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Short Communication

On the Computation of the Maximum Lyapunov Exponent in Condensed Matter Systems

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INTRODUCTION

A feature of a dynamical system that is often studied is its level of chaos. This is measured through the computation of a spectrum of quantities called Lyapunov exponents. Often λ_1, the maximum one, is assumed to be sufficient to characterize the whole dynamics. λ_1 determines the rate of separation of trajectories with infinitesimally close initial conditions; a positive value is taken as an indication that the system is chaotic [1].

A rigorous way to assess the Lyapunov spectrum is to compute the dynamics in the tangent space of the phase space using linearized equations of motion. While this procedure is possible for simple systems [2], its computational burden becomes extreme for more complex systems. Therefore, most of the computations of λ_1 are performed integrating the equations of motion of two trajectories, a reference trajectory and a perturbed one, initiating in nearby points of the phase space. In unbound systems this procedure may produce an exponential overflow of the distance between the two trajectories. However, in condensed matter systems, where the phase space available to atomic positions and momenta is bounded, the distance between the two trajectories reaches in time saturation values even when the system is chaotic, as the separation grows until it approaches a limit imposed by the geometric and energetic constraints of the system [3-5].

To avoid collecting useless data once the saturation region is reached, the distance between the two trajectories can be scaled at regular time intervals, before evolving a new segment of the two trajectories; λ_1 is then computed as the average of its values computed on each segment. This method was originally introduced to avoid an overflow of the distance between trajectories in unbound systems [6]. In the present Note we examine numerical features of this procedure when applied to a condensed matter system, focusing on the reaction of the system following the perturbation of the reference trajectory.

It will be shown that the scaling procedure, when applied to a condensed matter system, entails a source of error when it is applied, as it often is, without regard for a detailed observation of the system's reaction to the perturbation. As an example, the dynamical evolution of a system of 256 particles interacting via a Lennard-Jones (LJ) potential will be computed using the popular Verlet integrator [7]:

$$\mathbf{x}_i(t+h) = 2\mathbf{x}_i(t) - \mathbf{x}_i(t-h) + \mathbf{a}_i(t)h^2$$

$$\mathbf{v}_i(t) = (\mathbf{x}_i(t+h) - \mathbf{x}_i(t-h))/2h$$

Here $\mathbf{x}_i$ is the position of the i–th atom, $\mathbf{v}_i(t)$ its velocity, $\mathbf{a}_i(t)$ its acceleration; t is the time and h is the time step. Using this integrator the computed atomic positions are accurate up to a term $O(h^4)$, the velocities up to a term $O(h^2)$.

THE INITIAL PERTURBATION

There are several ways to perturb the reference trajectory. (A) A very intrusive one is the following. Given u, a random variable with uniform distribution between −0.5 and +0.5, each component of the vectors $\mathbf{x}_i(t)$ and $\mathbf{x}_i(t-h)$ ismultiplied by a factor $(1.0 + u \cdot S)$, where u is different for each component of each vector of each atom. S is a parameter tuning the overall strength of the perturbation. Because of the integration algorithm, the perturbation of the positions induces a perturbation also in the velocities. (B) A less intrusive perturbation is the one in which u is the same for the three components of $\mathbf{x}_i(t)$ and $\mathbf{x}_i(t-h)$, but is different for different atoms.

Here, because of the integration algorithm, the velocities are unperturbed at $t = 0$. In the following steps the perturbation of the positions produces a perturbation also of the velocities. It turns out that the results presented in this Note are qualitatively independent of the choice of the perturbation, whether A, B, or any perturbation created in between by applying differently the factor $(1.0 + u \cdot S)$.

Starting from the final point of an equilibrium trajectory of the system, the perturbation is applied at a time thereafter defined as $t = 0$. After the perturbation, a first segment of length Δ is integrated in parallel on the reference trajectory and on the perturbed trajectory; $\mathbf{d}(t)$, the distance in the phase space between the two trajectories, is recorded at every time step. At the end of this first segment, the vector $\mathbf{d}(t)$ is scaled, keeping its orientation but reducing its norm to the value at the beginning of the first segment. A new pair of segments of equal length is than computed, one segment being the continuation of the reference trajectory, and the other a new perturbed one initiating at the scaled end of vector $\mathbf{d}(t)$. This procedure is replicated on n following pairs of segments; the initial time of each segment is again defined as $t = 0$. At the end a local maximum Lyapunov exponent is computed via the following formula on each pair of segments:

$$\lambda_1 = (1/\Delta)\ln[d(\Delta)/d(0)]$$

where $d(t)$ is the norm of $\mathbf{d}(t)$. Finally, an effective maximum Lyapunov exponent is given by the average of the local exponents λ_1 computed on perturbations applied in different points along the reference trajectory, each followed by n perturbed segments. In the paper at hand this procedure is applied separately to the positions and momenta sub-spaces of the phase space, as their behaviour may be different. As all atoms have the same mass, the momenta sub-space is identical with the velocities sub-space.

The Lennard-Jones System

As an example we perturbed an equilibrium trajectory of a face centered cubic crystal composed of 256 LJ particles. As is customary, reduced LJ units were used in the computation: ϵ for the energy, σ for the distances $\tau = \sqrt{(m\sigma^2/\epsilon)}$ for the time. The corresponding physical values are, for Argon: $\epsilon = 1.654\times10^{-21}$ J; $\sigma = 3.405\times10^{-10}$ m; $\tau = 3.112\times10^{-13}$ s. The crystal's temperature is $T = 80$ K.

Figure 1 shows a typical result obtained using $S = 0.001$ in perturbation A, and computing in double precision 5 segments of 10 ps, with a time step of 2 fs. The figure shows the time evolution of the distance in the velocities sub-space in the 5 segments following the perturbation of the reference trajectory. These curves exhibit various features.

In this sub-space the first segment, that is the time evolution of the distance following the actual perturbation, behaves differently from all following ones. The distance grows rapidly from the initial perturbed value, and its following evolution separates it from the curves relating to the following, scaled perturbations. The latter initiate - because of the scaling algorithm - at the same value as the first segment, but evolve slowly toward higher values. These curves include three parts, characterized by different behaviours: a first, short part, where the slope of the curve is irregular; a second part, where the distance grows exponentially in time; a third part where the curves show an inflection, hinting at the onset of a saturation of the distance between trajectories. This saturation takes place both in the coordinates and velocities sub-spaces.

These different behaviours can be better appreciated switching the vertical scale to a logarithmic one, as shown in Figure 2. The curve of the first segment doesn't show an exponential growth, and the initial positive jump is

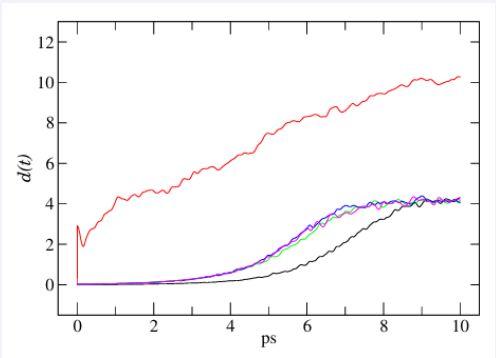


Figure 1 Solid LJ system, perturbation A. $S = 0.001$. Distance in the velocities sub-space, units σ/τ. Red curve: segment 1; black curve: segment 2; other colors: segments 3-5.

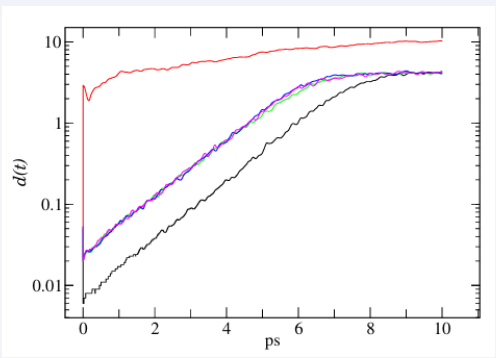


Figure 2 Same data as in Figure 1. Solid LJ system, perturbation A. $S = 0.001$. Distance in the velocities sub-space, units σ/τ. Red curve: segment 1; black curve: segment 2; other colors: segments 3-5.

due to a major reaction of the system to the perturbation. The second segment has at its beginning a dip, which means that the distance between the perturbed trajectory and the reference one is actually diminishing. This points at the condensed matter system's dynamic inertia: when the velocities of the atoms are changed, the system tries to recover the previous state, each atom feeling the reaction of its near environment to its displacement. This reaction has been noticed several years ago [4]. After the dip, the curve grows exponentially, as shown in the linear evolution in the logarithmic scale, between approximately t = 0.2 ps and 6.0 ps. In its last part, the evolution of the curve displays a saturation. In the last three segments the initial dip is less deep than in the second segment; this can be interpreted as a consequence of the first and second perturbation having shaped the system in such a way that the following scaled perturbations happen in a system already prepared to absorb them. These curves too grow exponentially between approximately t = 0.2 ps and 6.0 ps, and show a saturation in the last part of their evolution. The slope of segments 2 – 5 (and of 5 further following segments, not shown for clarity of the figure) are very similar, giving substance to the measurement of λ_1 as an average on these curves.

The system's dynamic inertia can be observed also in the position's sub-space. Figure 3 showcases in more detail the different behaviour of the first segment compared to the following ones, representing the time evolution after the scaled perturbations. Some segments following the first have at the beginning a very shallow negative dip, the origin of which has been explained above.

The 256 LJ particles system has been simulated also in the liquid state, at T = 85 K. Performing the analysis in the velocities sub-space one finds the results shown in Figure 4. Here all curves relative to the values S = 0.001, 0.01, 0.1 are shown. The results of these three cases cannot be distinguished; this means that varying the value of S over

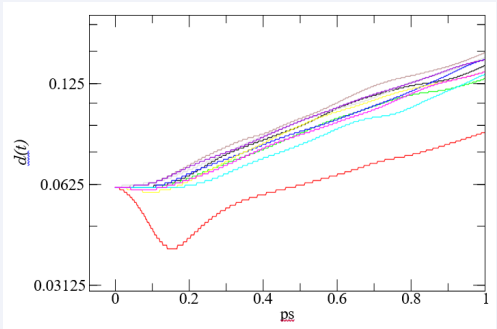


Figure 3 Solid LJ system, perturbation B. S = 0.01. Distance in the positions sub-space, units σ. Red curve: segment 1; other colors: segments 2-10.

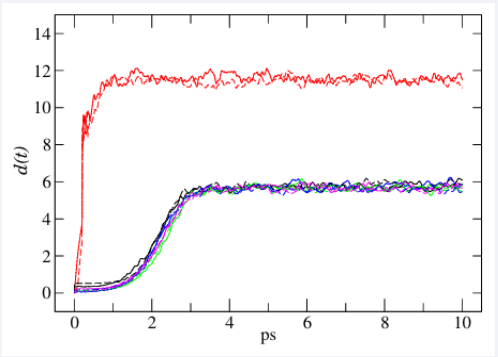


Figure 4 Liquid LJ system, perturbation B. Distance in the velocities sub-space, units σ/τ. Continuous lines: S = 0.001; dashed lines: S = 0.01; dotted lines: S = 0.1. Red curves: segments 1; other colors: segments 2-10.

two orders of magnitude doesn't change the behaviour of the system. Equivalent results (not shown) have been obtained for the positions sub-space in the liquid system, and for the positions and velocities sub-spaces in the solid system. In Figure 4 the curves relative to the first perturbed segment behave very differently from the following segments, as they don't have any portion growing at an exponential rate. The following perturbed segments have an exponential growth with similar slope between approximately 1.0 and 2.5, and the distances saturate at about 3 ps.

Figure 4 shows again the anomalous behaviour of the first perturbed segment, and an exponential growth of the following segments between approximately 0.3 and 2.5 ps. After t = 2.5 ps an inflection of the curves begins, pointing at the onset of a saturation of the distance between trajectories in the velocities sub-space.

If one wanted to compute λ_1 in the total phase space, comprising both positions and velocities, the time over which the divergence of trajectories should be measured would be the time interval in which both sets of variables exhibit an exponential growth. Moreover, it is advisable to discard the result of the first segment when computing λ_1 as the average on the series of segments that initiate by perturbing the reference trajectory.

CONCLUSION

In conclusion, the procedure to compute an average λ_1 in a condensed matter system (solid, liquid, macromolecule) is the following:

(1) Compute n segments of unperturbed and perturbed trajectories with the scaling procedure, as described above.(2) Draw two figures similar to Figure 2, one in the positions sub-space, and one in the velocities sub-space, with a logarithmic scale on the vertical axis $d(t)$. (3) Discard

the curve relative to the first segment. (4) Identify on the two figures the common time interval where the curves evolve linearly in the logarithmic scale, that is, where the distance between trajectories grows exponentially. (5) Compute the average λ_1 on all segments, but the first ones, from the slope of the curves in that common time interval.

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