A series expansion for the time autocorrelation of dynamical variables

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Abstract

We present here a general iterative formula which gives a (formal) series expansion for the time autocorrelation of smooth dynamical variables, for all Hamiltonian systems endowed with an invariant measure. We add some criteria, theoretical in nature, which enable one to decide whether the decay of the correlations is exponentially fast or not. One of these criteria is implemented numerically for the case of the Fermi–Pasta–Ulam system, and we find indications which might suggest a sub–exponentially decay for such a system.

1 Introduction

It is well known that one of the most important indicators of the chaotic behaviour of a dynamical system is the rate of decay to zero of the time autocorrelation of dynamical variables. A vast literature exists on this subject, mainly addressed to systems of some special class (for example, Anosov systems, see [1], or systems with few degrees of freedom, such as billiards, see [2]). In this paper we study the decay of correlations in the general frame of the dynamical theory of Hamiltonian systems, with an invariant measure. Such an approach has already provided interesting results, as it allows to obtain results holding in the thermodynamic limit (see [3, 4, 5]).

Here we provide a power series expansion (with respect to time) of the time autocorrelation of a smooth function f (Theorem 2, Section 2). It turns out that the coefficients of such a series are essentially the variances of the $L_H^n f$, where L_H is the Poisson bracket operator relative to the Hamiltonian H. We then establish sufficient conditions for its time–decay not to be exponential (Proposition 2, Section 3). We finally give a numerical application to the case of the Fermi–Pasta–Ulam problem. By truncating the series up to order 12, for system up to 364 degrees of freedom, we show that one sufficient condition for the exponential decay is satisfied up to that order.

In Section 2 the relevant notions on time correlation functions are recalled. In the same section we give a theorem which establishes a kind of continuity (with respect to a suitable distance) of time correlations in the L^2 space of the dynamical variables, and also Theorem 2 for the series expansion.

Section 3 is devoted to a study of some general properties of the series expansion. Here an interesting link with the Stieltjes moment problem is pointed out, and two sufficient criteria for the time–decay of the autocorrelation not to be exponential are given in Proposition 2

Then, the results of some numerical computations on the time autocorrelations of a significant variable in a FPU chain are reported in Section 4. Finally, in Section 5 some comments on the usefulness of the present method are also given, together with a conjecture on the exponential decay of the correlations.

2 Time correlations in their "natural" space

We recall here some standard concepts within the measure theoretic approach to dynamical systems. We consider a Hamiltonian system on a phase space $\mathcal{M}$ endowed with a probability measure μ invariant with respect to the time flow ϕ^t induced by the Hamiltonian H. We also consider the time evolution operator $\hat{U}_t$ acting on the space of the square integrable functions from $\mathcal{M}$ to $\mathbb{R}$, i.e., $L^2(\mu, \mathcal{M})$. The operator $\hat{U}_t$ maps f to $\hat{U}_t f = f \circ \phi^{-t}$. It is known after Koopman (see [6]) that $\hat{U}_t$ defines a one–parameter group of unitary operators, namely operators preserving the norm $\|\cdot\|$ in $L^2(\mu, \mathcal{M})$.

We are interested in the time autocorrelation of a dynamical variable $f \in L^2(\mu, \mathcal{M})$ defined as

$$\mathbf{C}_f(t) \stackrel{\text{def}}{=} \langle f_t\, f\rangle - \langle f\rangle^2 = \langle (f_t - \langle f\rangle)\,(f - \langle f\rangle)\rangle \ , \tag{1}$$

where f_t is a shorthand for $\hat{U}_t f$, and $\langle\cdot\rangle$ denotes the mean value with respect to the probability measure μ.

It will also be useful to consider the time correlation between two dynamical variables f and g, defined as

$$\mathbf{C}_{f,g}(t) \stackrel{\text{def}}{=} \langle f_t g\rangle - \langle f\rangle\langle g\rangle = \langle (f_t - \langle f\rangle)\,(g - \langle g\rangle)\rangle \ .$$

It is well known from probability theory that the concepts of variance and correlation acquire a geometrical meaning if the covariance between two random variables f and g is used as a scalar product. The covariance is defined as

$$\mathrm{cov}(f,g) \stackrel{\text{def}}{=} \langle (f - \langle f\rangle)\,(g - \langle g\rangle)\rangle = \mathbf{C}_{f,g}(0) \ ,$$

This choice leads to take as norm[1] of a dynamical variable f its standard

[1] We can adopt this quantity as a norm in strict sense only if all dynamical variables which differ only by a constant are identified. For a function with zero mean the covariance $\mathrm{cov}(f,f)$ actually coincides with the usual L^2 norm. In this paper we shall use both norms, keeping the usual symbol $\|\cdot\|$ for the L^2 norm.

deviation σ_f, defined by

$$\sigma_f^2 \stackrel{\text{def}}{=} \mathrm{cov}(f,f) = \|f\|^2 - \langle f\rangle^2 = \|f - \langle f\rangle\|^2 \ ,$$

σ_f^2 being the variance of f.

The notion that some relation exists between two random variables f and g is made quantitative through the correlation coefficient $\mathrm{r}(f,g)$ defined as

$$\mathrm{r}(f,g) \stackrel{\text{def}}{=} \mathrm{cov}(f,g)/\sigma_f\sigma_g \ .$$

Using the Schwarz inequality it is easily seen in our case that one has $|\mathrm{cov}(f,g)| \le \sigma_f\sigma_g$, so that $|\mathrm{r}(f,g)| \le 1$. Two variables are orthogonal in this metric if they are uncorrelated, i.e., if $\mathrm{r}(f,g) = 0$, and collinear if $\mathrm{r}(f,g) = \pm 1$.

We also emphasize that, in view of the above definitions, the time autocorrelation of a function f is nothing but the covariance between $\hat{U}_t f$ and f. Therefore one immediately has

$$\mathbf{C}_f(0) = \sigma_f^2 \quad \text{and } |\mathbf{C}_f(t)| \le \sigma_f^2 \ . \tag{2}$$

Thus, the variance of a dynamical variable is the natural scale of its time autocorrelation.

We come now to state two useful theorems. The first one points out an interesting property of the time correlation. The mere fact that two dynamical variables are strongly correlated (i.e., sufficiently collinear in the scalar product given by the covariance) entails a similar behaviour of their time autocorrelations. Equivalently, we can say that in the neighbourhood of each dynamical variable f, i.e., in the set of all dynamical variables strongly correlated with f, the behaviour of the time autocorrelations is determined by that of $\mathbf{C}_f(t)$.

Theorem 1 *Let μ be a probability measure on the phase space $\mathcal{M}$, invariant for the flow generated by H, and let f and g be dynamical variables belonging to $L^2(\mu,\mathcal{M})$ such that one has $|\mathrm{r}(f,g)| \ge 1 - \varepsilon^2/2$ for some $\varepsilon > 0$. Then there exists a multiple of f, namely $\tilde{f} \stackrel{\text{def}}{=} (\mathrm{sign}(\mathrm{r}(f,g))\sigma_g/\sigma_f)f$, such that*

$$\left|\mathbf{C}_{\tilde{f},g}(t) - \mathbf{C}_{\tilde{f}}(t)\right| \le \varepsilon\sigma_g^2 \tag{3}$$

and

$$\left|\mathbf{C}_g(t) - \mathbf{C}_{\tilde{f}}(t)\right| \le \left(\varepsilon^2 + 2\varepsilon\right)\sigma_g^2 \ . \tag{4}$$

Proof. Both inequalities come from the remark that

$$\sigma_{g-\tilde{f}} = \sigma_g^2 + \sigma_{\tilde{f}}^2 - 2\mathrm{cov}(\tilde{f},g) = 2\sigma_g^2 - 2\sigma_g^2\mathrm{r}(f,g) \le \varepsilon^2\sigma_g^2 \ ,$$

which is due to the identities $\sigma_{\tilde f} = \sigma_g$ and $\mathrm{r}(\tilde f, g) = \big|\mathrm{r}(f,g)\big|$. In fact, (3) hence follows by noting that

$$\big|\mathbf{C}_{\tilde f,g}(t) - \mathbf{C}_{\tilde f}(t)\big| = \big|\mathrm{cov}(\tilde f_t, g) - \mathrm{cov}(\tilde f_t, \tilde f)\big| = \big|\mathrm{cov}(\tilde f_t, g - \tilde f)\big| \le \sigma_g \sigma_{g-\tilde f} \ ,$$

while (4), in a similar way, comes from the following relations

$$\begin{aligned} \big|\mathbf{C}_g(t) - \mathbf{C}_{\tilde f}(t)\big| &= \big|\mathbf{C}_{g-\tilde f}(t) + \mathbf{C}_{g,\tilde f}(t) + \mathbf{C}_{\tilde f,g}(t) - 2\mathbf{C}_{\tilde f}(t)\big| \\ &\le \sigma^2_{g-\tilde f} + 2\sigma_g \sigma_{g-\tilde f} \ . \end{aligned}$$

Here, in the second line, use is made of the previous inequality and of the identity $\mathbf{C}_{g,\tilde f}(t) = \mathbf{C}_{\tilde f,g}(-t)$, due to the invariance of the measure.

Q.E.D.

A central role in this paper will be played by the formal power series expansion of $\mathbf{C}_f(t)$ with respect to time, which is given in the following theorem. Use will be made of the definition of the k–th order Lie derivative of f, for $k \ge 1$, namely $f^{(k)} \stackrel{\mathrm{def}}{=} [f^{(k-1)}, H]$, where $f^{(0)} \stackrel{\mathrm{def}}{=} f$ and $[\cdot,\cdot]$ denotes the Poisson brackets.

Theorem 2 *Let μ be a probability measure on the phase space $\mathcal{M}$, invariant for the flow generated by H, and let $n > 0$. Then, for any dynamical variable $f \in L^2(\mu, \mathcal{M})$ such that $f^{(k)} \in L^2(\mu, \mathcal{M})$ for all $k \le n$, one has*

$$\begin{aligned} \mathbf{C}_f(t) =& \sigma_f^2 + \sum_{k=1}^{n} (-)^k \big\|f^{(k)}\big\|^2 \frac{t^{2k}}{(2k)!} \\ &+ (-1)^{n+1} \int_0^t \mathrm{d}t_1 \ldots \int_0^{t_{2n-1}} \mathrm{d}t_{2n} \big\| f^{(n)}_{t_{2n}} - f^{(n)} \big\|^2 \ . \end{aligned} \tag{5}$$

Proof. We use the simple chain of identities

$$\|f_t - f\|^2 = 2\sigma_f^2 - 2\mathbf{C}_f(t) = 2\|f\|^2 - 2\langle f_t\, f\rangle \ , \tag{6}$$

which hold true for any invariant measure, and the remark that

$$f_t - f = \int_0^t \hat U_{t-s} \dot f ds, \tag{7}$$

where $\dot f = [f, H]$. One can check equations (6) by writing down the square at the l.h.s., while (7) comes [2] from the variation of constants formula applied to $f_t - f$.

[2] See [3] for a more detailed proof.

We go on by writing the l.h.s. of (6) as

$$
\begin{aligned}
\|f_t - f\|^2 &= \int \mathrm{d}\mu \int_0^t \mathrm{d}t' \int_0^t \mathrm{d}t'' \big(\hat{U}_{t-t'}\dot{f}\big)\big(\hat{U}_{t-t''}\dot{f}\big) \\
&= \int \mathrm{d}\mu \int_0^t \mathrm{d}t' \int_0^t \mathrm{d}t'' \big(\hat{U}_{t'-t''}\dot{f}\big)\dot{f} \qquad (8) \\
&= 2\int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t'' \left(\|\dot{f}\|^2 - \frac{1}{2}\|\dot{f}_{t''} - \dot{f}\|^2\right), \qquad (9)
\end{aligned}
$$

where, in the second line, the invariance of the measure with respect to the time evolution is used, so that the equality proceeds from a simple change of coordinates, and in the last line the same argument is used, as well as relation (6) applied to the variable $\dot{f}$. The order of the integrals can be exchanged if $\|\dot{f}\|$ is finite, because the integral (8) is absolutely convergent in this case, in virtue of Schwarz inequality. In (9) we repeat the same calculation for $\|\dot{f}_{t''} - \dot{f}\|^2$, using $\dot{f} = [f, H]$. This gives us the relation

$$
\begin{aligned}
\|f_t - f\|^2 &= 2\left(\|\dot{f}\|^2 \frac{t^2}{2!} - \|f^{(2)}\|^2 \frac{t^4}{4!}\right) \\
&\quad + \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_3 \int_0^{t_3} \mathrm{d}t_4 \|f_{t_4}^{(2)} - f^{(2)}\|^2 ,
\end{aligned}
$$

where $f^{(2)} = [\dot{f}, H]$. The same procedure can be iterated up to $k = n$ by recursively defining $f^{(k)} \stackrel{\text{def}}{=} [f^{(k-1)}, H]$, starting with $f^{(0)} \stackrel{\text{def}}{=} f$, and using the hypothesis that $f^{(k)} \in L^2(\mu, \mathcal{M})$. This completes the proof.

Q.E.D.

Remark 1. Theorem 2 suggests that one can express, at least in a formal way, the time autocorrelation of a dynamical variable f as a power series with respect to time

$$
\mathbf{C}_f(t) = \sigma_f^2 + \sum_{k=1}^{+\infty} (-)^k \|f^{(k)}\|^2 \frac{t^{2k}}{(2k)!} . \qquad (10)
$$

We could have got to this formula also by expressing f_t as a time power series through its Lie derivatives and by integrating by parts $\langle f_t\, f\rangle$, taking into account the observation that the mean value of any function which can be written as $[g, H]$ vanishes[3], since $\big\langle [g, H]\big\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\langle g\rangle$.

Remark 2. We emphasize that the term in the second line in equation (5), i.e., the remainder, turns out to be positive or negative accordingly to

[3]For the same reason, $\sigma_{f^{(k)}}$ can replace $\|f^{(k)}\|$ in all the previous formulas. We will keep the given notation, because this way it is more straightforward to understand how to compute the coefficients of the series.

n being odd or even, respectively. Therefore, the truncations of series (10) provide upper bounds for the time autocorrelation of f if truncated at an odd n, and lower bounds if truncated at an even n. Such bounds provide some informations on the behaviour of the time autocorrelation of f for finite times. The simplest example is that of the first order truncation, which has shown to be very helpful for the study of relaxation times in Hamiltonian setting (see [3, 4, 5]).

3 Properties of the series

Our aim now is to investigate the properties of the series expansion (10), which represents the formal expansion of the time autocorrelations. An especially interesting question concerns its asymptotic behaviour. In many cases one is indeed interested in determining whether the time correlation tends to zero as $t \to \infty$ and, if this is the case, which law controls this decay. Indeed, it is commonly stated that if the correlations decay exponentially fast (for a suitable and wide class of functions) then the system is chaotic. We are also interested in finding conditions under which the decay to zero is not exponentially fast.

Let us simplify the notations by defining

$$c_0 \overset{\text{def}}{=} \sigma_f^2 \ , \quad c_n \overset{\text{def}}{=} \left\| f^{(n)} \right\|^2 \text{ for } n > 0 \quad \text{and } a_n \overset{\text{def}}{=} \frac{c_n}{(2n)!} \ . \tag{11}$$

We point out that all these coefficients are positive.

For what concerns the problem of convergence, we just limit ourselves to recall that, in view of the Cauchy–Hadamard criterium, if the inequalities

$$a_n \leq D^n \quad \text{or, as is equivalent,} \quad c_n \leq D^n (2n)! \ , \tag{12}$$

are satisfied with $D > 0$, then series (10) uniformly converges near the origin to an analytic function.

We concentrate instead on two questions: first, what can be known *a priori* on the coefficients in view of the Schwarz inequality (2); second, which informations on the coefficients are needed in order to say something on the large time behaviour of the time correlations.

Proposition 1 *The coefficients a_n and c_n defined by (11) are such that the polynomials $P_n^l(y)$, $Q_n^l(y)$ defined as*

$$P_n^l(y) \overset{\text{def}}{=} 2a_0^l + \sum_{k=1}^{2n} (-)^k a_k^l y^k \ , \quad Q_n^l(y) \overset{\text{def}}{=} \sum_{k=0}^{2n} (-)^k a_{k+1}^l y^k \ , \tag{13}$$

with

$$a_n^l \overset{\text{def}}{=} a_{n+l} \cdot (2n+2l)!/(2n)! = c_{n+l}/(2n)! \ , \tag{14}$$

are positive semidefinite, for any $n, l \geq 0$.

Proof. Consider the series (5), and recall that the remainder has a definite sign. Due to the inequalities (2) we readily get the bounds

$$a_0 + \sum_{k=1}^{2n} (-)^k a_k t^{2k} \geq -a_0 \quad \text{and} \quad a_0 + \sum_{k=1}^{2n+1} (-)^k a_k t^{2k} \leq a_0 \ , \quad \forall t \in \mathbb{R} \ ,$$

which hold true because the remainder is negative in the first case and positive in the second one. Setting $y \stackrel{\text{def}}{=} t^2$, we get the inequalities

$$P_n(y) \stackrel{\text{def}}{=} 2a_0 + \sum_{k=1}^{2n} (-)^k a_k y^k \geq 0 \ , \tag{15}$$

$$Q_n(y) \stackrel{\text{def}}{=} \sum_{k=0}^{2n} (-)^k a_{k+1} y^k \geq 0 \ , \tag{16}$$

i.e., the polynomials $P_n(y)$ and $Q_n(y)$ are semidefinite positive for $y \geq 0$. Look now for the real roots of the equations $P_n(y) = -\varepsilon$ and $Q_n(y) = -\varepsilon$, with $0 < \varepsilon < \min\{a_0, a_1\}$. Since $P_n(y)$ and $Q_n(y)$ are polynomials of degree $2n$ in which $2n$ changes of sign occur, Descartes' rule of signs implies that such roots, if they exist, must be positive. Thus P_n and Q_n are positive semidefinite on the whole real axis, i.e., the inequalities (15) hold true for all $y \in \mathbb{R}$.
Consider now the dynamical variable $f^{(l)}$, calculated by recursive application of the Poisson bracket with H. By a straightforward application of Theorem 2 we get that the coefficients of f^l are precisely a_n^l as defined in (14). Since the argument above applies to any dynamical variable, then we get that the corresponding polynomials $P_n^l(y)$ and $Q_n^l(y)$ are positive semidefinite, too, as claimed. Q.E.D.

Let us add a remark. The statement of Proposition 1 entails further restrictions on the coefficients c_n, since $P_n^l(y)$ and $Q_n^l(y)$ are two–indexed sequences of positive semidefinite polynomials. Unfortunately, such relations can be expressed only in a quite complicated way, according to the Jacobi–Borchardt theorem (see, for example, [7]), which gives some relations among the roots of the polynomials. For any given positive definite polynomial of degree n, the quantities $S_m \stackrel{\text{def}}{=} \alpha_1^m + \ldots + \alpha_n^m$, where α_i are the roots of the polynomial, must be such that the sequence of determinants

$$S_0 \ , \quad \begin{vmatrix} S_0 & S_1 \\ S_1 & S_2 \end{vmatrix} \ , \quad \ldots \ , \quad \begin{vmatrix} S_0 & S_1 & \ldots & S_{n-1} \\ S_1 & S_2 & \ldots & S_n \\ \vdots & \vdots & \ddots & \vdots \\ S_{n-1} & S_n & \ldots & S_{2n-2} \end{vmatrix} \ ,$$

changes sign at each step, until they permanently vanish. On the other hand, due to Newton's identities, the S_m's can be written as functions of the coefficients of the considered polynomials.

We come now to the second question, namely investigating the long time behaviour of the correlations, and in particular their asymptotic decay.

We look at the Laplace transform $F(s)$, for $s \in \mathbb{C}$, of the time autocorrelation of f. It is known that an exponential decay of $C_f(t)$ implies that its Laplace transform $F(s)$ is analytic in the half plane $\mathrm{Re}\, s \geq 0$, including the imaginary axis $\mathrm{Re}\, s = 0$ as well. In our case the transform can be formally written as

$$F(s) \stackrel{\text{def}}{=} \int_0^{+\infty} \left(\sum_{n=0}^{+\infty} (-)^n a_n t^{2n} \right) e^{-st} \, \mathrm{d}t \tag{17}$$

$$= \sum_{n=0}^{+\infty} (-)^n \frac{c_n}{s^{2n+1}} \ , \tag{18}$$

provided it is possible to exchange the sum of the series with the integration over time. However, even if considered as a formal series, the series (18) can nevertheless provide interesting informations, as will be shown in a moment.

Assume first that the series (18) uniformly converges on the exterior of a circle of finite radius ρ. Then the decay of correlations cannot be exponential. Indeed, in order that the convergence hypothesis be satisfied, it is required that

$$\limsup_{n\to+\infty} \sqrt[n]{c_n} \leq \rho \quad \Longleftrightarrow \quad \limsup_{n\to+\infty} \sqrt[n]{a_n} = 0 \ ,$$

whence follows that series (10) converges uniformly on the whole complex plane, so that one is allowed to pass from (17) to (18). Vivanti's theorem, then, guarantees that the series defining $iF(iy)$, which has positive coefficients only, have at least a singular point in $y = \rho$ or $y = -\rho$. Thus, the Laplace transform $F(s)$ has at least a singularity on the imaginary axis and this rules out the exponentially fast decay to zero.

Consider now the case in which (18) is just a formal power series. The form itself of such a series reminds us of Stieltjes work [9] on the link between the asymptotic series, their expansion in continuous fractions and a particular kind of integral transform. In dealing with this subject he encountered the moment problem that now bares his name. We recall that, given a sequence of positive numbers c_n, the Stieltjes moment problem consists in checking whether there exists a measure Φ on $\mathbb{R}^+$ such that

$$\int_0^{+\infty} u^n \mathrm{d}\Phi(u) = c_n \ . \tag{19}$$

The solution exists if and only if

$$\det(\Delta_n) > 0 \quad \text{and} \quad \det(\tilde{\Delta}_n) > 0 \quad \forall n \ , \tag{20}$$

where the matrices Δ_n, $\tilde{\Delta}_n$ are defined by

$$\Delta_n \stackrel{\text{def}}{=} \begin{bmatrix} c_0 & c_1 & \cdots & c_n \\ c_1 & c_2 & \cdots & c_{n+1} \\ \vdots & \vdots & \ddots & \vdots \\ c_n & c_{n+1} & \cdots & c_{2n} \end{bmatrix}, \; \tilde{\Delta}_n \stackrel{\text{def}}{=} \begin{bmatrix} c_1 & c_2 & \cdots & c_{n+1} \\ c_2 & c_3 & \cdots & c_{n+2} \\ \vdots & \vdots & \ddots & \vdots \\ c_{n+1} & c_{n+2} & \cdots & c_{2n+1} \end{bmatrix}. \quad (21)$$

Furthermore, the solution is unique if condition (12) on the c_n's holds (for a proof with more recent methods, see [12]).

Coming back to our problem, we collect the results of paper [9] of interest to us in the following statement: *if the Stieltjes moment problem for the sequence c_n is uniquely solvable, then the Laplace transform $F(s)$ has at least a singularity on the imaginary axis.* As already pointed out, this implies that the decay of correlations cannot be exponentially fast.

The previous statement is proved this way. We consider series (18) as a function of $z \stackrel{\text{def}}{=} s^2$. Then such a series can be written as s multiplied by

$$\frac{c_0}{z} - \frac{c_1}{z^2} + \frac{c_2}{z^3} + \ldots \qquad .$$

Stieltjes statement is the following. Disregarding convergence, let the series in the previous line represent the formal solution of a given differential or integral equation, and let the c_n's satisfy conditions (20) and (12). Then there exists a measure Φ on $\mathbb{R}^+$ satisfying (19) such that the solution of the considered differential or integral equation takes the form

$$\int_0^{+\infty} \frac{\mathrm{d}\Phi(u)}{z+u} \ .$$

Applying this result to the integral equation (17), we conclude that the Laplace transform of the autocorrelation function can be written as

$$F(s) = s \int_0^{+\infty} \frac{\mathrm{d}\Phi(u)}{s^2+u} \ . \qquad (22)$$

The latter formula shows that the Laplace transform of series (10) has some singularty on the imaginary axis, so that, again, the decay of the correlation cannot be exponentially fast.

We have thus proven the following

Proposition 2 *The two following conditions are separately sufficient in order that the decay of the time autocorrelation of the dynamical variable f be not exponentially fast:*

- *there exists $\rho > 0$ such that $\limsup_{n\to+\infty} \sqrt[n]{c_n} \leq \rho$;*
- *conditions (20) are fulfilled.*

Remark 3. The former condition in Proposition 2 requires only to have an upper bound on the c_n, whereas the latter one asks for a more detailed knowledge on the coefficients c_n. We believe that the first one is seldom fulfilled (an example in which this happens is that of a harmonic oscillator). For, the n–th derivative of a function usually grows as $n!$, so that

$$\limsup_{n\to+\infty} \sqrt[n]{c_n} = +\infty \ .$$

The second requirement enables us to deal with a larger class of variables, but, as just said, it has the drawback of needing a very detailed knowledge of all coefficients, in order to check (20).

4 Numerical study on the FPU chain

Applying proposition 2 to a concrete problem is a major task, because it requires information on an infinite number of coefficients. Thus, as a first application, we made some numerical computations on a model which is widely studied in the literature and is of great relevance for the foundations of statistical mechanics, namely the Fermi–Pasta–Ulam model (FPU, see [10]). It describes a one–dimensional chain of $N+1$ particles interacting through nonlinear springs. The Hamiltonian of such a system, after a suitable rescaling, can be written as

$$H = \sum_{j=0}^{N} \frac{p_j^2}{2} + \sum_{j=0}^{N-1} \left[\frac{(q_j - q_{j+1})^2}{2} + \frac{\alpha\,(q_j - q_{j+1})^3}{3} + \frac{\beta\,(q_j - q_{j+1})^4}{4} \right] \ ,$$

where $p = (p_0, \ldots, p_N)$ and $q = (q_0, \ldots, q_N)$ are canonically conjugated variables, while α and β are parameters that control the size of the nonlinearity. We choose as invariant probability measure the Gibbs one, i.e., $\mathrm{d}\mu(p,q) \stackrel{\text{def}}{=} Z^{-1}(T)\exp(-H(p,q)/T)\mathrm{d}p\,\mathrm{d}q$, where $Z(T)$ is the partition function and $T>0$ the temperature, and for the purpose of speeding up the numerical evaluation of the integrals involving the measure, we consider here a chain with one end point fixed and the other one free, i.e, we impose only the boundary condition $q_0 = 0$, $p_0 = 0$ (see footnote 5 below). We note however that a few computations made on the model in which both end points are fixed have shown no significant difference. Concerning the parameters, we consider the often studied case in which $\alpha = \beta = 1/4$. The relevant fact is that as T approaches 0 the contribution due to the nonlinear terms becomes statistically negligible.

It is well known that if the nonlinear terms are neglected then the Hamiltonian is integrable, admitting N normal modes of oscillation, and that the motion is quasiperiodic so that, for every $k = 0, \ldots, N-1$, the energy E_k of the k–th mode is a constant of motion (and thus, as obvious, the time autocorrelation of such a dynamical variable is constant).[4] Our aim is to investigate what happens when the nonlinearity is introduced as a perturbation, namely, for T positive but close to 0. We are particularly interested in the exchange of energy among the normal modes. To this end, a good choice could be to consider the fraction of energy localized on the low frequency modes, defined, for example, as

$$S = \frac{1}{N} \sum_{k=0}^{N/2} E_k \ ,$$

since its time variation is a convenient indicator of the flow of energy from low to high frequency modes, and vice versa. As a numerical tool we want to compute numerically the coefficients of the series (10) for this function, since, in view of Proposition 2, they may give indication on the asymptotic behaviour of the autocorrelation.

As a matter of fact, we notice that the function S may not represent the best choice. For, it may happen that such a function is strongly correlated with the Hamiltonian, so that, in virtue of Theorem 1, its autocorrelation could remain close to that of the Hamiltonian, thus remaining far from zero. This happens, indeed, so we rather took a suitable modification of S, namely, the projection of S, via the Gram–Schmidt orthogonalization process, on the space of the dynamical variables uncorrelated with H. Thus we consider the dynamical variable $\tilde{S} \stackrel{\text{def}}{=} S - \text{cov}(S,H)H/\sigma_H^2$.

Our calculation proceeds as follows. We extract a sample in phase space according to the Gibbs measure[5] and we estimate the L^2–norm $\|\tilde{S}^{(n)}\|^2$ of the functions $\tilde{S}^{(n)} = [\tilde{S}^{(n-1)}, H]$ generated by $\tilde{S}^{(0)} = \tilde{S}$ taking the mean value on our sample.[6] A direct evaluation of $\mathbf{C}_{\tilde{S}}(t)$ through the series (10) is unpractical, since it generally turns out to be a power series in t with a finite convergence radius. Fruitful results are instead provided by its Laplace transform (18). Following the procedure of Stieltjes, we approximate the Laplace transform up to order n with rational functions, and look for the

[4]It may be useful to recall that, in our case, the explicit expression of the energy of the k–th mode as a function of p and q is

$$E_k \stackrel{\text{def}}{=} \frac{4}{N+1/2} \left(\sin\left(\pi \frac{k+1/2}{2N+1}\right) \sum_{j=1}^{N} q_j \sin\left(\pi \frac{j(k+1/2)}{N+1/2}\right)\right)^2 + \frac{1}{N+1/2} \left(\sum_{j=1}^{N} p_j \sin\left(\pi \frac{j(k+1/2)}{N+1/2}\right)\right)^2 \ .$$

[5]We extract p_j and $r_j \stackrel{\text{def}}{=} q_j - q_{j-1}$, for $j = 1, \ldots, N$, which are stocastically independent variables for the Gibbs measure with respect to the present Hamiltonian. Here lies the great advantage of studying the chain with one end point free.

[6]Recall that the $\tilde{S}^{(n)}$'s are certain functions of p and q, which can be expressed via Faà di Bruno's formula for the derivatives of any order of a composed function.

poles of such an approximating function in the complex plane (see chapter 2 of the memoir [9]). The most striking fact is that the poles are foumd to lie on the imaginary axis, for any temperature T and any number N of particles we investigated (see below), at least up to the orders for which the outcome was found to be numerically reliable.

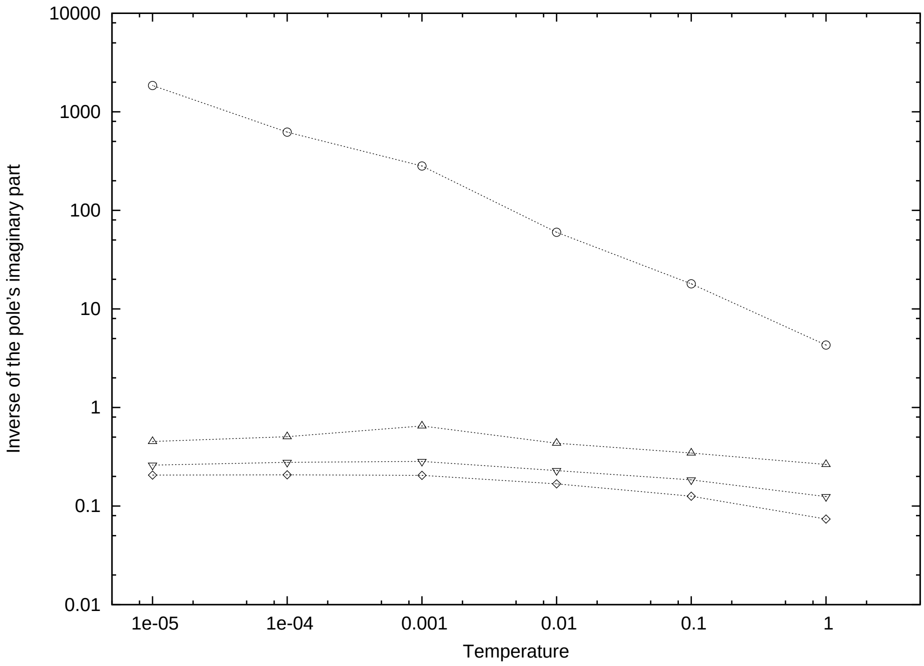

Figure 1: Inverse of the immaginary part of the four poles of the Laplace transform of the time autocorrelation of $\tilde{S}$ versus temperature, in logarithmic scale. Here the number of particles is $N = 40$. Notice that the real part is vanishing.

Let us describe the results in some detail. From analytical considerations one has that, by approximating the Laplace transform at order $2n$ with a rational function having polynomials of degree $2n$ as numerator and denominator, one finds $2n$ complex conjugated poles, $z_k = i\omega_k$, $\bar{z}_k = -i\omega_k$ say. The inverses of the ω's so found are plotted in fig. 1. The first pole that shows up in our calculation is the upper curve in the figure. It is due to oscillation of quite large period, growing as $1/T^{1/2}$ as T decreases to zero. The actual value changes a little when the approximation increases, keeping however the same order of magnitude. The plotted data correspond to the approximation order $n = 4$. We have also noted that the values found do not significantly change with the number N of particles, with N up to 364. The frequencies represented by the lower curves appear at successive orders $n = 2, 3, 4$, and correspond to oscillations of short period, close to the period of the normal modes. They appear to remain almost constant with T.

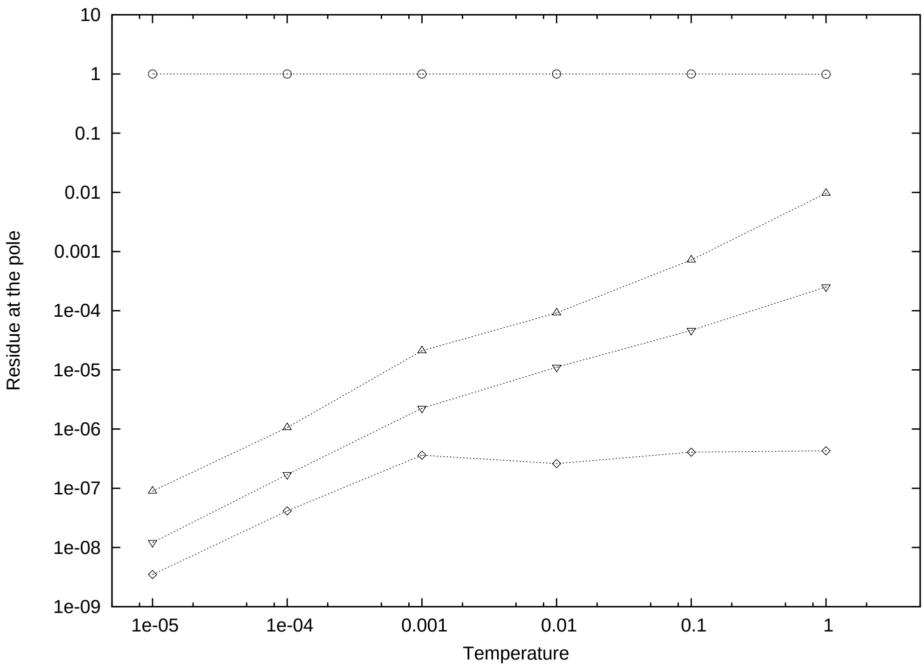

Figure 2: Residues at the four poles, whose imaginary parts are reported in fig. 1 versus temperature, in logarithmic scale. Here the number of particles is $N = 40$.

A further information is provided by the residues of the poles, which are the amplitudes of the oscillations. The quantities for the four poles of fig. 1 are reported in fig. 2, after a normalization defined by setting the sum of the residues equal to one. The remarkable fact is that the amplitude corresponding to the longest period is the largest one. Even for $T = 1$ the amplitudes of the shorter periods do not exceed one percent of the total.

Let us add a few considerations concerning the actual difficulty of the calculation. The main task is to calculate a determinant of increasing order, with coefficients determined via a Monte Carlo approximation of an integral. Thus the coefficients are subject to a numerical error. If the sequence of determinants (21) remains positive, then the poles lie on the imaginary axis. The difficulty is that increasing the order requires also a correspondingly increase of the precision, and so a longer and longer calculation in order to decrease the error on the coefficients. This makes the whole procedure unpractical even at not too high orders, and for this reason we performed most calculations up to order 8 only, thus finding 4 frequencies. In a few cases we computed two more frequencies, working with extended precision, and the result was that the determinants were still positive. We observed indeed that in some cases, as the order is increased, a new determinant turns out to be negative, with values strongly dependent on both the numerical precision and the size of the sample. On the other hand, a further increase of both the sample and the precision made these determinants to become stabilized with a positive value.

5 Conclusions

In view of the results found at low orders we may advance the conjecture that the conditions (20) are satisfied at every order, and that, as a consequence, the decay of correlations in the present system is not exponentially fast. An interesting question is whether it is possible to prove that conditions (20) are always satisfied, in virtue of Proposition 1, possibly with some supplementary hypothesis easier to check than (20). In our opinion this is an algebraic problem which is worth attention, in view of the great relevance of the exponential decay in the characterization of the chaotic behaviour of a given system.

References

[1] C. Liverani, Ann. Math. **159**, (2004) 1275-1312.

[2] N. Chernov, R. Markarian, *Chaotic billiards*, AMS (Providence, 2006).

[3] A. Carati, J. Stat. Phys. **128**, (2007) 1057-1077.

[4] A.M. Maiocchi, A. Carati, Commun. Math. Phys. **297**, (2010) 427-445.

[5] A. Carati, A.M. Maiocchi, *Exponentially long stability times in the thermodynamic limit*, Commun. Math. Phys. (2011), in press

[6] B. O. Koopman, Proc. Natl. Acad. Sci. USA **17**, (1931) 315-318.

[7] N. Obreškov, *Verteilung und Berechnung der Nullstellen reeller Polynome*, VEB Deutscher Verlag der Wissenschaften, (Berlin, 1963).

[8] G. Dötsch, *Anwendungen der Laplace–Transformation*, 1^{st} ed., Birkhauser (Basel, 1956).

[9] T. J. Stieltjes, Ann. Fac. Sci. Toulouse Sér. 1, **8**, J1-J122 (1894) and **9**, A5-A47 (1895).

[10] E. Fermi, J. Pasta, S. Ulam, in *E. Fermi Collected Papers*, The University Chicago Press (Chicago, 1965), vol. 2, pagg. 977-988.

[11] A. Carati, L. Galgani, A. Giorgilli, S. Paleari, Phys. Rev. E **76**, (2007) 022104.

[12] M. Reed, B. Simon, *Methods of mathematical physics*, Academic Press (San Diego, 1975).