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Equivalence of kinetic-theory and random-matrix approaches to Lyapunov spectra of hard-sphere systems

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ABSTRACT

In the study of chaotic behaviour of systems of many hard spheres, Lyapunov exponents of small absolute values exhibit interesting characteristics leading to speculations about connections to non-equilibrium statistical mechanics. Analytical approaches to these exponents so far can be divided into two groups, macroscopically oriented approaches, using kinetic theory or hydrodynamics, and more microscopically oriented random-matrix approaches in quasi-one-dimensional systems. In this paper, I present an approach using random matrices and weak-disorder expansion in an arbitrary number of dimensions. Correlations between subsequent collisions of a particle are taken into account. It is shown that the results are identical to those of a previous approach based on an extended Enskog equation. I conclude that each approach has its merits, and provides different insights into the approximations made, which include the Stoßzahlansatz, the continuum limit, and the long wavelength approximation. The comparison also gives insight into possible connections between Lyapunov exponents and fluctuations.

1. Introduction

In recent years, investigations into the connections between the theory of dynamical systems and non-equilibrium statistical mechanics have yielded many interesting and important results. Gallavotti and Cohen [1,2], for instance, conjectured that many-particle systems as studied by statistical mechanics will generally be strongly chaotic. This has prompted a great deal of interest in the connections between chaos on the one hand and the decay to equilibrium and transport coefficients on the other (see for instance Ref. [3]). A central role in the study of chaos and related properties is played by the Lyapunov exponents, which describe the exponential divergence or convergence of nearby trajectories in phase space.

Some of this interest has been directed towards the Lyapunov exponents of the propotype system of many hard spheres. Several analytical calculations of, among other things, the largest Lyapunov exponent and the sum of all positive Lyapunov exponents have been performed [4–9]. Lyapunov exponents of many-particle systems have also been evaluated numerically in molecular-dynamics simulations (see, for instance Ref. [10–12]). Because of their unexpected behaviour, in particular the Lyapunov exponents of small but nonzero absolute value have received attention. A step structure occurs in the Lyapunov spectrum near zero whenever the system is large enough compared to the mean free path, as was first noted by Posch and Hirschl [13] and later also found in other systems (see, for example, Refs. [11,14]). These Lyapunov exponents differ from the exponents of larger absolute value, in the sense that all particles contribute to them, much like in the case of the zero Lyapunov exponents, and the corresponding modes appear to be, on average and to first approximation, linear combinations of these zero modes with a sinusoidal modulation in the position. Initially, it was hoped that describing the Lyapunov modes through a macroscopically oriented approach such as hydrodynamics or an Enskog equation might provide insight into possible connections between chaos and transport. In Ref. [7], it has been shown that the small exponents can in fact be viewed to belong to Goldstone modes and that the behaviour found in simulations [13] can be understood from this. A set of equations was derived for these exponents by the use of an extended Enskog equation and values for the exponents were obtained. Other attempts to understand these exponents have been based on hydrodynamic equations [15], and, although limited to quasi-one-dimensional systems, random matrices along with approximations of weak disorder [16–18].

In view of the two distinct approaches to the Goldstone modes, through random matrices on the one hand and through the Enskog

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equation on the other, it is of interest to investigate whether the results of Ref. [7] can also be derived using techniques from random-matrix theory. In this paper, instead of starting from the Enskog equation, I make use of random matrices and the weak-disorder expansion. Unlike the previous random-matrix approaches mentioned above, the present derivation is not limited to quasi-one-dimensional systems. The approximations needed to arrive at quantitative results can be studied more carefully in some cases, and are similar to those used in the derivation of Ref. [7]. By comparing the Enskog and random-matrix approaches, one gains insight into the approximations made in both approaches and the associated inaccuracies. Of special interest are the consequences of the thermodynamic limit, since finite-size effects in the Lyapunov exponents may be related to fluctuations and decay of correlations.

This paper is organised as follows. In Section 2, Lyapunov exponents are briefly introduced as well as the dynamics in tangent space of freely moving hard spheres in tangent space. Next, in Section 3, a summary is given of the Goldstone modes and the calculation of Ref. [7] by the use of an extended Enskog equation. In Sections 4–6, it is explained how the results found from the extended Enskog equation can also be derived through the use of random matrices. The approaches are compared in Section 7, and the approximations needed are discussed. Possible corrections are considered and it is pointed out how these may lead to insight in the connections between non-equilibrium behaviour and chaotic properties.

2. Lyapunov exponents and the dynamics in tangent space

Consider a d-dimensional system of N particles moving in a $2dN$-dimensional phase space Γ. At time $t = 0$, the system is assumed to be in an initial point $\boldsymbol{\gamma}_0$ in this phase space, from which it evolves with time according to $\boldsymbol{\gamma}(\boldsymbol{\gamma}_0, t)$. If the initial conditions are perturbed infinitesimally by $\delta\boldsymbol{\gamma}_0$, the system evolves along an infinitesimally different path $\gamma(\gamma_0, t) + \delta\gamma(\gamma_0, t)$, where $\delta\gamma$ denotes a coordinate in the tangent space $\delta\Gamma$, and $\delta\gamma(\gamma_0, 0) = \delta\boldsymbol{\gamma}_0$. The evolution of a vector in the tangent space is described by

$$\delta\boldsymbol{\gamma}(\boldsymbol{\gamma}_0, t) = \mathsf{M}_{\boldsymbol{\gamma}_0}(t) \cdot \delta\boldsymbol{\gamma}_0, \tag{1}$$

where $\mathsf{M}_{\boldsymbol{\gamma}_0}(t)$ is a $2dN$-dimensional matrix defined by

$$\mathsf{M}_{\boldsymbol{\gamma}_0}(t) = \frac{\mathrm{d}\boldsymbol{\gamma}(\boldsymbol{\gamma}_0, t)}{\mathrm{d}\boldsymbol{\gamma}_0}. \tag{2}$$

The Lyapunov exponents are the possible average asymptotic growth rates of infinitesimal perturbations $\delta\gamma_i(\gamma, t)$ associated with the eigenvalues $\mu_i(t)$ of $\mathsf{M}_{\boldsymbol{\gamma}_0}(t)$, i.e.,

$$\lambda_i = \lim_{t\to\infty} \frac{1}{t} \left(\ln|\mu_i(t)| + i \arg \mu_i(t)\right). \tag{3}$$

If the system is ergodic, it will eventually come arbitrarily close to any point in phase space for all initial conditions except for a set of measure zero. The Lyapunov exponents are thus the same for almost all initial conditions. In the literature, one also finds the Lyapunov exponents defined with reference to the eigenvalues of $[\mathsf{M}_{\boldsymbol{\gamma}_0}(t)^\dagger \cdot \mathsf{M}_{\boldsymbol{\gamma}_0}(t)]^{\frac{1}{2}}$, in which case they are real.

The symmetries of the dynamics of the system generate vectors in tangent space which do not grow or shrink exponentially and therefore have Lyapunov exponents equal to zero. For a system of hard spheres under periodic boundary conditions, these symmetries and their corresponding zero modes are uniform translations, Galilei transformations, time translations, and velocity scaling.

We now consider a gas of identical hard spheres of diameter a and mass m in d dimensions in the absence of external fields. As there are no internal degrees of freedom, the phase space may be represented by the positions $\mathbf{r}_i$ and velocities $\mathbf{v}_i$ of all particles, enumerated by i, and similarly the tangent space by infinitesimal deviations $\delta\mathbf{r}_i$ and $\delta\mathbf{v}_i$. The evolution of the system in phase space consists of a sequence of free flights interrupted by collisions. During the free flights, the particles do not interact and their positions change linearly with the velocities; similarly, $\delta\mathbf{r}$ changes linearly with $\delta\mathbf{v}$. For rigid spheres the collisions are instantaneous. At the moment of the collision, momentum is exchanged between the two particles involved along the collision normal $\hat{\boldsymbol{\sigma}} = (\mathbf{r}_i - \mathbf{r}_j)/a$ at impact, as shown in Fig. 1. At the instant of the collision, none of the other particles are assumed to interact.

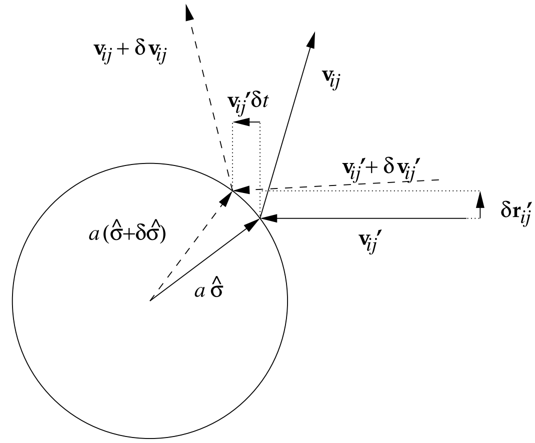

Fig. 1. Geometry of a collision of two particles i and j of diameter a, in relative position $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ and with the relative velocity $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$. The collision normal $\hat{\boldsymbol{\sigma}}$ is the unit vector pointing from the centre of particle j to the centre of particle i. The circle drawn represents the locus of closest approach. Coordinates before the collision are marked with a prime. The dashed lines indicate an infinitesimally displaced path.

From Eq. (2) and the phase space dynamics, the dynamics in tangent space can be derived [4,19]. During the free flight between the instant of a collision t_z (z being the number of the collision in the sequence) and t, there is no interaction between the particles and the components of the tangent-space vector transform according to

$$\begin{pmatrix} \delta\mathbf{r}_i \\ \delta\mathbf{v}_i \end{pmatrix}_t = \mathcal{Z}(t - t_z) \cdot \begin{pmatrix} \delta\mathbf{r}_i \\ \delta\mathbf{v}_i \end{pmatrix}_{t_z}, \tag{4}$$

$$\mathcal{Z}(t - t_z) = \begin{pmatrix} \mathsf{I} & (t - t_z)\mathsf{I} \\ 0 & \mathsf{I} \end{pmatrix}, \tag{5}$$

in which I is the $d \times d$ identity matrix.

As shown in Fig. 1, infinitesimal differences in the positions and velocities of the particles lead to infinitesimal changes in the collision normal and collision time. This, in turn, leads to infinitesimal changes in both positions and velocities right after the collision. Throughout the paper, primes denote coordinates in phase space and tangent phase space just before a collision while non-primed quantities refer to coordinates just after the collision. For colliding particles i and j, one finds

$$\begin{pmatrix} \delta\mathbf{r}_i \\ \delta\mathbf{r}_j \\ \delta\mathbf{v}_i \\ \delta\mathbf{v}_j \end{pmatrix} = (\mathcal{L} + \mathcal{I}) \cdot \begin{pmatrix} \delta\mathbf{r}'_i \\ \delta\mathbf{r}'_j \\ \delta\mathbf{v}'_i \\ \delta\mathbf{v}'_j \end{pmatrix} = \begin{pmatrix} \mathsf{I}-\mathsf{S} & \mathsf{S} & 0 & 0 \\ \mathsf{S} & \mathsf{I}-\mathsf{S} & 0 & 0 \\ -\mathsf{Q} & \mathsf{Q} & \mathsf{I}-\mathsf{S} & \mathsf{S} \\ \mathsf{Q} & -\mathsf{Q} & \mathsf{S} & \mathsf{I}-\mathsf{S} \end{pmatrix} \cdot \begin{pmatrix} \delta\mathbf{r}'_i \\ \delta\mathbf{r}'_j \\ \delta\mathbf{v}'_i \\ \delta\mathbf{v}'_j \end{pmatrix}, \tag{6}$$

where $\mathcal{I}$ and I are the $4d \times 4d$ and $d \times d$ identity matrices, respectively, and $\mathcal{L}$ is the $4d \times 4d$ collision matrix, which can be written in terms of $d \times d$ matrices S and Q specifying the collision dynamics in tangent space (see, for instance, Refs. [4,7]).

Let $\mathsf{Z}(t)$ be the $2dN \times 2dN$ matrix which performs the single-particle transformations $\mathcal{Z}(t)$ for all particles during free flight