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Lyapunov Modes of Two-Dimensional Many-Body Systems; Soft Disks, Hard Disks, and Rotors

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The dynamical instability of many-body systems can best be characterized through the local Lyapunov spectrum $\{\lambda\}$, its associated eigenvectors $\{\delta\}$, and the time-averaged spectrum $\{\langle\lambda\rangle\}$. Each *local* Lyapunov exponent λ describes the degree of instability associated with a well-defined direction—given by the associated unit vector δ—in the full many-body phase space. For a variety of *hard*-particle systems it is by now well-established that *several* of the δ vectors, all with relatively-small values of the time-averaged exponent $\langle\lambda\rangle$, correspond to quite well-defined long-wavelength "modes." We investigate *soft* particles from the same viewpoint here, and find no convincing evidence for corresponding modes. The situation is similar—no firm evidence for modes—in a simple two-dimensional lattice-rotor model. We believe that these differences are related to the form of the time-averaged Lyapunov spectrum near $\langle\lambda\rangle = 0$.

KEY WORDS: Local Lyapunov exponents; Lyapunov modes; hard disk fluid; soft disk fluid.

1. INTRODUCTION

Nonequilibrium molecular dynamics has been used to establish a close link between microscopic dynamical phase-space instabilities and the macroscopic irreversible dissipation associated with the second law of thermodynamics.[(1–5)] The simplest such connection between microscopic dynamics

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and macroscopic dissipation results when a Nosé-Hoover thermostat is used to control a nonequilibrium steady state. In this case the instantaneous external entropy production rate (due to heat extracted by the thermostat) is proportional to the sum of the instantaneous Lyapunov exponents:

$$\dot{S}/k \equiv -\sum \lambda.$$

Such microscopic-to-macroscopic connections have focussed attention on these instantaneous (or "local") Lyapunov exponents, $\{\lambda\}$, and their time averages, $\{\langle\lambda\rangle\}$. A very recent development is the discovery of "modes"[(6–13)] corresponding to the exponents. Because our current theoretical understanding of these modes, as well as the exponents themselves, is still rudimentary, the present work treats only equilibrium systems. These results can serve as a basis for extending our understanding to the far-from-equilibrium systems which are a strong focus of current research in many-body dynamics.

At equilibrium, and away, the local exponents together with their associated eigenvectors provide the fundamental microscopic description of phase-space instability. Recent investigations[(6–13)] have shown that some of the Lyapunov exponents, those describing relatively-weak instabilities with near-zero growth rates, correspond to *wavelike* eigenvectors, both longitudinal and transverse. The phase relations in these eigenvectors differ from those of acoustic waves. The coordinate and momentum displacements in the Lyapunov "modes" are "in phase" reflecting the exponential time dependence $e^{\lambda t}$ of Lyapunov instability. In acoustic waves the coordinate and momentum displacements have a phase difference of $\frac{\pi}{2}$, reflecting their periodic time dependence $e^{i\omega t}$.

Computing these instantaneous eigenvectors requires additional N-body solutions, one for each vector, so that the work for a complete description varies as the *square* of the number of particles, N^2. Worse yet, the additional computational effort involved in keeping of the order of N^2 eigenvectors orthonormal, where each eigenvector has of the order of N components, varies as N^3. Nevertheless, presentday gigahertz serial-processor work stations are capable of following the complete spectrum of eigenvalues and eigenvectors for systems of a thousand particles.

The present work describes detailed computations for *soft* disks at equilibrium. Though some qualitative modelike character is present in the soft-disk results the evidence is much less convincing than corresponding hard-disk simulations. Likewise, lattice-rotor simulations give no firm evidence for modes in two dimensions.

We review the definition and evaluation of the Lyapunov exponents and their associated δ vectors in the next section. Numerical results follow, for a dense soft-disk fluid, and we include corresponding observations for lattice-rotor problems. Our exploration of the fundamental question "Modes or Not?" and our overall conclusions make up the final two sections.

It is our great pleasure to dedicate this work to Bob Dorfman, whose generous, careful, and perceptive exploration of statistical mechanics[5] has enriched the field and our appreciation of it.

2. LOCAL LYAPUNOV EXPONENTS

The "local" (or "instantaneous") Lyapunov exponents quantify a special set of *comoving and corotating* (moving, and rotating, in the neighborhood of a particular "reference solution" in phase space) orthogonal expansion and contraction rates. For a *two*-dimensional system of N particles, the complete $\{x, y, p_x, p_y\}$ phase space is $4N$-dimensional, and $4N$ local Lyapunov exponents $\{\lambda\}$ describe the expansion and contraction rates of an infinitesimal "ball" (or "extension in phase") centered on the reference trajectory. The usual "global" Lyapunov exponents $\{\langle\lambda\rangle\}$ are the long-time-averaged values of the local exponents. It is also possible to carry out simulations restricted to the $4N-1$-dimensional energy shell, in which case there are $4N-1$ local Lyapunov exponents. The instantaneous $\{\lambda\}$ and $\{\delta\}$, as well as their fluctuations, depend upon the coordinate system chosen to describe the system, while the long-time-averaged spectrum of exponents $\{\langle\lambda\rangle\}$ does not.[14]

For the chosen coordinate system we have to follow the changing *orientations* of the vectors—along which the orthogonal rates are calculated—empirically. The rates and orientations both follow from continuous Gram–Schmidt orthonormalization of vectors linking the central "reference trajectory" to $4N$ infinitesimally-separated nearby "satellite trajectories." In the Hamiltonian case (which we treat here) and also in some special homogenous nonequilibrium situations,[15] the exponents and their eigenvectors have a symmetry property—"pairing"—which makes it unnecessary to calculate the whole spectrum. In these cases the sums of *pairs* of exponents, $\lambda_1+\lambda_{4N}$, $\lambda_2+\lambda_{4N-1}$, $\lambda_3+\lambda_{4N-2}$,... are identical, so that only half the spectrum, $\{\lambda_{1\leqslant j\leqslant 2N}\}$, needs to be calculated. In all of our work here the sum of the complete spectrum of exponents vanishes as a consequence of the underlying Hamiltonian mechanics.

The dependence of the local exponents and their δ vectors on the chosen coordinate system is easy to demonstrate in Hamiltonian mechanics.[14] With Cartesian coordinates the introduction of a simple scale factor s into the Hamiltonian, (analogous to simple changes of length and mass units which leave phase volume unchanged)

$$\mathscr{H} = \Phi + K \longrightarrow (\Phi/s) + Ks,$$

where the potential energy is the usual pairwise-additive sum:

$$\Phi \equiv \sum_{i<j} \phi_{ij}; \qquad K \equiv \sum p^2/(2m),$$

leaves the dynamics, $\{q(t), \dot{q}(t), \ddot{q}(t),...\}$ unchanged, but *does* change the relative contributions of the coordinates $\{q\}$ and momenta $\{p\}$ to the *local* Lyapunov exponents and to their associated δ vectors.

The *directions* in which the growth and decay rates are measured at a particular phase-space point represent the integrated past history in the neighborhood of the trajectory passing through the point. There are several algorithms for the numerical evaluation of the local exponents. For the relatively large systems described here, with N of order 1000, the rescaling approach discovered by Stoddard and Ford,[16] by Benettin and his coworkers,[17] and by Shimada and Nagashima[18] is the only practical choice. It should be mentioned that Stoddard and Ford considered only the largest Lyapunov exponent in their work.

In our case we find the positive half of the Lyapunov spectrum by starting with $2N$ orthogonal $4N$-dimensional vectors $\{\delta\}$. These vectors describe the locations of $2N$ satellite trajectories infinitesimally close to the reference trajectory. All $2N+1$ trajectories are advanced in time by dt and the resulting new vectors are orthonormalized using the Gram–Schmidt procedure. That is, for each new vector δ_j, the projections of all earlier vectors $\{\delta_{k<j}\}$ in the direction of the new one are subtracted before the complete set of vectors $\{\delta\}$ is normalized. The normalization step provides estimates for the instantaneous exponents,

$$\lambda(t) \simeq (1/dt) \ln[\delta(t+\tfrac{dt}{2})/\delta(t-\tfrac{dt}{2})],$$

with the estimates becoming exact for sufficiently small dt. The time averages of these estimates $\{\langle\lambda\rangle\}$ then give the conventional Lyapunov spectrum.

3. RESULTS FOR SOFT DISKS

The eigenvector δ_1 associated with the largest (when time-averaged) Lyapunov exponent, $\langle\lambda_1\rangle$ has been carefully studied for series of fairly large dense-fluid systems, with as many as one million particles.[19–21] In that work a specially smooth short-ranged potential was used to eliminate the influence of force-law singularities on the (fourth-order Runge–Kutta) numerical integration errors. Here we consider the same dense two-dimensional fluid, but at equilibrium.

The specially smooth soft-disk potential function is pairwise-additive:

$$\Phi = \sum_{i<j} \phi_{ij}; \qquad \phi = 100(1-r^2)^4,$$

and vanishes beyond the cutoff distance $r = 1$. Both the energy per particle,

$$(\Phi + K)/N = \left[\sum_{i<j} \phi_{ij} + \sum_i (p_i^2/2m) \right] \Big/ N,$$

and the volume (area) per particle, L^2/N, are chosen equal to unity in all of our numerical work. With these choices the potential energy of the system is about 30% of the total energy:

$$\langle \Phi/N \rangle \simeq 0.30; \qquad \langle K/N \rangle \simeq 0.70.$$

A timestep of $dt = 0.01$ and an initial reference-to-satellite vector length—at the beginning of each timestep—of 0.00001 are good choices for this problem. We also carried out tangent-space simulations, which correspond to the limit of an infinitesimal reference-to-satellite vector length. The tangent-space simulations were carried out with a timestep of $dt = 0.002$ with a Gram–Schmidt orthonormalization carried out every five steps. Simulations both with and without constraints on the center of mass of the satellite trajectories were analyzed. All these varied approaches led to substantially similar results.

We studied typical results for systems of 4×4, 8×8, 16×16, and 32×32 particles, all with square periodic boundaries. The Lyapunov spectra for all these systems converge nicely to smooth featureless curves (two samples are shown in Fig. 1), showing none of the discontinuous stairstep structures now familiar from the hard-particle simulations of Dellago, Forster, Hirschl, Hoover, MacNamara, Mareschal, Milanović, and Posch. For comparison, two hard-disk spectra are shown in Fig. 2. The more complicated hard-disk spectrum (upper curve) has an aspect ratio of $\sqrt{0.75}$ rather than unity.

The statistical uncertainties in the exponents and the vectors decrease with time. For the positive exponents they follow, fairly well, an exponential decay:

$$\Delta \langle \lambda_i \rangle_t \simeq e^{-t\langle \lambda_i \rangle_\infty}.$$

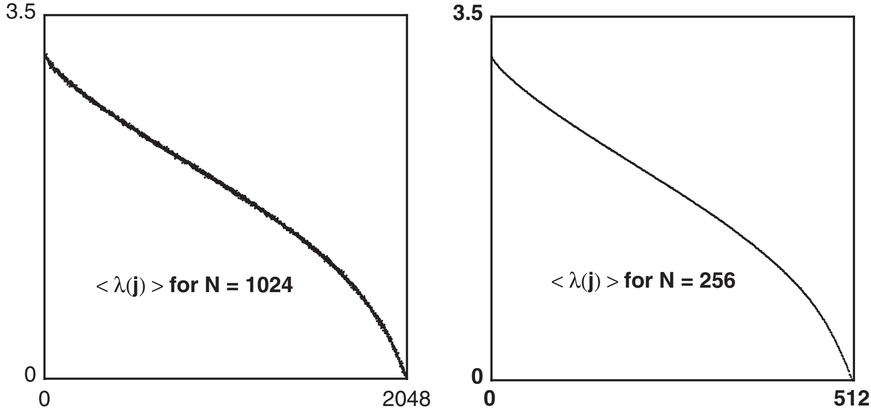

Fig. 1. Spectra of time-averaged Lyapunov exponents for 256 (right) and 1024 (left) soft disks. In both cases the largest $2N$ of the $4N$ exponents are shown.

We followed the 256-particle system to a time of 5000 in order to make sure that the gross features of the spectrum, which converge in a time of order 10, underwent no qualitative changes at longer times. Our 1024-particle system, though necessarily followed for a much shorter time, seems to behave in a similar manner. For 1024 particles the last positive exponent, $\langle \lambda_{2045} \rangle$, was in error by about 0.03 after 2000 timesteps of 0.01 each.

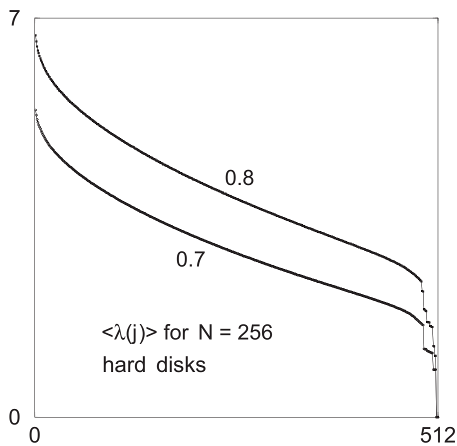

Fig. 2. Spectra of time-averaged Lyapunov exponents for 256 hard disks of diameter σ, with $\frac{N\sigma^2}{V} = 0.70$ and 0.80. The upper hard-disk spectrum (0.80) was computed with geometric aspect ratio $L_x/L_y = \sqrt{0.75}$. Compare this to the lower spectrum (0.70), with an aspect ratio of unity, to appreciate the effect of aspect ratio on "mode" degeneracy.

In the absence of center-of-mass constraints the eigenvectors corresponding to the last three of the calculated modes,

$$\{\delta_{2N}, \delta_{2N-1}, \delta_{2N-2}\},$$

all correspond to constants of the motion for our equilibrium system. In the full spectrum of $4N$ exponents, there are *six* vanishing exponents corresponding to the summed-up x and y coordinates, the summed-up p_x and p_y momenta, the energy, and the long-time-averaged stationarity of satellite displacements parallel to the phase-space flow direction. In energy-shell calculations, with $4N-1$ exponents there are only five vanishing exponents.

For plotting, we interpolated the individual components of the reference-to-satellite vectors onto a regular spatial grid by using a smooth-particle weighting function with a range of 2, 3, or 4.[4] We found that the resulting "modes" (that is, the coordinate or momentum components of the eigenvectors) all looked rather similar, with several highly-irregular oscillations within the periodic box length. Though qualitative indications of modal structure remain, with longer wavelengths more prominent for time-averaged exponents nearer zero, as is illustrated in Fig. 3, the structure is much less distinct than that found for disks. Detailed results for disks will soon be published by two of us.[10, 22]

To further characterize the δ vectors we followed Milanović,[10] computing both instantaneous and time-averaged values of the various second moments,

$$\{\langle\delta x^2\rangle, \langle\delta y^2\rangle, \langle\delta p_x^2\rangle, \langle\delta p_y^2\rangle, \langle\delta x\cdot\delta p_x\rangle, \langle\delta y\cdot\delta p_y\rangle\},$$

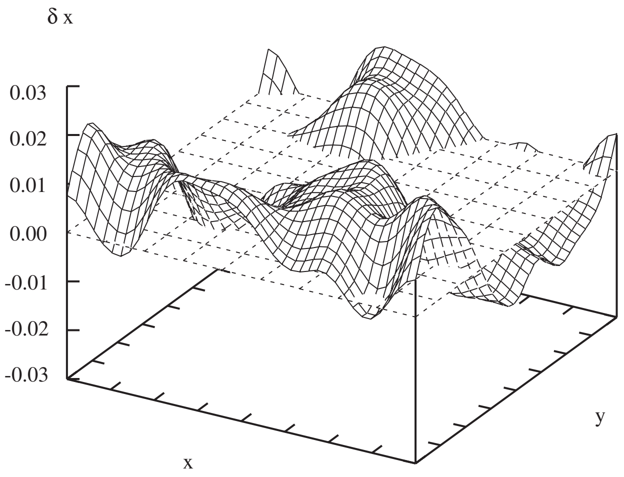

Fig. 3. Positive values of x components of δ_{508} are shown for a system of 256 soft disks.

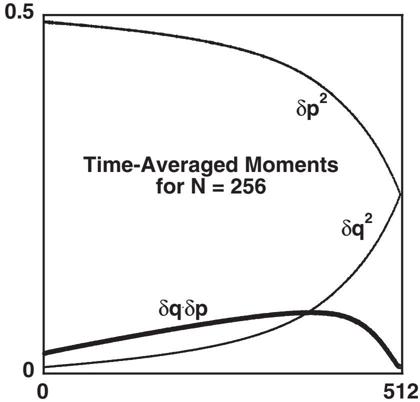

Fig. 4. Time-averaged components for the Lyapunov Exponents: $\langle \delta x^2 \rangle$, $\langle \delta y^2 \rangle$, $\langle \delta p_x^2 \rangle$, $\langle \delta p_y^2 \rangle$, $\langle \delta x \cdot \delta p_x \rangle$, $\langle \delta y \cdot \delta p_y \rangle$ for 256 soft disks.

for all the vectors. Representative results for 256 soft disks are shown in Fig. 4.

Like the spectra of exponents, these moments also follow rather featureless curves. Similar curves, not shown here, are obtained using hard disks.[10, 22] It is interesting to see the positive correlation between the coordinate and momentum components of the vectors [$\langle \delta x \cdot \delta p_x \rangle$ and [$\langle \delta y \cdot \delta p_y \rangle$]. This correlation is precisely what would be expected for

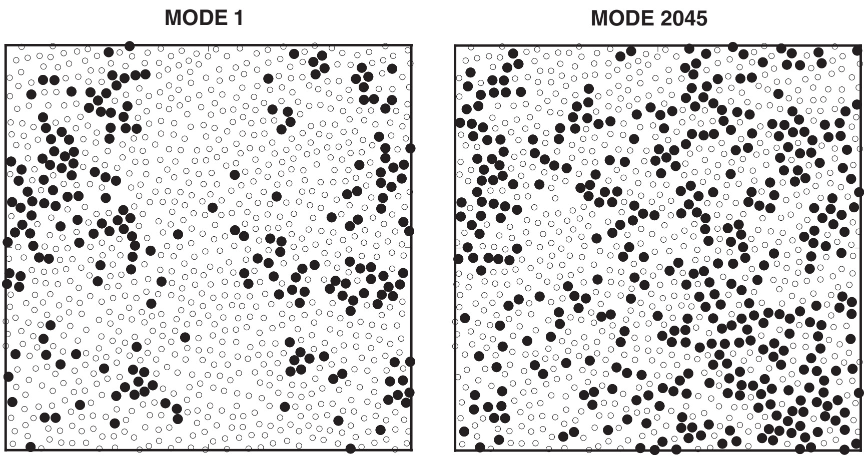

Fig. 5. Particles making above-average/below-average contributions to δ_1 and δ_{2045} for 1024 soft disks are shown as larger/smaller disks.

modes growing (or decaying) exponentially in the time, but it appears throughout the spectrum.

Apart from the three special modes with vanishing (when averaged for long times) Lyapunov exponents the remaining δ vectors show no particular irregularities. The spectrum is smooth and featureless. In Fig. 5 we emphasize those particles making above-average contributions to the first and last of the positive modes (numbers 1 and 2045 for the 1024-particle system) by showing the above-average contributors as larger disks. In the lower-frequency "mode," number 2045, the significant particles are more numerous than in the higher-frequency mode, but display no special sinusoidal character.

4. MODES OR NOT?

To determine whether or not "modes" are a useful concept for soft potentials it is necessary first to develop one or more quantitative criteria for modes and then to study the number-dependence of these criteria in order to assess the large-system limit. Evidently the simplest possible modes would display purely sinusoidal eigenvector components. The longest possible wavelength, $\sqrt{N}$, should correspond to the eigenvectors corresponding to the smallest positive eigenvalues. Unfortunately a visual inspection of these components gives ambiguous results. The small-eigenvalue eigenvectors appear to contain *several* Fourier components. Time averaging does not help.

A second characteristic of each eigenvector is its fluctuation in time. One would expect that "modes" should exhibit smaller fluctuations than representative eigenvectors from the continuous part of the spectrum. Plots of the (time-averaged) squares of the Lyapunov exponents are suggestive. For soft disks the squares follow a smooth curve, with larger fluctuations for both the smaller and the larger exponents, and a minimum for eigenvalues near the middle of the positive part of the spectrum. The *size* of these exponent fluctuations decreases with increasing N. Fluctuations for the exponents near the two ends of the spectrum vary approximately as $1/N$, with a finite value for the large-N limit of $\langle \lambda_1^2 \rangle - \langle \lambda_1 \rangle^2$. For the large-exponent end the number-dependence of the fluctuations is somewhat better fitted as $c + O(N^{-0.7})$. After the directions of the δ vectors have converged there are five vectors with relatively-small fluctuations—three of these small fluctuations are precisely zero. These three correspond to the five zero exponents expected for a system studied on the constant-energy shell. Unrestricted simulations provide similar spectra, and fluctuations, but with six rather than five vanishing exponents.

Instantaneous snapshots of the vectors near $\langle\lambda\rangle = 0$ do not show pure modes. Time averaging provides smoothing, as well as reduced amplitudes, but still no convincing evidence for modes. The strongest evidence for the lack of modes in the soft-disk case comes from comparing eigenvectors for the *same* modes, but generated with *different* computer programs or different initial conditions. Although all the long-time-averaged moments agree (as they must) there is no evident correlation between the "modes" themselves generated with different computer programs.

Based on this computational evidence we have to conclude that neither the Lyapunov spectrum nor the corresponding vectors show the clear and interesting modal structure revealed in the hard-particle work. Lattice-rotor eigenvector results, based on the extended XY model introduced by Domany, Schick, and Swendsen,[23] yield Lyapunov spectra[24, 25] resembling those for soft disks. In that model the square-lattice nearest-neighbor forcelaw is a simple monotonic function of the angular difference $\Delta\theta$ of two adjacent rotors. Visual inspection of the eigenvectors for systems of up to 256 rotors showed no particular modal structures.

For soft disks there is a gradual loss of spatial correlations as $|\langle\lambda\rangle|$ decreases, with rather different sets of particles contributing to the corresponding δ vectors for $\langle\lambda\rangle$ near zero. On the other hand, the highly-correlated localization of the more unstable modes, for large values of $|\langle\lambda\rangle|$, which can be well-characterized for much larger systems because only a few δ vectors need to be calculated, shows the same behavior for soft and hard systems: relatively few particles, localized in coordinate space, make the major contributions to both the coordinate and momentum parts of the corresponding δ vectors.[21]

5. CONCLUSIONS

Our investigation of Lyapunov vectors for a soft dense fluid and for the lattice-rotor model indicates an absence of definite modes like those found for hard disks and dumbbells. For soft disks the structures of *all* the eigenvectors appear instead to reflect noise and fluctuations. It seems to us that this finding is probably linked to the smooth continuous spectra associated with the softer systems, with exponents going smoothly through zero.

What difference is there between hard-particle and soft-particle systems with continuous differentiable potentials? The hard particles, at least for the small systems that can be examined now, have shown a distinct gap between the positive and negative Lyapunov exponents. This gap will likely disappear in the large-system limit,[7, 10] but with the spectrum [λ *versus* (j/N), where j indexes the modes] showing an infinite slope.[10]

There is certainly no corresponding gap with soft potentials. We have to conclude that the modes have no special hydrodynamic significance, since their very existence seems to hinge on the detailed nature of the interparticle forces and, perhaps, on system size. This finding seems to contradict the general considerations used by McNamara and Mareschal to "predict" modes.[11] Theoretical understanding of what it takes to generate modes is still missing, even in the simplest equilibrium case considered here. Some interesting efforts have been made[26] by studying the spectra characterizing large random matrices. But that work also fails to allow for qualitative differences. At a minimum it would seem necessary to generalize these efforts so as to reproduce the qualitative dependence of the spectra on both dimensionality (two or three) and phase (fluid or solid).

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