Detecting Microscopic Chaos in a Time Series of a Macroscopic Observable

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Extracting reliable indications of chaos from a single experimental time series is a challenging task, in particular, for systems with many degrees of freedom. The techniques available for this purpose often require unachievably long time series. In this paper, we propose a new method to discriminate chaotic from multi-periodic integrable motion for a short time series provided it is very accurately measured. The method is based on analyzing higher order time derivatives of the time series. It exploits the fact that power spectra of chaotic time series exhibit exponential high-frequency tails, while, in the integrable systems, the power spectra are normally terminated at a finite frequency. We apply the above method to analysing signals generated by integrable and non-integrable systems of many interacting classical spins.

The problem of detecting deterministic chaos in an experimental time series is of fundamental interest for the foundations of statistical physics1, 2. It also arises in other contexts, e.g., in biomedical applications3. In a typical difficult situation, a system having many degrees of freedom is suspected to be chaotic, but one can access the time evolution of only one degree of freedom. This means that the primary indicator of chaos, namely, the Lyapunov instability in the many-dimensional phase space cannot be investigated directly. A notable example in this regard was an attempt of Ref.3 to identify microscopic chaos in the measured trace of a Brownian particle. The approach of Ref.3 was to analyze the rate of information entropy (IE) production by this trace. The limiting value of this rate in the chaotic systems is known to be equal to the sum of the positive Lyapunov exponents. The results of Ref.3 were consistent with the possible presence of microscopic chaos, but, at the same time, were criticized as leaving open the possibility that the same signatures might be produced by non-chaotic systems4, 5. Detection of microscopic chaos means that it should be discriminated from (i) a stochastic noise process characterized by the infinite limiting rate of IE-production and from (ii) a multi-periodic integrable motion characterized by the zero rate of IE-production. The difficulty here is that extracting the true limiting behavior of the rate of IE-production in many-particle systems typically requires unachievably long time series.

The present paper focuses on issue (ii) above and proposes a new method to discriminate chaos from a multi-periodic non-chaotic motion in a short very accurately measured time series. We consider time series generated by many-dimensional Hamiltonian systems, where both chaotic and non-chaotic motions are smooth in time, and where the non-chaotic motion is characterized by a sufficiently large number of frequencies that cannot be resolved by the Fourier transform of the time series. The method is based on analyzing the higher order time derivatives of the time series. It exploits the fact, which we demonstrate numerically, that the power spectra of time series generated by many-dimensional Hamiltonian chaotic systems have exponential high-frequency tails. To the best of our knowledge, the existence of these tails has never been proven rigorously, but otherwise reported in the studies of non-Hamiltonian or low-dimensional chaotic systems6–10. In contrast, the power spectra of integrable systems normally have a high-frequency cutoff, and their high-frequency behavior is non-universal. Taking time derivatives of a time series progressively suppresses the low frequency parts of the power spectra and amplifies the high-frequency part, thereby producing a number of clearly detectable signatures of chaos. Particularly intriguing is the possibility to apply this method to the time series obtained by monitoring large quantum systems. Should a quantum time series produce the same signatures of chaos as expected for classical systems, such a result would shed a new light on the notion of quantum chaos.

The above method is likely to be limited by the experimental noise11. This limitation can be partially dealt with by using ultra-low noise sensing devices and by an appropriate high-frequency filtering of the signal. But, more importantly, it can be overcome by applying the method to the time series representing equilibrium fluctuations of extensive macroscopic variables, such as, e.g., the total magnetization of a spin system, in which case, the signal-to-noise ratio can be decreased by measuring these fluctuations in larger systems.

We introduce our method by applying it to the time series of the total spin polarization for large clusters of interacting classical spins. These clusters are known to exhibit relaxation properties11 that were linked to microscopic chaos12, 14, but the interaction can also be chosen to lead to a non-chaotic multi-periodic dynamics. We mostly consider two $6 \times 6 \times 6$ cubic clusters with periodic boundary conditions. One of these clusters is
integrable, while the other is not. We first demonstrate the chaotic character of the non-integrable cluster by calculating its largest Lyapunov exponent. After that, we generate rather long time series for the two clusters and demonstrate that one cannot discriminate between the chaotic and non-chaotic time series on the basis of the numerically accessible rate of IE-production. We then proceed with calculating the higher order time derivatives for the two time series and show that their seventh derivatives already look qualitatively different to discriminate the chaotic from the non-chaotic time series simply by visual inspection. We further introduce several quantitative criteria characterizing this difference. Finally, we demonstrate the utility of our method by applying it to very short time series.

The $6 \times 6 \times 6$ spin clusters are characterized by the nearest-neighbor (NN) interaction Hamiltonian

$$H = \sum_{i<j}^{\text{NN}} J_{ix} S_i^x S_j^x + J_{iy} S_i^y S_j^y + J_z S_i^z S_j^z,$$

where $(S_i^x, S_i^y, S_i^z)$ are the components of the $i$th classical spin normalized by the condition $S_i^2 + S_i^y + S_i^z = 1$, and $J_x, J_y$ and $J_z$ are the coupling constants. For the integrable cluster, we select the Ising Hamiltonian characterized by $J_x = J_y = 0$ and $J_z = 1$, while, for the chaotic cluster, we select $J_x = -0.65$, $J_y = -0.3$, $J_z = 0.7$. In the Ising case, the motion is integrable, because the $z$-component of each spin is a constant of motion, while the $x$- and the $y$-components simply precess in the local fields created by the frozen $z$-components of the neighbors. Therefore, the non-chaotic time series to be computed below is characterized by the superposition of 216 different frequencies. The characteristic time scale of the dynamics of the both clusters is made equal since, in the both cases, $J_x^2 + J_y^2 + J_z^2 = 1$. The equations of motion for the Hamiltonian (1) were solved numerically using the discretization routine of Ref. [1]. This routine conserves the energy of the system exactly. The typical discretization time step $\Delta t$ was 0.01. The discretization errors were controlled by looking at the effects of the change of $\Delta t$ on the Lyapunov exponents and on the power spectra of the time series. The initial orientations of spins were chosen randomly. Therefore, the energy of the system was close to zero.

We have computed the largest Lyapunov exponent for both clusters using the method of Ref. [13]. The method consists of choosing small initial distance $d_0$ between two phase space trajectories, letting them diverge during time $\tau$ and then resetting this distance back to $d_0$ along the displacement direction just before the reset, and so on, repeating the above manipulation many times. If the system is chaotic, the spread of the two trajectories is eventually controlled by the largest Lyapunov exponent, which can be calculated as the limiting value of the expression $\lambda_{\text{max}} = \frac{1}{\tau} \sum_{j=1}^{k} \log \left( \frac{d_j}{d_0} \right)$, where $j$ is the reset index, $k$ is the total number of resets, and $d_j$ is the distance between the two trajectories just before the $j$th reset. For a fixed value of $\tau$, integrable systems can also produce small but finite value of $\lambda_{\text{max}}$ because of the polynomial spread of the trajectories. However, for the polynomial spread, $\lambda_{\text{max}} \sim 1/\tau$ (up to a logarithmic prefactor), while for the exponential spread the value of $\lambda_{\text{max}}$ should not depend on $\tau$. The dependences of $\lambda_{\text{max}}$ on $\tau$ for the two clusters are shown in Fig. [1]. For the Ising cluster, $\lambda_{\text{max}}$ approaches zero approximately as $1/\tau$ as expected for an integrable system. The chaotic cluster exhibits $\tau$-independent value $\lambda_{\text{max}} = 0.63$. The insets of Figs. [1](a) and (b) show that distance growth between two resets is exponential in the chaotic case, and slower than exponential in the integrable case.

We now compute for each of the two clusters the time series of length $T = 1000$ for the $x$-component of the total spin polarization, $M_x(t)$ and try to discriminate between chaotic and non-chaotic time series. The two time series look very similar as illustrated in Figs. [2](a) and (b).

In an attempt to detect the difference between the two time series, we investigated their rates of the $(\varepsilon, \tau)$ information entropy production [1]. For this purpose, we “coarse-grained” the time and the magnetization axes in steps of $\tau$ and $\varepsilon$, respectively, to obtain a newly discretized version of the time series (a stream of symbols). The $(\varepsilon, \tau)$ Shannon information entropy for patterns of length $N$ is given by $H_{\text{Sh}}(\varepsilon, \tau, N) = -\sum P_i \log P_i$, where $i$ is the pattern index, and $P_i$ is the pattern probability. The Shannon $(\varepsilon, \tau)$ entropy per unit time is defined as $\lim_{N \to \infty} h_{\text{Sh}}(\varepsilon, \tau, N)$, where $h_{\text{Sh}}(\varepsilon, \tau, N) = \frac{1}{T} \left[ H_{\text{Sh}}(\varepsilon, \tau, N + 1) - H_{\text{Sh}}(\varepsilon, \tau, N) \right]$. For a chaotic system, $h_{\text{Sh}}(\varepsilon, \tau, N)$ is expected to approach the constant value equal to the sum of the positive Lyapunov exponents in the limit $T \to \infty$, $N \to \infty$, $\varepsilon \to 0$ and $\tau \to 0$. However, for many-dimensional systems, the above limit is, typically, impossible to reach in practice, because, as $N$ increases or $\varepsilon$ decreases, any finite time series quickly becomes too short to fairly represent the statistics of all possible patterns of length $N$. Once this happens, each pattern, that occurs, occurs only once,

![FIG. 1: (Color online) Numerical values of the maximum Lyapunov exponent $\lambda_{\text{max}}$ for the chaotic (a) and the integrable (b) systems as a function of the reset time $\tau$ (dots). The lines represent the fits by a constant in (a) and by function $\text{Log}(1+\varepsilon^\tau)$ in (b). The insets illustrate the growth of the distance between a pair of trajectories during 5 reset intervals.](image-url)
and, as a result, $h_{sh}(\epsilon, \tau, N) \to 0$. We, nevertheless, calculated $h_{sh}(\epsilon, \tau, 2)$ in order to check if there is any indication of chaos before the effect of the finite length of the time series sets in. The results presented in Fig. 2 are nearly identical for both chaotic and non-chaotic time series. Similar results were also obtained for the Cohen-Procaccia entropy $[16]$.

We now demonstrate, that one can easily identify chaos in the time series of $M_x(t)$ by looking at its derivatives of the $n$-th order, which we denote as $M^{(n)}_x(t)$. In Figs. 3(c) and (d), we exemplify this statement by presenting the time evolution of the 7th time derivative $M^{(7)}_x(t)$ for the seemingly indistinguishable time series appearing in Figs. 3(a) and (b). (The plots for the lower-order derivatives are given in [16].) For the chaotic time series, $M^{(7)}_x(t)$ fluctuates noticeably faster than $M_x(t)$ and has a rather random appearance, while, for the non-chaotic time series, $M^{(7)}_x(t)$ has the appearance of a slowly modulated periodic signal with period of the order of the characteristic time of $M_x(t)$.

The clear difference between Figs. 3(c) and (d) can be understood from the fact that the power spectrum of the original time series, $P(\omega)$, and the power spectrum of the $n$th time derivative $P^{(n)}(\omega)$ are related as $P^{(n)}(\omega) = \omega^{2n}P(\omega)$. Both $P(\omega)$ and $P^{(7)}(\omega)$ for each time series are presented in Figs. 3(c) and (f). In the non-integrable case, $P(\omega)$ has exponential tail $e^{-\gamma \abs{\omega}}$, where $\gamma$ is a constant. As a result, for sufficiently large $n$,

$$P^{(n)}(\omega) \simeq \omega^{2n}e^{-\gamma \abs{\omega}}. \quad (2)$$

We propose to use this dependence as a quantitative signature of chaos. Figure 3(e) includes the fit to $P^{(7)}(\omega)$ of the form $\omega^{14}e^{-\gamma \abs{\omega}}$. The important aspect of this dependence is not that it becomes exponential at sufficiently large frequencies, but that, before it becomes exponential, it has the universally shaped broad maximum shifting with $n$ to increasingly high frequencies. On the contrary, the power spectrum for the integrable cluster is terminated sharply at a certain maximum frequency $\omega_{max}$. As a result, the shape of $\omega^{2n}P(\omega)$ for sufficiently large $n$ becomes narrowly peaked around $\omega_{max}$. Therefore, $\omega_{max}$ becomes the carrier frequency for the modulations observed in Fig. 3(d), while the inverse width of this peak characterizes the modulation time scale.

We further propose two related criteria of chaos. The first of them characterizes the root-mean-squared (RMS) values of $M^{(n)}_x(t)$, denoted as $M^{(n)}_{rms}$. In Fig. 3(a), we plot the quantity $R_n = M^{(n)}_{rms}/M^{(n-1)}_{rms}$ as a function of $n$. For the non-chaotic time series, $R_n$ exhibits saturation, while for the chaotic time series it increases nearly linearly without apparent limit. The second criterion looks at the evolution of $v_n$ defined as the square root of the variance for the positive-$\omega$ part of $P^{(n)}(\omega)$ [$v_0$ corresponds to $P(\omega)$]. In Fig. 3(a), we plot $W_n \equiv v_n/v_0$. Here the difference is that, in the chaotic case, $W_n$ asymptotically increases with $n$, while in the non-chaotic case it decreases, asymptotically approaching zero.

Finally, the fact that the higher-order derivatives look more random for the chaotic time series should also have
quantifiable consequences in terms of the rate of the $(\varepsilon, \tau)$-entropy production.[10]

In the power spectrum of the non-chaotic time series shown in Fig. 3(e) one can distinguish some discrete frequencies, which is an indication of integrability. The chaos indicators proposed above are mainly intended for the situations when this discreteness is not discernible due to either too large number of discrete frequencies or too short length of the time series. In Fig. 4 we illustrate the effectiveness of our method by applying it to a very short time series of length $T = 10$ produced by two $4 \times 4$ square lattice spin clusters with the same nearest neighbor coupling coefficients as the previously considered two clusters. Detecting chaos from such a short time series using just the power spectrum of $M_x(t)$ is difficult, because it is contaminated by the oscillations and the power-law decays associated with the short length of the time series. However, taking the 7th derivative reveals the expected qualitative difference between the chaotic and integrable systems and the good quality fit of form (2).

One potentially promising application of our method would be to analyze the equilibrium fluctuations of nuclear spin polarization in solids[17]. These fluctuations were measured by several NMR groups[18, 19] although not yet with high enough accuracy. The exponential high-frequency tail in the Fourier transform of the NMR free induction decay[20] suggests that the signatures of chaos may be directly observable in this case.

In conclusion, we have demonstrated that examining the behavior of higher-order time derivatives is an effective way to distinguish between chaotic and integrable systems on the basis of a finite time series, provided the time series can be measured with a sufficient accuracy. For the time series with zero average, the criterion of chaos can be based on Eq. (2) and its observable consequences. We are grateful to H. Kantz, P. Gaspard and D. Shepelyansky for discussions.

FIG. 4: (Color online) Statistical characteristics of the time series of $M^{(n)}_x(t)$ for the chaotic and the integrable systems: (a) ratios $R_n$ of the RMS value of $M^{(n)}_x(t)$ to the RMS value of $M^{(n-1)}_x(t)$; (b) relative width $W_n$ of the power spectrum $P^{(n)}(\omega)$ with respect to the width of $P(\omega)$.

FIG. 5: (Color online) Time series of $M_x(t)$ for $4 \times 4$ spin lattices. Same notations as in Fig. 4. Frames (a,b,c,d) now represent the entire time series used to obtain frames (e,f).

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A. Comparison between derivatives of the time series produced by the chaotic and the integrable systems

In Fig. 3 of the main article, we presented the fragments of two time series $M_x(t)$ of the total spin polarization for the chaotic and the integrable $6 \times 6 \times 6$ spin clusters together with their respective 7th derivatives, $M_x^{(7)}(t)$. In Fig. S1 below, we show the plots for all the derivatives $M_x^{(n)}(t)$ of the same two time series up to the 9th order. We used the standard finite-difference numerical procedure for computing these derivatives. Namely, if the discretized time series in a given order was $\{..., \left(t_i, M_x^{(n)}\right), \left(t_{i+1}, M_x^{(n)}\right), \left(t_{i+2}, M_x^{(n)}\right), ...\}$, then the next-order derivative was obtained as $\{..., \left(t_i, \frac{M_x^{(n)}(t_{i+1}) - M_x^{(n)}(t_i)}{t_{i+1} - t_i}\right), \left(t_{i+1}, \frac{M_x^{(n)}(t_{i+2}) - M_x^{(n)}(t_{i+1})}{t_{i+2} - t_{i+1}}\right), ...\}$. The numerical derivatives beginning with the ninth in the integrable case and tenth in the chaotic case show signs of numerical noise associated with the accumulated rounding errors. In order to exclude this concern, the presentation in the main article was limited to the 7th derivative.
B. Rate of the Cohen-Procaccia \((\varepsilon, \tau)\)-entropy production for the chaotic and the integrable systems

It was pointed out in the main article that (i) the results similar to those presented in Fig. 2 can be obtained on the basis of the Cohen-Procaccia (CP) entropy [A. Cohen and I. Procaccia, Phys. Rev. A 31, 1872 (1985)]; and (ii) the apparent impression that the 7th derivative of the time series in Fig. 3 looks more random for the chaotic system than for the integrable system is likely to have signatures in terms of the rate the \((\varepsilon, \tau)\)-entropy production. In this section, we present evidence supporting both of the above statements.

In Fig. 2, we show the CP \((\varepsilon, \tau)\)-entropy plots corresponding to the same data set as those analysed in Fig. 2 of the main article with the help of the Shannon entropy. The magnetization axis is not discretized for the calculation of the CP \((\varepsilon, \tau)\)-entropy. Instead, the distance between two patterns of length \(N\) is given by the maximum of the differences between each pair of time-discretized points. To calculate the CP \((\varepsilon, \tau)\)-entropy, \(H_{CP}(\varepsilon, \tau, N)\), a group of \(R = 100\) reference patterns of length \(N\) is selected randomly, and the probability of each of them is obtained by counting the number of all other patterns occurring in the time series which are within distance \(\varepsilon\) from that reference pattern. The CP \((\varepsilon, \tau)\)-entropy is given by

\[
H_{CP}(\varepsilon, \tau, N) = -\frac{1}{R} \sum_{\{R\}} \log P_i. \tag{3}
\]

The limiting rate of the CP \((\varepsilon, \tau)\)-entropy production is defined as \(\lim_{N \to \infty} h_{CP}(\varepsilon, \tau, N)\), where

\[
h_{CP}(\varepsilon, \tau, N) = \frac{1}{\tau} [H(\varepsilon, \tau, N + 1) - H(\varepsilon, \tau, N)]. \tag{4}
\]

In Fig. S2, we used \(\tau = 0.1\) (10 discretization time steps) for one pattern element and varied \(N\) from 10 to 19 in different plots. It is evident from Fig. S2 that one cannot distinguish integrable from chaotic dynamics on the basis of numerically accessible behavior of \(h_{CP}(\varepsilon, \tau, N)\) because of the finite length \((T = 1000)\) of our otherwise very long time series.

FIG. S2: Comparison between \(h_{CP}(\varepsilon, \tau, N)\) with \(\tau = 0.1\) and various values of \(N\) for the chaotic time series (solid lines) and the integrable time series (dashed lines). Curves reaching higher maximum values of \(h_{CP}\) correspond to the smaller values of \(N\).
With regard to the seventh time derivatives of the both time series, we do notice some qualitative difference between the chaotic and the integrable cases, when we compare the CP \((\varepsilon, \tau)\)-entropy for each of these derivatives with the CP \((\varepsilon, \tau)\)-entropy for the original time series. In Fig. S3, we present the average of \(h_{CP}(\varepsilon, \tau, N)\) over different \(N\) for the original time series and for the 7th time derivatives using the set of values of \(N\) given in Fig. S2. The plotted values of \(\varepsilon\) for \(h_{CP}(\varepsilon, \tau, N)\) associated with the 7th derivative were rescaled by dividing the true values by the following factors: \(1.13 \times 10^4\) in the chaotic case and \(1.31 \times 10^3\) in the integrable case. These factors were chosen such to make the spread between the maximum and the minimum values of \(M^{(7)}(t)\) equal to that of the corresponding \(M_x(t)\). Despite the apparent drawbacks of the above \(N\)-averaging procedure, it does indicate, that the maximum accessible values of \(h_{CP}(\varepsilon, \tau, N)\) for fixed \(\tau\) and \(N\) are reduced for the integrable system, while staying about the same for the chaotic system. This suggests that the derivatives of the time series for the integrable system produce less information when the order of the derivatives increases, while, for the chaotic time series, this is not the case.

**C. Details on the calculation of the power spectra in Fig. 3 of the main article**

The power spectra in Fig. 3 of the main article were obtained by calculating the absolute value of the Discrete Fourier Transform (DFT) of the respective time series multiplied by a smooth-shaped window \(\{w_i\}\) to mitigate the spectral leakage from low frequencies to high frequencies due to the finite length of the time series. That is, if the original time series is \(\{..., (t_i, M^{(n)}_{x,i}), ...,\}\), then the modified time series is \(\{..., (t_i, w_i M^{(n)}_{x,i}), ...,\}\). We used the ten-percent Tukey window [F. Harris, Proceedings of the IEEE 66, 51 (1978); J. Tukey, *Spectral analysis of time series*, (Wiley, 1967)] defined as:

\[
w_i = 0.5 \left\{ 1 - \cos \left[ \frac{2\pi i}{0.1N_t} \right] \right\} \quad \text{for} \quad 0 \leq i \leq 0.05N_t, \]

\[
w_i = 1 \quad \text{for} \quad 0.05N_t \leq i \leq 0.95N_t, \]

\[
w_i = 0.5 \left\{ 1 - \cos \left[ \frac{2\pi (i - N_t)}{0.1N_t} \right] \right\} \quad \text{for} \quad 0.95N_t \leq i \leq N_t, \]

where \(N_t\) is the index of the last discretized time point in \(\{t_0, ..., t_i, ..., t_{N_t}\}\). This window smoothly suppresses the time series to zero at \(t_0\) and \(t_{N_t}\) to reduce the finite-time-length effects.

**FIG. S3:** The \(N\)-averaged values of \(h_{CP}(\varepsilon, \tau, N)\) calculated for both \(M_x(t)\) [blue] and \(M^{(7)}_x(t)\) [red] as described in the text. The values of \(\varepsilon\) for \(M^{(7)}_x(t)\) are rescaled by the factors given in the text.
We did not use the above procedure for the power series presented in Fig. 5 of the main article, because, in that case, the time series was very short ($T = 10$), and, as a result, the window function $w_i$ would contaminate the relevant part of the power spectrum.