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The average Riemann curvature of conservative systems in classical mechanics

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Abstract. The average value $\bar{R}$ of the Riemann scalar R over the configuration space is defined for conservative systems in classical mechanics. Positive $\bar{R}$ is associated with integrability, negative $\bar{R}$ with ergodicity, mixing etc. The average is calculated for a number of model systems. Oscillator systems and 8-particle Lennard–Jones systems are characterised by $\bar{R}>0$. For low densities this also applies to 8- and 27-particle Debye–Hückel systems. For high densities and small energies the calculations suggest that $R<0$ everywhere on the accessible part of configuration space. In a larger part of the density, energy plane $\bar{R}<0$.

1. Introduction

An interesting question in the classical mechanics of many-body systems is whether there exists a computable quantity which shows by its sign (or size) that the system is integrable, ergodic, mixing, or that it has some other well defined ergodic property. Proving the integrability or ergodicity of a system would thereby be reduced to computing that quantity, or to showing that it has the required sign (or size). Since ergodic properties are intrinsic properties of the system, the quantity should not depend on the particular way in which the coordinates have been chosen. In other words, it should be an invariant with respect to coordinate transformations.

One such quantity is the Kolmogorov entropy (Arnol'd and Avez 1968). Ergodic properties are associated with positive entropy. For example, K-systems have positive entropy. About the implications of positive entropy not much useful seems to be known. But positive entropy is not necessary for mixing of all orders: there are systems with zero entropy which have that property (Newton and Parry 1966).

Pesin (1977) gives a formula which relates the Kolmogorov entropy with the Liapunov characteristic numbers. Computation of these numbers thereby provides a practical method for the computation of the entropy. This method has been applied by Benettin *et al* (1979). A disadvantage of the method is that it is not local: in order to compute the Liapunov characteristic numbers one has to integrate the equations of motion. One would prefer to avoid this in systems where exponential growth of errors or perturbations is to be expected.

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A property even less tangible than positive entropy is 'completely positive entropy' (Rokhlin 1967). If a system has this property, then it is ergodic (Rokhlin 1967). The power of this theorem is offset by the lack of a practical way of verifying completely positive entropy.

2. The Riemann invariant $\bar{R}$

A local quantity which might be useful for the purpose stated above is the Riemann tensor (van Velsen 1980, to be referred to as I). With respect to ergodic properties it can be used to define a hierarchy of 'chaos'. The most chaotic situation is represented by negative curvature. Negative curvature means that all sectional curvatures are negative everywhere. At each point of an N-dimensional manifold the number of independent sectional curvatures or conditions is of the order N^2.

If a system has negative curvature, neighbouring trajectories diverge uniformly. Two neighbouring trajectories do not intersect more than once (Milnor 1969, lemma 19.1). A theorem of Anosov (1967) states that a system with negative curvature is a K-system.

A weaker condition is that for each direction neighbouring trajectories diverge only on the average. This can be written as a condition on the Ricci tensor. At each point of configuration space one has of the order of N conditions. If on the other hand the eigenvalues of the Ricci tensor are (strictly) positive, then every sufficiently long part of a trajectory is intersected at least twice by a neighbouring trajectory (Myers 1941).

Averaging the eigenvalues of the Ricci tensor yields the Riemann scalar R. The next level in the hierarchy is therefore defined by the condition $R<0$.

It remains to average over the configuration manifold. In order to give a precise definition of this average it is necessary first to define a few fundamental quantities. Let E be the energy and $V(q)$ the potential of the configuration $q=q^1, \ldots, q^N$. Then the configuration manifold M is defined by the condition that the kinetic energy is positive: $E-V(q)>0$. The metric tensor g_{ij} has determinant g, and the invariant volume element has the form $\sqrt{g}\,\mathrm{d}q^1 \ldots \mathrm{d}q^N$. It follows that the invariant average $\bar{R}$ of the Riemann scalar over the configuration manifold is given by

$$\bar{R}=\left(\int_M R\sqrt{g}\,\mathrm{d}q^1\ldots \mathrm{d}q^N\right)\left(\int_M \sqrt{g}\,\mathrm{d}q^1\ldots \mathrm{d}q^N\right)^{-1}. \tag{1}$$

It is obvious that $\bar{R}$ has something to do with the integrability or ergodicity of the system. But except for the two-dimensional case little is known about the implications of the condition $\bar{R}<0$ for the topology of the trajectories, and similarly the relation between $\bar{R}$ and the Kolmogorov entropy is poorly understood. For a two-dimensional closed manifold Kramli (1973) (cited by Pesin 1977) has shown that the flow is ergodic if $\bar{R}<0$.

According to I it may be assumed that $g_{ij}=(E-V)\delta_{ij}$ and, consequently, $g=(E-V)^N$. In the same paper it is shown that

$$R=(N-1)\{(E-V)\,\mathrm{Tr}\,\nu_{ij}-\tfrac{1}{4}(N-6)\,\mathrm{Tr}\,\nu_i\nu_j\}/(E-V)^3 \tag{2}$$

where ν_i and ν_{ij} are the first and second derivatives of the potential $V(q)$. These two quantities do not depend on E. Therefore, if $R<0$ for some energy E_0, then $R<0$ for all $V<E<E_0$. Note that (2) explicitly shows that R is a local quantity.

For $E \to \infty$ the effect of the potential on the motion of the system vanishes, the trajectories are straightened out and the curvatures tend to zero. In particular also $R \to 0$.

Substituting the expression (2) for R into (1) one obtains

$$\bar{R} = \left[(N-1)\int_M (E-V)^{\frac{1}{2}N-3}\left\{(E-V(q))\,\mathrm{Tr}\,\nu_{ij} - \tfrac{1}{4}(N-6)\,\mathrm{Tr}\,\nu_i\nu_j\right\}\mathrm{d}q^1\ldots\mathrm{d}q^N\right] \times\left[\int_M (E-V(q))^{\frac{1}{2}N}\,\mathrm{d}q^1\ldots\mathrm{d}q^N\right]^{-1}. \tag{3}$$

The average is seen to exist for $N \geq 6$. If $V(q)$ is bounded from above $\bar{R} \to 0$ as $E \to \infty$. With decreasing E the domain $E - V > 0$ decreases. This, together with the property of R just mentioned, shows that if $\bar{R} < 0$ for some E_0, then $\bar{R} < 0$ for $E < E_0$.

3. Analytical calculations of $\bar{R}$

In this section and the following one, some examples of calculations of $\bar{R}$ will be given. Our aim is to find out whether $\bar{R}$ is an interesting quantity in the sense that it does not always have the same sign. This turns out to be the case, thereby leading one to conjecture that $\bar{R} = 0$ corresponds to a definite point in the series: ergodicity, mixing, n-mixing, etc. Systems with $\bar{R} > 0$ are to the left of that point, systems with $\bar{R} < 0$ to the right.

Even though the Riemann scalar R is a local quantity, its calculation need not be simple in many-body systems where each of the bodies interacts with many others. In general one will have to do the calculation numerically. A second problem is the integration of R over the configuration manifold. As will be seen below, the main contribution occasionally comes from a very small part of configuration space (as measured in ordinary coordinates).

In this section we shall consider two simple systems, where formal expressions for $\bar{R}$ can be derived. The first is the trivial example of the ideal gas. It is defined by $V = 0$. The derivatives of V obviously vanish, and (3) therefore shows that $\bar{R} = 0$. Actually all components of the full Riemann tensor are zero everywhere, which is another way of saying that all trajectories are straight lines.

More interesting is the potential

$$V(x_1, \ldots, x_N) = \sum_{i=1}^{N} x_i^2. \tag{4}$$

It describes a system of N independent linear oscillators. This is an example of an integrable system. It is found that

$$\bar{R} = 4\frac{N(N-1)^2}{N-4}\frac{1}{E^2}. \tag{5}$$

This result is compatible with the hypothesis that integrable systems have positive $\bar{R}$ and systems high in the ergodicity hierarchy negative $\bar{R}$.

It may also be noticed that $\bar{R} \to 0$ as $E \to \infty$. Putting $E = N\varepsilon$ and taking the limit $N \to \infty$ yields $\bar{R}_\infty = 4/\varepsilon^2$.

4. The Riemann invariant of some Debye–Hückel and Lennard–Jones systems

To see what $\bar{R}$ becomes in simple models for a plasma and a noble gas we consider Debye–Hückel and Lennard–Jones systems with eight or more particles. Curvature statistics for such systems were reported in I. There the weight function of the distributions was taken to be unity. Invariant distributions may be obtained by adopting the weight function $\sqrt{g}$.

An N_p particle Debye–Hückel (DH) system is defined by the potential

$$V(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{N_p}) = \sum_{\substack{i,j=1 \\ i<j}}^{N_p} \exp(-r_{ij})/r_{ij}, \qquad r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|. \tag{6}$$

The trace of the matrix ν_{ij} of the second derivatives of V is given by

$$\mathrm{Tr}\, \nu_{ij} = \sum_{k \neq l} \exp(-r_{kl})/r_{kl}. \tag{7}$$

It is obviously strictly positive definite. Together with (3) this fact shows that $\bar{R} > 0$ for sufficiently large E. The main problem is therefore to determine the behaviour for (relatively) small energies.

The results of the calculations for systems with $N_p = 8$ are given in table 1, those for $N_p = 27$ particles are given in table 2. The method of calculation is described in § 6 of I. The present tables are based on samples of 10^4–10^5 configurations. Beside the value of $\bar{R}$ the tables give the ratio f_+ of the invariant volume of the domain where $R > 0$ to the total invariant volume.

The results can be summarised as follows.

(i) The qualitative behaviour of the computed quantities is the same for the 8- and 27-particle systems.

(ii) For sufficiently small densities $\bar{R} > 0$ for all E. (To be precise: an upper limit has been set on the value of E_0.)

(iii) For higher densities there is an energy E_0 such that $\bar{R} < 0$ for $E < E_0$ and $\bar{R} > 0$ for $E > E_0$.

Table 1. $\bar{R}$ and f_+ as a function of the density n and energy E for an 8-particle Debye–Hückel system.

n	E	$\bar{R}$	f_+
0.001	10^{-4}	$(5.6 \pm 0.2) \times 10^4$	0.975 ± 0.001
	0.001	$(3.67 \pm 0.06) \times 10^3$	0.966 ± 0.002
	0.01	202 ± 2	0.974 ± 0.001
	0.1	9.5 ± 0.1	0.9824 ± 0.0005
	1	0.316 ± 0.004	0.9902 ± 0.0006
1	10	-16 ± 1	0.04 ± 0.02
	50	-0.215 ± 0.010	0.739 ± 0.005
	100	$(-0.24 \pm 0.03) \times 10^{-1}$	0.847 ± 0.004
	10^3	$(-0.25 \pm 0.18) \times 10^{-3}$	0.9725 ± 0.0005
	10^4	$(+0.35 \pm 0.04) \times 10^{-5}$	0.9962 ± 0.0002
1000	250	-132 ± 8	0.00
	10^3	-1.361 ± 0.011	0.00000
	10^4	$(-0.75 \pm 0.20) \times 10^{-2}$	$(8.25 \pm 0.15) \times 10^{-2}$

Table 2. $\bar{R}$ and f_+ as a function of the density n and energy E for a 27-particle Debye–Hückel system.

n	E	$\bar{R}$	f_+
0.001	0.1	59.2 ± 1.1	0.946 ± 0.006
	1.0	2.37 ± 0.02	0.952 ± 0.002
	10	0.0627 ± 0.0005	0.975 ± 0.001
1	100	-1.38 ± 0.10	0.22 ± 0.03
	200	-0.175 ± 0.004	0.64 ± 0.01
	500	0.189 ± 0.005	0.833 ± 0.004
	10^3	$(0.42 \pm 0.05) \times 10^{-2}$	0.900 ± 0.003
	10^4	$(0.13 \pm 0.12) \times 10^{-4}$	0.981 ± 0.001
1000	2500	-21.2 ± 0.7	0.0000
	10^4	-0.208 ± 0.006	0.0000
	10^5	$(-1.4 \pm 0.8) \times 10^{-2}$	0.435 ± 0.003
	10^6		0.944 ± 0.002

(iv) Moreover, for sufficiently large densities and sufficiently small energies the Riemann scalar is negative everywhere on the configuration manifold.

Of course, the last remark is actually a hypothesis. In fact our computations showed that for all 250000 8-particle configurations and all 50000 27-particle configurations chosen at random $R < 0$.

A Lennard–Jones (LJ) system with N_p particles is defined by the potential

$$V(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{N_p}) = \sum_{\substack{i,j=1 \\ i<j}}^{N_p} \left(\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}} \right). \tag{8}$$

We consider 8-particle systems, $N_p = 8$. The results are given in table 3.

The most remarkable result is that $\bar{R} > 0$ for $n = 0.001$ and $E = 0$. This is remarkable because in I negative curvature was found for more than half of the configurations. Similarly, here it is found that the fraction of configurations having $R > 0$ is only 0.006. The table shows, however, that the invariant volume of the configurations with $R < 0$ is small with respect to the invariant volume of the configurations with $R > 0$. This situation is caused by the well in the LJ potential. For small energy the kinetic energy of a configuration is small (and of the same order of magnitude), except when

Table 3. $\bar{R}$ and f_+ as a function of the density n and energy E for an 8-particle Lennard–Jones system.

n	E	$\bar{R}$	f_+
0.001	0	$(1.9 \pm 0.3) \times 10^3$	0.85 ± 0.05
	0.1	$(1.34 \pm 0.19) \times 10^3$	0.8 ± 0.1
	1	34 ± 1	0.115 ± 0.002
$1/\sqrt{2}$	0	$(0.71 \pm 0.03) \times 10^3$	0.968 ± 0.004
	10^2	5.28 ± 0.08	0.982 ± 0.001
	10^4	$(3.38 \pm 0.06) \times 10^{-2}$	0.992 ± 0.001

there is a close pair of particles. Since T appears in (3) with the exponent $\frac{1}{2}N-3$ these last configurations carry great weight.

Furthermore, the well gives rise to relatively large derivatives ν_i and ν_{ij}. The absolute values of $\mathrm{Tr}\nu_{ij}$ and $\mathrm{Tr}\nu_i\nu_j$ are larger by orders of magnitude for configurations with at least one close pair as compared with other configurations. Moreover, it turns out that they are characterised by

$$2(E-V)\,\mathrm{Tr}\,\nu_{ij}-\tfrac{1}{2}(N-6)\,\mathrm{Tr}\,\nu_i\nu_j>0,$$

i.e. by $R>0$. The main contribution to the integrals in (3) therefore comes from these configurations. In particular the numerator is positive. Still, the positive values in the sum approximating the numerator have a large spread, and it is difficult to obtain a reliable value for $\bar{R}$. The relative accuracy of 16 % for $n=0.001$ and $E=0$ (see table 3) was obtained by taking a sample of 5×10^6 configurations.

The minimum of $1/r^{12}-1/r^6$ is $-\frac{1}{4}$. Therefore, the weights of configurations with and without close pairs are of the same order of magnitude if $E\geqslant 0(1)$. In table 3 this shows up in the reduction of f_+ from 0.8 at $E=0.1$ to 0.1 at $E=1$. The Riemann invariant is seen to remain positive during this transition.

At liquid densities virtually all configurations contain close pairs. The statistics are much better, so that the accuracy of the results for $n=1/\sqrt{2}$ in table 3 could already be obtained by taking samples of 10^4 configurations.

5. Conclusion

If the above results and those of I are taken together the following picture emerges.

In DH systems configurations with negative curvature are extremely rare, if they exist at all. Nonetheless, the evidence suggests that in part of the n, E-plane $R<0$ everywhere on the manifold $E-V(q)>0$. Obviously, a larger part of the n, E-plane has the weaker property $\bar{R}<0$.

The LJ systems are very different. For n and E sufficiently small, negative curvature is found in a domain of the configuration manifold that has a relatively small invariant volume. The occurrence of negative curvature seems to have little effect on the overall curvature properties however: no case of $R<0$ was encountered in our survey, and $\bar{R}>0$ for all n, E in table 3.

In § 3 we had already seen that $\bar{R}=0$ for the ideal gas, and that for the integrable many-oscillator system $\bar{R}>0$. Thus it has been shown that the selected model systems display a wide variety of curvature properties. This leaves one the more curious as to the precise implications of these properties in terms of integrability and ergodic properties.

Finally, it may be worth noticing that the Riemann tensor depends continuously on the potential. If, therefore, $\bar{R}>0$ or $\bar{R}<0$ for a specific potential, the same inequality will in general hold for all potentials in a neighbourhood of the given one.

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