Coherent Behaviour of Single Degrees of Freedom in an Order-to-Chaos Transition

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Introduction

A quite relevant theme in biological physics is the coherent energy transduction at the macromolecular level. One of the main theoretical problems in this field is the construction of a realistic model for nondissipative intramolecular energy transfer, through a nonlinear coupling among different degrees of freedom (DOFs).

In the recent past a soliton model, originally proposed by Davydov, has been extensively studied [1] in the general context of energy transport in proteins. We contributed [2,3,4] to the subject with a molecular dynamics study of acetanilide (ACN), a model for α-helical regions in proteins. In our work on ACN chains we have investigated the dynamics of the DOFs involved in the soliton generation and propagation. If a soliton travels along such a chain, one may have an ordered dynamics in a limited region of space, and for a limited time; the ordered region would move along the chain with the soliton. Because of the need to recognize those vibrations that can sustain ordered motions over adequate time scales, in a background of chaotic uncorrelated motions, we have elaborated new diagnostic tools to analyse the dynamical coherence of each DOF in a complex molecular system.

In a highly chaotic regime one does not expect to observe qualitatively different behaviours among the different DOFs: equipartition of energy holds and memory of the initial conditions is rapidly lost. However, in the transition from a fully chaotic regime to a regime dominated by ordered motions, one expects to find a mixed situation where part of the system may have a degree of chaoticity which is different from the rest of the system, and which could also vary in time. The usual indicators of order and chaos (e.g. Lyapunov spectra [5], fractal dimensions [6], spectral entropies [7]), which give a global information on the system and are based on asymptotic time scale estimates, would not be useful, e.g., in identifying in the complex structure of a molecular chain the DOFs involved in a soliton. In this work we propose new indicators: partial Lyapunov exponents, computed from the dynamics of the tangent space vector associated with a given dynamical system. The finite time analysis of the growth rate of the components of this vector will give the required knowledge on the chaoticity of the single DOFs. In order to test our diagnostics we study here a simple dynamical system exhibiting a large range of characteristic frequencies.

The model

Our model consists of a system of five nonlinearly coupled linear oscillators. The hamiltonian of the model is given by:

$$H = \frac{1}{2}\sum_{i=1}^{5}\left(p_i^2 + \omega_i^2 q_i^2\right) + \frac{1}{2}\sum_{i\neq j}^{1,5} q_i^2 q_j^2. \tag{1}$$

In one case, which we call the single gap system (SG), the values of the frequencies are the following: $\omega_1 = 1$, $\omega_2 = \frac{\pi}{2}$, $\omega_3 = 2$, $\omega_4 = 10e$, and $\omega_5 = 30$; in another case, which we call the double gap system (DG), we put $\omega_5 = 90$. The choice of the last two frequencies, an order of magnitude higher than the first three, is aimed at showing the influence of a broad range of frequencies with a gap on the dynamics of the various DOFs.

We have numerically integrated both the equations of motion and the variation equations of motion with the central difference algorithm. In our case the second order equations of motion are:

$$\ddot{q}_i = -\omega_i^2 q_i - 2\sum_{j(\neq i)}^{1,5} q_j^2 q_i \qquad i = 1,\ldots,5. \tag{2}$$

The equations of motion in the tangent space (variation equations) are related to the stability of the orbits; they are usually written as first order equations, obtainable from the hamiltonian equations of the system. If $\dot{x}_i = F_i(\{x_j\})$ are the hamiltonian equations of motion, where x_i is one of the q_i or one of the p_i, then the equations of motion of the tangent space vector $\vec{y}$ corresponding to the variation of $\vec{x}$ are given by:

$$\dot{y}_i = \sum_k \frac{\partial F_i(\{x_j\})}{\partial x_k} y_k \tag{3}$$

where the factor of y_k is computed along the trajectory $\vec{x}(t)$. Here we write (3) as second order equations:

$$\ddot{\xi}_i = -\left(\omega_i^2 + 2\sum_{j(\neq i)}^{1,5} q_j^2(t)\right)\xi_i - 4\sum_{j(\neq i)}^{1,5} q_i(t)q_j(t)\xi_j, \qquad \eta_i \equiv \dot{\xi}_i,$$

$$i = 1,\ldots,5, \tag{4}$$

where $(\xi_1,\ldots,\xi_5,\eta_1,\ldots,\eta_5) \equiv \vec{y}$, with ξ_i and η_i corresponding to the variations of q_i and p_i respectively.

From eqs. (4) one can compute the Lyapunov spectrum in the usual way [5]; in particular, the maximum Lyapunov exponent is given by:

$$\lambda_M = \lim_{t\to+\infty} \lambda(t), \qquad \lambda(t) = \frac{1}{t} Log \frac{|\vec{y}(t)|}{|\vec{y}(0)|} \tag{5}$$

where $\vec{y}(0)$ is the initial vector in the tangent space, taken randomly. We have defined new partial Lyapunov exponents (PLEs), referring to single DOFs:

$$\lambda_i = \lim_{t\to+\infty} \lambda_i(t), \qquad \lambda_i(t) = \frac{1}{2t} Log \frac{\omega_i^2 \xi_i^2(t) + \eta_i^2(t)}{\omega_i^2 \xi_i^2(0) + \eta_i^2(0)}, \qquad i = 1, \ldots, 5. \tag{6}$$

We want to remark the following point. It is a necessary condition that at least one of the λ_i is equal to λ_M, the maximum Lyapunov exponent defined in (5); but, a priori, some of them could be smaller. However, a generic initial vector in the tangent space will expand in modulus like $e^{\lambda_M t}$ when $t \to \infty$ with probability one. Therefore, also λ_i, for each i, should be equal to λ_M with probability one. However, this is true only in the asymptotic limit; it is not to be expected that the $\lambda_i(t)$s, at finite times, should be equal. As a matter of fact, their differences are a central point of our investigation. It turns out that, in the transition region between ordered and chaotic motions, there are still significant differences in the values of the $\lambda_i(t)$s for times three or four orders of magnitude higher than the characteristic periods of the oscillators. This is the manifestation of a qualitative diversity in the behaviour of the single DOFs. We have studied the differences among the $\lambda_i(t)$s by computing the quantities $\delta_i(t) = (\lambda(t) - \lambda_i(t))/\lambda_M$, and we have defined a characteristic "coherence time" for each DOF through:

$$\tau_i = \frac{1}{T} \int_0^T t\delta_i(t)dt. \tag{7}$$

Maximum Lyapunov exponents

We have studied the two versions of our model at different values of ϵ, the energy per DOF, or energy density. We have computed the maximum Lyapunov exponent (λ_M) to find out whether a transition in the dynamics takes place and the energy range in which this happens. In Fig. 1 we show λ_M at different energy densities for the SG version of our model. It is evident from the sharp change in the slope of $Log(\lambda_M)$ that such a transition takes place indeed [8], and is located between $\epsilon = 0.9$ and $\epsilon = 1$. Below this threshold the slope is strongly positive: λ_M changes by four orders of magnitude, passing from $\epsilon = 0.7$ to $\epsilon = 1$. Above the threshold the slope becomes small. The value of λ_M for the DG version at $\epsilon = 0.7$ is 1.04×10^{-3}, much larger than the corresponding value in the SG version (0.79×10^{-4}). This point will be discussed in the last section.

In the frame of the KAM theorem [9] it is interesting to contrast the values of λ_M with the anharmonicity of the system. We have computed the ratio R of the anharmonic to the total harmonic energy, and we report in Table I its values at the different energies that we have simulated. It is interesting to note that at $\epsilon = 0.6$, where the system SG gives $\lambda_M = 0$, the anharmonicity R is still as high as 4.7% . This shows that for this system - with a significant gap in the frequency spectrum - the ratio of the perturbed part of the hamiltonian to the harmonic part may reach quite relevant values before the KAM tori begin being destroyed.

TABLE I

ϵ	0.6	0.7	0.8	0.9	1.0	1.5	2.0
$R(\%)$	4.7	5.1	5.5	4.5	5.8	6.4	7.4

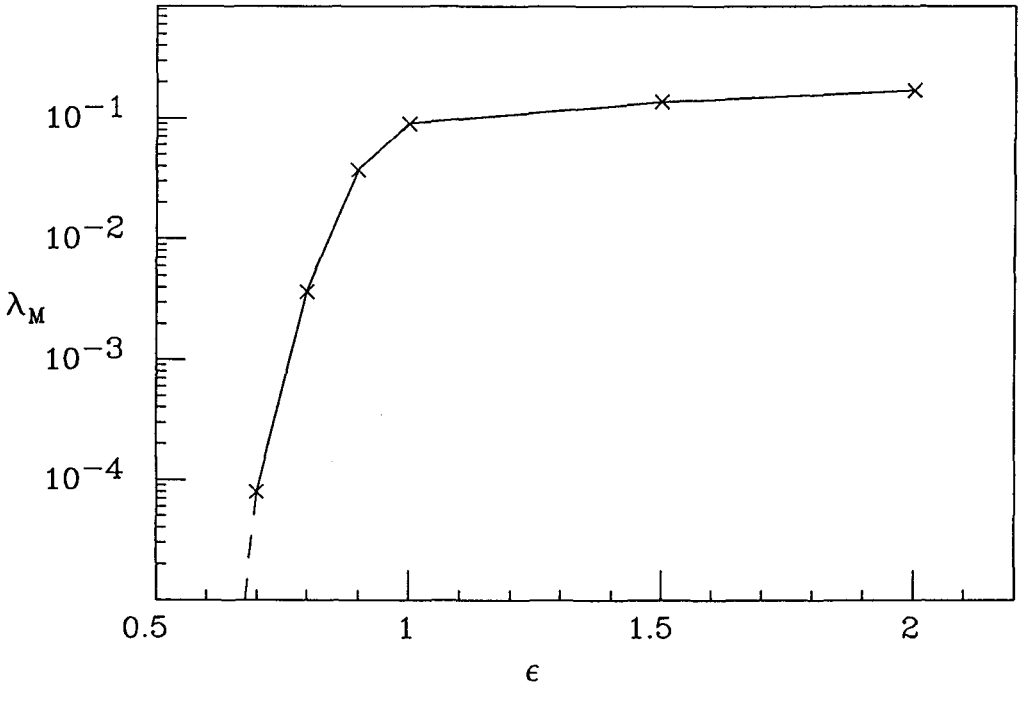

Fig. 1. Maximum Lyapunov exponent vs. energy density (SG case).

Correlation functions

The statistical properties of the dynamics of the single DOFs may be characterized by the autocorrelation functions (ACFs). We have collected in Fig. 2 these functions for the harmonic energies of the different DOFs for the SG case, at total energy density $\epsilon = 0.9$.

Some of the graphs are symmetric with respect to the zero line. This happens because in Fig. 2 only maxima and minima over groups of 100 computed points are plotted, in order to have clear graphs over large times. In the case of an ACF rapidly oscillating around zero this appears as a symmetrical graph. This way of plotting is sufficient if one is interested in studying the decay of the ACFs. From this point of view, they exhibit quite different patterns: there is a clear distinction between the high-

and low-frequency DOFs at that energy; while the high-frequency ACFs show a short decay time, the low-frequency ones exhibit a large decay time.

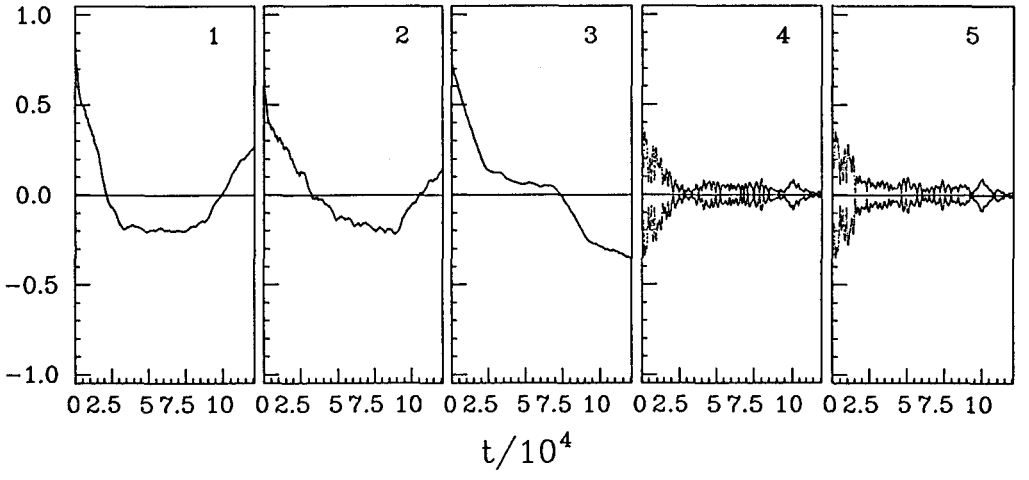

Fig. 2. Autocorrelation functions of the harmonic energy for the five degrees of freedom (SG case), at $\epsilon = 0.9$.

Partial Lyapunov Exponents

We have computed the PLEs for the five degrees of freedom of our system at energies near to the transition point individuated by λ_M. In Fig. 3 we show a graph with five curves corresponding to the DOFs for the SG case, at $\epsilon = 0.9$. It is clear that, because of the gap, the curves behave in very different ways; a group, corresponding to the DOFs with small eigenfrequencies, oscillates around zero; a second group, corresponding to the large frequencies, decays to zero only over large times. It should be noted here that the dynamical behaviour of the individual DOFs, as derived from the PLEs, is not related in a systematic way to the complementary information that can be deduced from the ACFs. Thus, while the PLEs of the high-frequency DOFs show a slower divergence of those DOFs for nearby trajectories (i.e., a localized ordered behaviour) than for the low-frequency DOFs, the corresponding ACFs at the same energy give a different indication, i.e., that the autocorrelation time is shorter for the high frequencies.

Using (7), one finds $\tau_4 = 182$ and $\tau_5 = 192$. The values computed for the low-frequency DOFs are not significant because the variance of the integrand in (7) is so large (in particular, larger than τ_i) that τ_i itself loses its meaning, as it could be expected looking at Fig. 3. The variance of the integrand in (7) for $i = 4, 5$ is small, which shows that the corresponding functions $\delta_i(t)$ are close to hyperbola with the x-axis as asymptote.

A point has to be remarked. One could try to assign a characteristic decay time to the ACFs shown in the previous section. It is evident, inspecting Fig. 2, that the shape of the ACFs in most cases does not allow to define a characteristic time of a

decay process. Indeed, either the ACFs are correlated over times which are even greater than the whole simulation time (DOFs 1, 2 and 3), or the structure is quite irregular (DOFs 4 and 5). At best, in the last case, one could roughly identify in the ACFs a superposition of two decaying processes with completely different characteristic times [10].

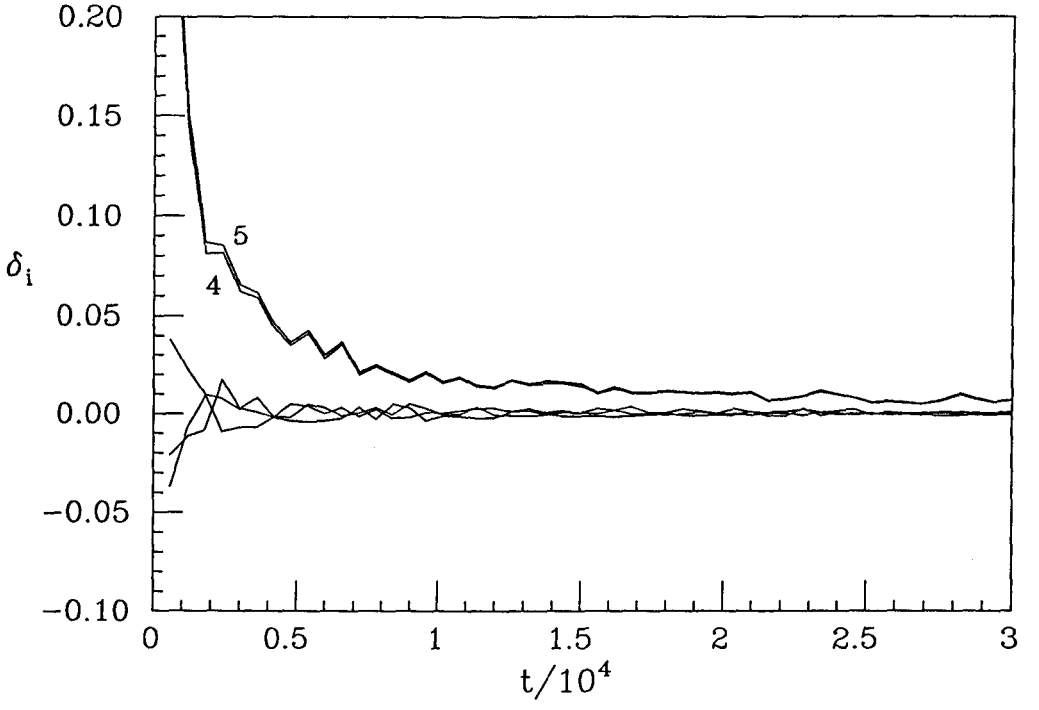

Fig. 3. Functions δ_i vs. time at $\epsilon = 0.9$ (SG case).

We have computed the LPEs also for the DG version at $\epsilon = 0.7$. The LPEs are shown in Fig. 4, using the same method as in Fig. 3. One can see that in this version, where the high frequencies are separated, the corresponding $\delta_i(t)$s are also separated, giving rise to quite different τ_is: $\tau_4 = 5400$, $\tau_5 = 7800$. Each τ_i of the high-frequency DOFs turns out to be approximately inversely proportional to λ_M, when ϵ is changed; the proportionality constant is approximately the same in both versions of the model for $i = 4$. More generally, looking at all the results, this constant seems to depend only on the frequency of each DOF.

Discussion and Comments

As noted before, the DG version has a λ_M which is much larger, at $\epsilon = 0.7$, than the λ_M of the SG version. That is, the system with the larger frequency gap is more

chaotic. This shows how a prediction of the qualitative features of the dynamics of a system based simply on an inspection of the frequencies (or frequency differences) of the DOFs may be misleading. On the other hand, the characteristic coherence times τ_i here introduced are able to single out the behaviour of each DOF also in a complex situation, in which a clear definition of a correlation time through the ACFs may not be possible (as shown in Fig. 2).

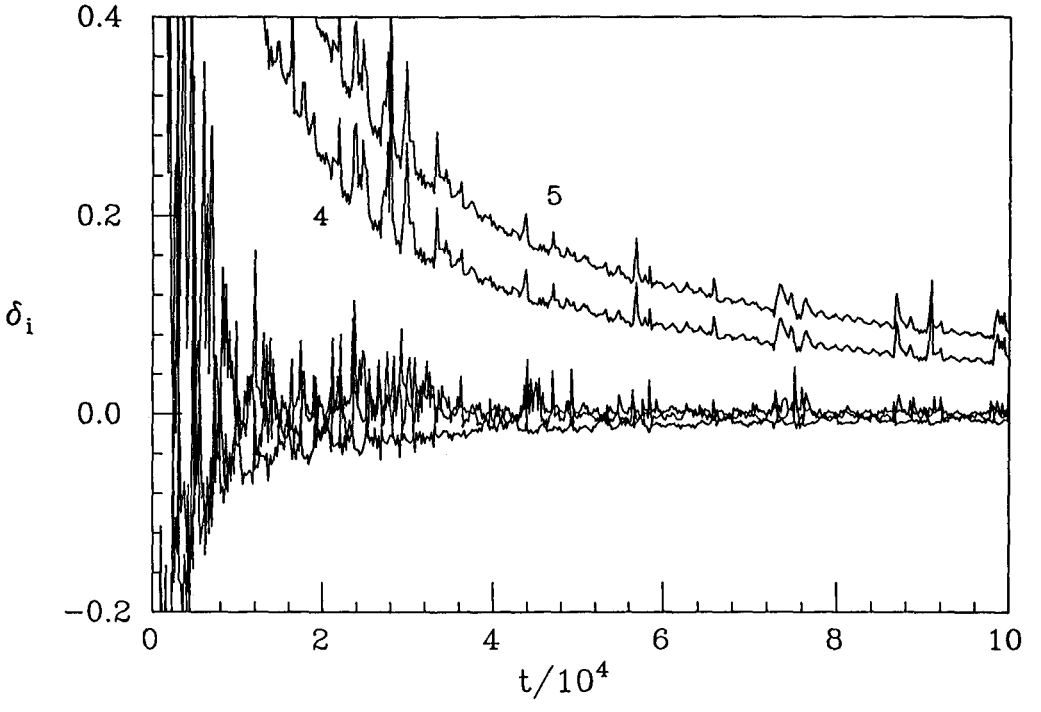

Fig. 4. Functions δ_i vs. time at $\epsilon = 0.7$ (DG case).

The shape of the curves given in Fig. 4 allows also to gain insight into the intermittent character of the dynamics of a single DOF. The peaks which accompany the time decrease of the curves indicate that the corresponding DOF have just had transient phases of more coherent dynamics, i.e., of lower values of the corresponding $\lambda_i(t)$. If one computed the $\lambda_i(t)$s over time intervals comparable with the average width of the peaks, one whould find a step-wise pattern, with short intervals of very coherent dynamics for the single DOFs. The coincidence of these peaks in different curves gives a clear indication of a cross-correlation of the coherent character in the dynamics of the DOFs.

In conclusion, we would like to stress an important feature of the new diagnostics we have introduced. When simulating a real system, one has always to use simplified models; it is therefore necessary to ask oneself if the results derived from the computer experiments are reliable. In this context the question of structural stability of the

equations of the model is of utmost importance. As this question is usually very difficult to answer for complex systems, one can think of using the PLEs to check whether the DOFs which are more relevant in the description of the phenomena of interest in the simulation have long coherence times. If this were the case, one could argue that these DOFs would also be structurally stable for small changes introduced in the equations of motion, in the same way in which they keep coherence for small perturbations of their trajectory.

More fundamentally, the computation of the coherence times of the DOFs in a realistic system, say in a biological macromolecule, could be a clue to understand how certain specific DOFs are able to perform ordered dynamical sequences over time intervals which are orders of magnitude larger than their characteristic period, while the others simply vibrate in a disordered, thermal way.

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