the periodic orbit that we find, the dependency gives a clue to understand the link between averaged values (e.g., the largest Lyapunov exponent and the expectation value of a macroscopic variable) and a microscopic point of view (e.g., a periodic orbit). In general, it is difficult to discuss such a dependency, due to the lack of the number of periodic orbits. As a matter of fact, in the Fermi-Pasta-Ulam-\(\beta\) model, the number of such periodic orbits is five.\textsuperscript{16} To discuss the dependency, we need a chaotic model in which many periodic orbits are easily found. If the expressions of these periodic orbits are analytically written, these expressions give analytical expressions of linear growth rates along the orbits. It is noted here that there is a work in Ref.,\textsuperscript{18} where they have compared with two periodic orbits in a different point of view.

In this paper, we study the periodic orbit dependencies on (a) the method predicting the largest Lyapunov exponent\textsuperscript{15} consisting of the three steps mentioned above, and (b) substituting the expression of a periodic orbit into the definition of a macroscopic variable. We treat the discrete nonlinear Schrödinger equation, in which we exactly calculate the modulational estimates along \(N\) periodic orbits with \(N\) being the number of lattice sites. The fact that there are a number of analytically expressed periodic orbits is a feature peculiar to the discrete nonlinear Schrödinger equation. The existence of \(N\) exact periodic orbits allows us to discuss the periodic orbit dependencies for (a) and (b). Using these approach, we bridge some averaged quantities and a microscopic point of view: the largest Lyapunov exponent and the expectation value of a macroscopic variable from a periodic orbit.

\section*{2. Theoretical Prediction and Numerical Simulation}

The equations of motion and the Hamiltonian for the discrete nonlinear Schrödinger equation are

\[
\frac{du_j}{dt} = -i(u_{j+1} + u_{j-1} - 2u_j + \gamma |u_j|^2 u_j) = \frac{\partial H}{\partial u_j^*},
\]

(2.1)
\[ \frac{d u_j^*}{dt} = -\frac{\partial H}{\partial u_j}, \quad H = i \sum_{j=0}^{N-1} (|u_{j+1} - u_j|^2 - \frac{\gamma}{2} |u_j|^4), \]

with conditions \( u_{j+N} = u_j \), \( N \) being the number of degrees of freedom. We restrict ourselves to the case that \( N \) is even. Here \( u_j \) are complex variables and \( \gamma \) is a real parameter. The system (2.1) has the conserved quantity \( I := \sum_{j=0}^{N-1} |u_j|^2 \), in addition to the Hamiltonian.

In the next subsection, we theoretically predict the largest Lyapunov exponent and the expectation value of a macroscopic variable.

2.1. Theoretical Prediction

First, we concentrate on the Lyapunov exponent. We predict the largest Lyapunov exponent with the three steps that are introduced in §2.1.

As the step (1), we find the following \( N \) periodic orbits in this model,
\[
\begin{align*}
    u_j^{PO}(t) &= A_k \exp\{i(2\pi kj/N - \omega_k(|A_k|^2)t)\}, \\
    \omega_k(|A_k|^2) &= -4\sin^2(\pi k/N) + \gamma |A_k|^2,
\end{align*}
\]
where \( k = 0, \ldots, N-1 \), and \( A_k \in \mathbb{C} \) are the amplitudes of the orbits. It is noted that we do not make any approximation to express these unstable periodic orbits.

As the step (2), we calculate the growth rate along \( u_j^{PO}(t) \). To calculate the growth rates of the orbits, we substitute \( u_j = u_j^{PO}(1 + \mu_j), |\mu_j| \ll 1 \) into Eq. (2.1), where \( \mu_j \) are complex variables describing the tangent phase space along \( u_j^{PO}(t) \). After taking into account the linear terms only and using the Fourier transformation, we obtain the linearized equations around \( u_j^{PO}(t) \) in Fourier space,
\[
\frac{d}{dt} \left( \begin{array}{c} \hat{\mu}_{m-k} \\ \hat{\mu}_{k-m} \end{array} \right) = \left( \begin{array}{cc} -iB & -iC \\ iC & iB \end{array} \right) \left( \begin{array}{c} \hat{\mu}_{m-k} \\ \hat{\mu}_{k-m} \end{array} \right). \tag{2.3}
\]

Here
\[
\hat{\mu}_m := \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} \mu_j e^{-i2\pi mj/N}, \quad \hat{\mu}_m = \frac{1}{\sqrt{N}} \sum_{m=0}^{N-1} \mu_m e^{i2\pi mj/N},
\]
where \( m = 0, \ldots, N-1 \), and \( B, C \in \mathbb{R} \) are given by
\[
B = 4\{\sin^2(\pi k/N) - \sin^2(\pi m/N)\} + \gamma |A_k|^2, \\
C = \gamma |A_k|^2.
\]

The growth rates of the periodic orbits (2.2) are obtained as the eigenvalues of the linearized equation (2.3). The squared eigenvalues are calculated as follows,
\[
\tau(k; m)^2 = -16 \left( \sin^2\left(\frac{\pi k}{N}\right) - \sin^2\left(\frac{\pi m}{N}\right) \right)^2 \\
-8\gamma |A_k|^2 \left( \sin^2\left(\frac{\pi k}{N}\right) - \sin^2\left(\frac{\pi m}{N}\right) \right).
\tag{2.4}
\]

Then we have the pairs of eigenvalues \( \tau_{\pm}(k; m) \). It should be noted that the stability analysis has also been done without any approximation. The expression of eigenvalues shows the following symmetries for \( \tau_{\pm}(k; m) \),
\[
\tau_{\pm}(k; k) = 0, \\
\tau_{\pm}(k, N/2 - m) = \tau_{\pm}(k, N/2 + m), \\
\tau_{\pm}(N/2 - k, m) = \tau_{\pm}(N/2 + k, m).
\tag{2.5}
\]
When $\tau^2(k; m)$ is positive, the periodic orbit labeled by $k$ is unstable. On the other hand, when $\tau^2(k; m)$ is negative, the periodic orbit is stable. Substituting Eq. (2.2) into Eq. (2.1), we have the relation between the absolute value of the amplitude and the energy density $\epsilon := H/N$, $\langle H = iH \rangle$,

$$|A_k|^2 = \sqrt{\left(\frac{4}{\gamma}\right)^2 \sin^4 \left(\frac{\pi k}{N}\right) - \frac{2\epsilon}{\gamma} + \left(\frac{4}{\gamma}\right) \sin^2 \left(\frac{\pi k}{N}\right)}.$$ 

As the step (3), the linear stability analysis gives an analytical prediction of the largest Lyapunov exponent,

$$\lambda_1 = \frac{2}{N} \sum_{m=0}^{N/2-1} \tau_+(k; m),$$

and this can be viewed as the average of the growth rates. Here this expression of $\lambda_1$ depends on both the parameter $k$ and the energy density $\epsilon$.

Second, we predict the time-averaged value of a macroscopic variable using a substitution of the periodic orbit. This substitution is introduced in Eq. (2.7). As one of the macroscopic variables, we take

$$\Xi := \frac{1}{I} \sum_{j=0}^{N-1} \frac{d\omega_j}{dt} \frac{d\omega_j^*}{dt}.$$ 

Substituting the periodic orbits into Eq. (2.7), we predict the time-averaged values of the macroscopic variable $\Xi$. Then we have $\langle \Xi \rangle_{PO} = \omega_k^2(|A_k|^2)$. In the high energy limit, we predict $\langle \Xi \rangle_{PO} \sim \gamma^2 |A_k|^4 \sim (-2\epsilon\gamma)$ provided $\epsilon\gamma < 0$, and $\langle \Xi \rangle_{PO}$ does not depend on $k$ in this limit. In the low energy limit, there is a periodic orbit dependency.

### 2.2. Numerical Simulation and discussion

Let us compare our predictions with numerical simulations. We restrict ourselves to the case $\gamma < 0$. Numerical integrations of the canonical equation of motion are performed using a second symplectic integrator.\(^{19-21}\) The time step of the integrator is set at 0.005 and it suppresses the relative energy error $\max_{0 \leq t \leq 50000} \{(H(t) - H(0))/H(0)\} \sim 10^{-4}$. Our initial conditions of $u_j(0)$ are as follows. For $Re\{u_j(0)\}$, small perturbation terms are added to $\propto \cos(\pi j)$, and $Im\{u_j(0)\}$ are exactly zero. The amplitudes of $u_j(0)$ determine the value of the energy. The computing time is set to more than 50000 so that the time-averages converge, which are to obtain the largest Lyapunov exponent and the expectation value of the macroscopic variable. We do not take any ensemble average to obtain numerical data.

First, we study the largest Lyapunov exponent. In Fig. 1, we compare the largest Lyapunov exponent $\lambda_1$ obtained both the predictions (2.6) with the numerical calculations for the model with $N = 512$. This figure shows that the analytical estimate depends on $k$, and that the prediction by taking $k = 116$ is best fitted to the numerical data in the regime $0.1 \lesssim E/N \lesssim 100$. We denote it by $k_*$, and the value of $k_*$ gives $k_*/N \sim 0.227$ for $N = 512$. For $N = 128$, the best fitting parameter is $k_* = 28$ (i.e., $k_*/N \sim 0.219$), as shown in Fig. 2. Although we do not show any figure for cases $N < 128$, we find the non-trivial rule $k_*/N \sim 0.22$. In Fig. 2 the $\gamma$ dependency is shown for models with $N = 128$. For all $\gamma$ which we study, $k_*$ are the same each other. Then the rule $k_*/N \sim 0.22$ can be applied for a wide range parameter regime.

Let us look for the origin of the non-trivial rule $k_*/N \sim 0.22$. Here we attempt to bridge the rule for the choice of the periodic orbit and components of the Lyapunov vector. Due to the definition of the largest Lyapunov exponent, the origin of the rule $k_*/N \sim 0.22$ should be discussed in both the tangent phase space and phase space, not only in the phase space. When the rule $k_*/N \sim 0.22$ is applied to the periodic orbit (2.2), we can obtain the approximate periodicity in space, $u_{j+4,5} \sim u_j$. We identify these values, $4 \sim 5$, with the correlation length. On the other hand, it is worth to note here that the localization phenomenon of components
Fig. 1. For the discrete nonlinear Schrödinger equation with $N = 512$ and $\gamma = -1$. Comparison of the analytical estimate with numerical data for the largest Lyapunov exponents. Pluses denote the numerically obtained the largest Lyapunov exponents and lines the predicted ones. The prediction using the periodic orbit labeled by $k = 116$ is the best fit to the numerical data.

Fig. 2. For the discrete nonlinear Schrödinger equation with $\gamma = -0.1, -1, -2$ and $N = 128$. Comparison of the analytical estimate with numerical data for the largest Lyapunov exponents. Pluses, crosses and asterisks denote numerically obtained the largest Lyapunov exponents and lines the predicted ones with $k = 28$. Predictions by periodic orbits labeled by $k = 28$ are best fit to the numerical data.

of the Lyapunov vector has been studied in Ref.\textsuperscript{15}) In this paper, we calculate the normalized correlation length of components of the Lyapunov vector numerically as shown in Fig. 3. Here we define the correlation function for components of the Lyapunov vector as

$$
\zeta(j) = \lim_{t \to \infty} \frac{1}{t - t_0} \int_{t_0}^{t} dt' |du_j(t')du^*_j(t')|^2.
$$

(2.8)

Here $t_0$ is taken as 100 for our calculations, $du_j(t)$ denote the $j$-th component of the tangent vector associated with the orbit $u_j(t)$. Fitting the normalized correlation function to a sum of a Lorentzian curve and an exponential curve, we extract the correlation length from the tangent space of the phase space. The fitting function which we use here is then

$$
\frac{\zeta(j)}{\zeta(0)} = \left( \frac{\Gamma}{2} \right)^2 \frac{1 - E}{j^2 + (\Gamma/2)^2} + E \exp(-j/J),
$$

where $E, \Gamma$ and $J$ are the fitting parameters. The value of this function equals unity at $j = 0$ for any values of $E, \Gamma$ and $J$. Due to this fitting function, we have two typical length scales. One of
them is from the width of the Lorentzian curve, $\Gamma$, and the other is from the exponential curve, $J$. The correlation lengths obtained by $J$ are approximately $4.5 \sim 5$ for the large energy density regime. For example, the correlation length is $4.6$ for the model with $N = 128$ and $\gamma = -1$ in the high energy regime as shown in Fig. 3. We can say that the correlation length in the tangent dynamics can be estimated using $J$. For the system with $N = 128$ and $\gamma = -0.1$, although the value of $J$ is in between $4.5 \sim 5$ in the high energy regime, such correlation length is far from it, about $12$ in the low energy regime. Then this explanation for the rule $k_s/N \sim 0.22$ is valid only in the high energy regime. Combining the consideration of components of the Lyapunov vector and that of the approximate spatial periodicity by applying the rule $k/N \sim 0.22$ to the periodic orbit, we could say that the emergence of the non-trivial rule is from the localization of the tangent dynamics in the high energy regime. It could be one of the reasons why the rule $k_s/N \sim 0.22$ appears, at least in the high energy regime.

Let us consider the validity of the definition of the instability entropy. If we define another version of the instability entropy, $S_{IE}' = \sum_{m=0}^{N-1} (\lambda_{(k;m)}^+ > 0) \lambda_{+(k;m)}$, the largest Lyapunov exponent could be predicted as $\lambda_{1}' = (2/N) \sum_{m=0}^{N-1} (\lambda_{(k;m)}^+ > 0) \lambda_{+(k;m)}$, by making the assumption that the Kolmogorov Sinai entropy is equal to $S_{IE}'$. This new expression $\lambda_1'$, which is different from Eq. (2.6), cannot predict numerical data for the largest Lyapunov exponents in the whole energy density regime (no figure given). When we look for the parameter $k_s'$ which gives the best fit to the numerically obtained data in the high energy regime, we find $k_s'/N \sim 0.16$ for the models with $N = 512, 128$ and $\gamma = -1$.

Next, we compare the prediction for the time-averaged value of $\Xi$ with numerical simulation. Fig. 4 shows that, in the high enough energy regime, each prediction labeled by $k$ is in good agreement with numerically obtained data. In contrast to the success of the prediction in the high energy regime, it is difficult to conclude what happens in the low energy regime. Although we do not show any figure, in the low energy regime $E/N \lesssim 100$, the time-averaged values of $\Xi$ do not converge fast in time. However, from the edge of the low energy regime, $E/N \sim 50$ in Fig. 4, even the best fitted prediction, labeled by $k = N/2$, differs from the data obtained numerically. Similar tendency is observed for the cases $N < 512$.

Let us look for the reason why every periodic orbit (222) can predict the time-averaged values of $\Xi$ in the high energy regime. Because the interaction range of this system is short, the system has additivity. For such an additive Hamiltonian system in a fully developed chaotic regime, we can define some macroscopic subsystems whose sizes are macroscopically arbitrary.
§3. CONCLUSIONS

We have studied which and how periodic orbits predict both (a) the largest Lyapunov exponent and (b) the time-averaged value of a macroscopic variable in a Hamiltonian lattice.

To clarify these questions, we have studied the discrete nonlinear Schrödinger equation in which there are $N$ analytically expressed periodic orbits. In the nonlinear Schrödinger equation, we have exactly constructed the modulational estimates along the $N$ periodic orbits and compared with numerical simulation. Then we have observed that the analytically predicted largest Lyapunov exponent depends on the periodic orbit and that there is a suitable periodic orbit for the prediction. The reason has been discussed in the phase space and the tangent phase space by studying components of the Lyapunov vector. On the other hand, to predict the time-averaged value of a macroscopic variable, we have substituted the analytical expression of the orbits into the definition of the macroscopic variable. The prediction is in good agreement with numerically obtained data in the high energy limit. The reason has been discussed in the phase space by considering the range of interactions.

In this paper, we have focused on a way to bridge between the dynamics and statistics. Further investigations are necessary to quantitatively understand why the special periodic orbit can only predict the largest Lyapunov exponent even in a relatively low energy regime, and every periodic orbit can be used for predicting the time-averaged values of macroscopic variables in the high energy regime. We believe that this kind of investigations can help to elucidate the study of Hamiltonian systems with many degrees of freedom.
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