$1/f$ Fluctuations in FPU Lattices

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Abstract

We have found $1/f$ fluctuations in the Fermi-Pasta-Ulam equation, which is one of the simplest lattice models to describe fundamental properties of lattice vibrations of real substances. The crossover frequency f_c between the $1/f$ and f^0 behavior of the power spectrum density varies as a function of the strength of the non-linear interaction λ as $f_c \sim \sqrt{\lambda}$. Larger the system size becomes, smaller f_c becomes. Our result indicates that small non-linearity $\lambda \leq 1$ in the system generates $1/f$ fluctuations even in a very small system $N = 8$. The large number of degrees of freedom cannot be the origin of $1/f$ fluctuations even in the realistic systems like Fermi-Pasta-Ulam equation.

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$1/f$ fluctuations have been seen over a wide variety of phenomena such as those in several devices, human activities, and social phenomena [1–5]. Phenomena which show $1/f$ fluctuations cover a lot of different scales. The name "$1/f$ fluctuations" has been given to these phenomena since $1/f$ dependence is observed in the lowest frequency range of the power spectrum density (PSD). When the time sequence is stationary, its PSD integrated all over the frequency range is equal to the variance. On the other hand, $1/f$ fluctuations cause the divergence of variance, which implies non-stationarity. No one has succeeded in explaining the origin of this non-stationarity. There is no established explanation of $1/f$ PSD so far.

It is known that $1/f$ PSD is observed in one dimensional maps with the intermittency chaos [6–8]. However, models with excessive fidelity to real substances would have too many unessential factors, which obscure the true origin of the 1/f phenomena. In this respect, the equation proposed by Fermi, Pasta and Ulam(FPU) is an ideal test ground.

Statistical physics based upon approximations using harmonic potentials can explain a lot of properties such as specific heat for realistic substances, but such systems are not ergodic. Assuming that small non-linearity in the system recovers ergodicity, Fermi, Pasta, and Ulam investigated the energy transfers between eigenmodes in one dimensional anharmonic lattices in 1950's [9], which is known as the first computer experiment. The FPU equation they adopted is composed of harmonic linear terms and small non-linear terms (quadratic, cubic, and broken linear forces). The FPU equation is simple and yet general enough to describe the fundamental properties of non-linear lattices. It also satisfies the energy conservation and translational invariance.

In this letter we investigate the FPU equation with non-linear cubic terms in one dimension. This equation is so general and simple that our result well reflects essential properties of real substances. Our FPU equation shows $1/f$ PSD even in N = 8 small system. The PSD has a typical $1/f$ PSD structure where $1/f$ PSD in the sufficiently low frequency region and white noise in the higher frequency region. The crossover frequency between these two types of behaviors depends on a non-linear parameter and the system size N. Since the

whole shape of PSD does not change for $8 \leq N \leq 32$, it is concluded that the fundamental mechanism to generate $1/f$ PSD does not require large degrees of freedom even in realistic models. This new feature of $1/f$ fluctuations has been clarified in this letter.

The general form of the equation of motion for a one-dimensional ring of classic atoms is

$$\partial^2 u_i/\partial t^2 = \phi'(u_{i+1} - u_i) - \phi'(u_i - u_{i-1}) \tag{1}$$

where ϕ' represents the derivative of the potential ϕ. When the displacement of u_i is sufficiently small, we may approximate the potential as $\phi(x) \propto x^2/2 + \lambda x^4/4$, where λ is a parameter for non-linearity. After an appropriate renormalization, we obtain the following FPU equation:

$$\partial^2 u_i/\partial t^2 = u_{i+1} - 2u_i + u_{i-1} + \lambda\{(u_{i+1} - u_i)^Q - (u_i - u_{i-1})^Q\} \tag{2}$$

where Q is 3 in our case and i runs from 1 to N. We adopt the periodic boundary condition. This FPU system has a Hamiltonian, the energy conservation, translational and reflective invariance ($u_i \rightarrow -u_i$). This property indicates that the FPU equation has more physically reasonable aspects than mathematical maps [7,8].

Let us first consider the computational technique for Hamilton systems. In a Hamilton system, it is important to calculate a time development with several conserved physical quantities such as the total energy and the total momentum. From the view point of differential geometry, a Hamilton system is symplectic two forms [10]. The Symplectic Integrator (SI) is known as an effective computational method for symplectic forms [11]. The fundamental formalism of the SI consists of a Trotter decomposition of symplectic two forms. The SI conserves symplectic two forms with high accuracy. When we use the SI to take a time development of our system, the typical relative truncation error can be estimated phenomenologically by systematic time step changes (e.g., 0.01, 0.02, 0.04..) as about 10^{-9} for time sequences of u_i when the time step is 0.01. This accuracy is sufficient to estimate the PSD up to $10^{-3} \sim 10^{-4}$ Hz.

In the following we investigate phonon number fluctuations defined as follows. The FPU equation with the periodic boundary condition starts from the initial condition that the

initial amplitude of u_i is set as a random number between -1 and 1 and the initial velocity is set to zero at all sites. We expand the amplitude u_i as $u_i = \sum_n a_n exp(2\pi i n\sqrt{-1}/N)$. When $\lambda = 0$, the amplitude of the nth eigenmode of lattice vibrations is a_n, where $|a_n|^2$ is identified with the number of excited phonon. We have investigated $|a_n|^2$ at a fixed n to study the phonon number fluctuations. The $|a_n|^2$ oscillates regularly but sometimes bursts. We can observe similar phenomena in intermittency chaos [7,8]. We take PSD of $|a_n(t)|^2$ by Fast Fourier Transform [12] using 2^{13} points picked up in a single time sequence. To drop the dependence of PSD upon the initial conditions, we renormalize PSD so that it has the same variance obtained from time sequence of $|a_n|^2$. The variance obtained from time sequence of $|a_n|^2$ yields a good estimate of the renomalizaion of PSD since $\int S(f)df$ is equal to the variance of $|a_n(t)|^2$ when stationary. In other words, we renormalize PSD, $S(f)$, as $S(f)/\int S(f)df$ for each initial condition. After this renormalization, the sample average runs over the PSDs which have different initial conditions for each parameter set.

FIGURES

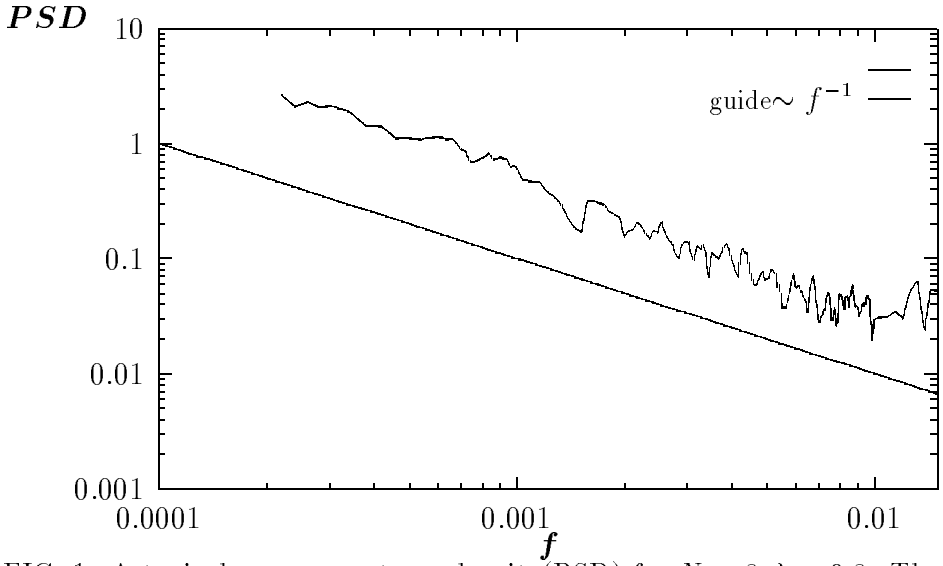

FIG. 1. A typical power spectrum density(PSD) for $N = 8, \lambda = 0.8$. The PSD has $1/f$ in the lowest frequency region and leads to the white noise as the frequency becomes large.

The PSD at sufficiently low frequency shows $1/f$ dependence (see Fig. 1). $1/f$ at the lowest frequency does not saturate with $f \to 0$ to the white noise in our computation, which is coincident with observation in real phenomena [1]. Fig. 1 shows that the PSD varies smoothly from $1/f$ to white noise as the frequency becomes larger. It is a crossover between $1/f$ and f^0 PSD(e.g. a little below 10^{-2} in Fig. 1). This is also often observed in real phenomena [1].

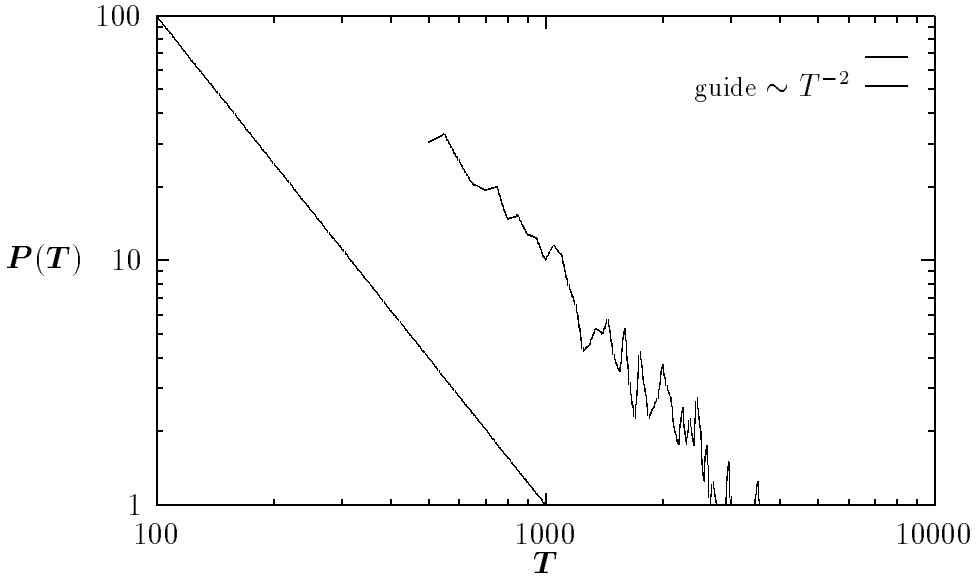

FIG. 2. The distribution function $P(T)$ of time T which is a period between bursts in time sequences of $|a_n|^2$. This figure is for N = 8, $\lambda = 0.8$, which is obtained over 100 runs with different initial conditions. In this case we determine that a burst is a period when $|a_n|^2$ is over 90 % of the maximum of $|a_n|^2$. The form of the distribution function is not sensitive to the critical value 90. $1/f$ region in PSD begins at $f \sim 10^{-2}$, corresponding to $T \geq 100$ in this figure. The distribution function behaves like a T^{-2} over 100 sec.

$1/f$ behavior in the PSD is also characterized by the distribution of time staying in a state. See Fig. 2. The distribution function $P(T)$ is defined as the distribution of the time pausing in states where T is a period of almost regular oscillation between bursts in time series of some physical quantities. We determine that a burst is a period when $|a_n^2|$ is over some threshold value e.g. 90 % of the maximum of $|a_n(t)|^2$. This state is usually short.

In other words for simplicity we divide the time sequence into two states and make a symbolic sequence composed of two states [1]. In our case the physical quantities are $|a_n|^2$ or eigenmode energies. We investigate $P(T)$ over several physical quantities and threshold values, but the result $P(T)$ is insensitive to these conditions. We obtain the same $P(T) \sim T^{-2}$. It is known in chaos theory of small degrees of freedom that $P(T)$ is $P(T) \sim T^{-2}$ when $1/f$ PSD is observed [13]. Our result is well consistent with chaos theory of small degrees of freedom. This characterizes and ensures the $1/f$ behavior of our PSD.

Let us consider the dependence of the crossover frequency upon the non-linear parameter and the system size. We define the crossover frequency as follows: Let us assume that PSD, $S(f)$, behaves as $S(f) \sim a/f + b$ where a and b are constants. The two extrapolated lines a/f and b cross each other at $f_c = a/b$. $\partial lnS(f)/\partial lnf$ is -1 in the $1/f$ region and 0 in the white noise region.(Actually the $\partial lnS(f)/\partial lnf$ varies smoothly). $f_c = a/b$ corresponds to $\partial lnS(f_c)/\partial lnf_c = -0.5$ for $f_c = a/b$. and $\partial ln(f_c S(f_c))/\partial lnf_c = 0.5$. We define the crossover frequency f_c where two conditions above are satisfied. It is useful to define the

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[1] e.g. '0100000010000...' where '1' is a burst state.

crossover frequency in two ways to obtain a better estimation of crossover and to compute the crossover frequency automatically.

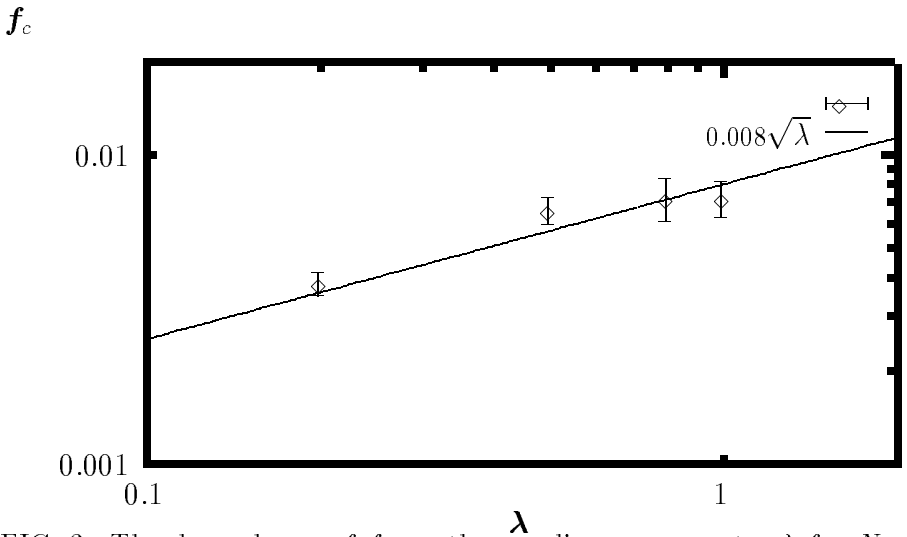

FIG. 3. The dependence of f_c on the non-linear parameter λ for $N = 12$. We estimate the errorbar by sample average over five data of f_c. One datum of f_c is evaluated using a PSD already sample-averaged over ten PSDs with other initial conditions. The line represents the relation $f_c \sim \sqrt{\lambda}$. The experimental data is taken at $\lambda = 0.2 \sim 1$ from the second mode data. This result suggests that it is difficult to observe $1/f$ fluctuations in realistic phenomena which must have small non-linearity.

Fig. 3 shows how f_c varies with the non-linear parameter λ under the condition that the system size is fixed. The line in Fig. 3 represents $f_c \sim \sqrt{\lambda}$, which fits data points well [2]. The smaller non-linearity becomes, the more difficult it becomes to see $1/f$ PSD since f_c becomes too small.

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[2]It is interesting that our result is also consistent with the scaling relation that the characteristic time scales $\sim 1/\sqrt{\lambda}$ assuming that the amplitude of the displacements is fixed by the energy, though it is not apparent that the crossover between $1/f$ region and the white noise region obeys the usual scaling.

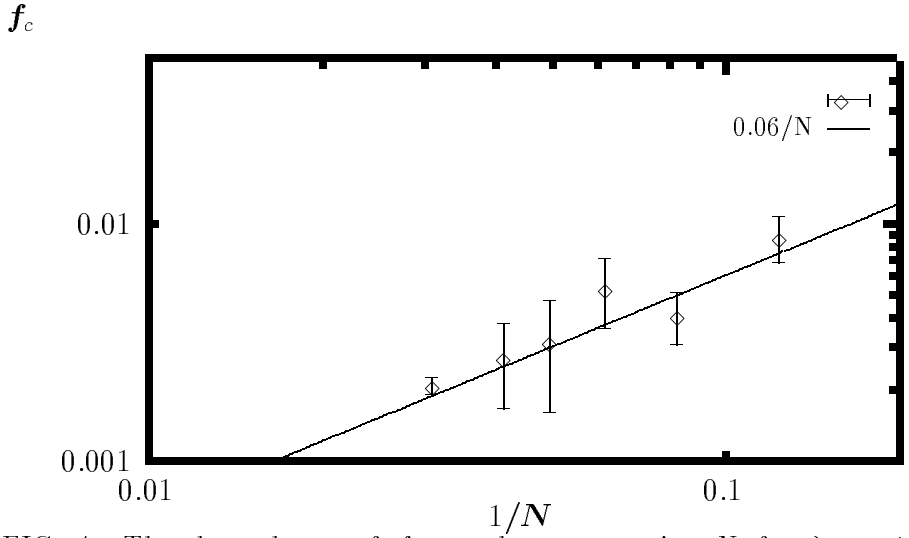

FIG. 4. The dependence of f_c on the system size N for $\lambda = 1$. Data are taken at $N = 8, 12, 16, 24$, and 32 from the second mode data. In the same way mentioned above, we estimate the errorbar by sample average over three data of f_c. One datum of f_c is evaluated using a PSD already sample-averaged over five PSDs with other initial conditions. The line $f_c \sim 1/N$ is just a guide for the eye. In thermodynamic limit f_c becomes ~ 0, so it must be difficult to observe the $1/f$ fluctuations.

In the same way we have investigated the system size N dependence of f_c at a fixed non-linear parameter $\lambda = 1$ (Fig. 4). The full line in Fig. 4 represents the relation $f_c = 0.06/N$, which fits data points. Our interest is independence of f_c on system sizes and non-linearity in the limit of large system sizes and small non-linearity. Under such a condition corresponding to real substances properties of low excited modes should be important, so we consider only low excited modes. We investigate the lowest first mode to fourth mode. f_c is evaluated for each system size N at this fixed non-linear parameter and the fixed mode. Since the number of knots is fixed, the wave number varies as $1/N$ with the system size N. For small wave numbers, the phonon wave number is linear to the phonon frequency. Hence the characteristic structure of PSD such as eigen frequencies shifts as $1/N$. The whole structure of PSD including $1/f$ structure may also shift as $1/N$, but it is not apparent. The whole structure of our PSD behaves roughly like $1/N$ shift. Fig. 4 shows the trend of the $1/N$ shift. In other words f_c is almost the same at the fixed wave number as the system size

varies. Low excited modes contribute to only the lowest frequency region of PSD. When the contribution from low excited modes is important, $1/f$ region from low excited modes is seen in only the lowest frequency region of PSD. This fact indicates that it is in general difficult to observe $1/f$ PSD in the limit of large system sizes [3] and small non-linearity, which limit corresponds to the condition of real substances. Our result suggests that increase of the number of degrees of freedom does not affect qualitative properties of $1/f$ PSD very much. Hence we clarify that $1/f$ fluctuations do not come from properties in the large number of degrees of freedom.

In summary we have investigated the FPU equation to find that it shows the $1/f$ fluctuations at sufficiently low frequency and the crossover frequency obeys $f_c \sim \sqrt{\lambda}/N$. No qualitative difference appears among investigated parameter ranges. Our result suggests that $1/f$ fluctuations do not come from the large number of degrees of freedom. We may be able to understand the fundamental mechanism of $1/f$ fluctuations based on theories like intermittency chaos where systems have been investigated in small degrees of freedom.

Lastly we consider the relation to experiments. One of the famous samples which show $1/f$ fluctuations is quartz oscillators. Musha et al. [2] observed the fluctuation of the imaginary part of quartz dielectric response to find that it shows $1/f$ fluctuations. They suggested that $1/f$ mechanism is closely related to fluctuations of thermally activated phonons. For the direct observation of phonon fluctuations, Musha et al. [3] took a laser-light-scattering experiment where the flux fluctuations directly represent the phonon number fluctuations. They found that the phonon number fluctuates as $1/f$. Our computation agrees with their experimental results.

In this computation we have investigated the FPU equation in one dimension. We should investigate qualitative and quantitative change of the PSD structure in higher dimensions.

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[3]We should remark here that the deviation from our result may happen in more and more large system size as seen in e.g. coupled maps of very large degrees of freedom [14].

It is also important whether the specific forms of non-linear terms are essential or not. The fact that we can see $1/f$ PSD even for small degrees of freedom may enable us to investigate motions in the phase space directly.

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