Radius of curvature approach to the Kolmogorov-Sinai entropy of dilute hard particles in equilibrium

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We consider the Kolmogorov-Sinai entropy for dilute gases of N hard disks or spheres. This can be expanded in density as $h_{KS} \approx nN \ln na^d + B + O(na^d) + O(1/N)$, with a the diameter of the sphere or disk, n the density, and d the dimensionality of the system. We estimate the constant B by solving a linear differential equation for the approximate distribution of eigenvalues of the inverse radius of curvature tensor. We compare the resulting values of B both to previous estimates and to existing simulation results, finding very good agreement with the latter. Also, we compare the distribution of eigenvalues of the inverse radius of curvature tensor resulting from our calculations to new simulation results. For most of the spectrum the agreement between our calculations and the simulations again is very good.

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I. INTRODUCTION

It is generally believed that the approach to equilibrium of a typical many-particle system, such as a gas or liquid will depend on its dynamical properties. Specifically, the more chaotic the system, the more rapidly its approach to (at least local) equilibrium will proceed. Furthermore, the apparent randomness of these systems, in spite of their fully deterministic microscopic behavior (at least for classical systems) has also been attributed to the chaotic nature of their dynamics. Discussions of this can be found e.g. in books by Dorfman [1] and Gaspard [2] and review papers by Van Zon et al. [3, 4]. A very common and generally used measure of chaos is the Kolmogorov-Sinai entropy, which we will denote by $h_{KS}$. In systems which are closed, the Kolmogorov-Sinai entropy $h_{KS}$ equals the sum of all positive Lyapunov exponents, the average rates over very long times of divergence (or convergence) of infinitesimal perturbations. It describes the rate at which the system produces information about its phase-space trajectories, or equivalently about the distribution of density over phase space in some ensemble. In systems with escape, the Kolmogorov-Sinai entropy has also been connected to transport coefficients [3,8]. In such systems it is no longer equal to the sum of all positive Lyapunov exponents.

Chaotic properties such as the Lyapunov spectrum of systems of low [8,11] as well as high [12] dimensionality, such as moving hard spheres or disks, have been studied frequently. Extensive simulation work has been done on their Lyapunov spectra [13,15], and for low densities analytic calculations have been done for the largest Lyapunov exponent [3,16,18], the Kolmogorov-Sinai entropy [11,16] and for the smallest positive Lyapunov exponents [19,20]. Analytic methods employing kinetic theory have been applied to calculate chaotic properties. Agreement between analytic calculations and numerical results is generally good, but with respect to the KS-entropy there is one notorious exception, which is the central issue of the present paper.

In this paper we consider a system consisting of N hard, spherical particles, of diameter a, at small number density n, in d dimensions ($d = 2, 3$). We calculate the Kolmogorov-Sinai entropy in the low density approximation, where it is expected to behave as [11]

$$h_{KS} = N \bar{v} A \left[ - \ln(na^d) + B + O(na^d) + O\left(\frac{1}{N}\right) \right].$$

(1)

The constant A has been calculated by Van Beijeren et al. in [11], but the results found there for B were unsatisfactory.

In this paper we present a more successful calculation of B, through the distribution of eigenvalues of the inverse radius of curvature tensor. The calculation presented here differs from that presented by De Wijn in Ref. [21], in that it is far more elegant and less cumbersome and the agreement of the results with values found in simulations is better. On the other hand, the calculation here is less systematic and it is not clear how to apply the results of this paper to calculating specific Lyapunov exponents, as can be done [22] with the results of Ref. [21].

The paper is organized as follows: In section II we introduce Lyapunov exponents and review the properties...
of hard sphere dynamics in tangent space (the space in which the dynamics is described of infinitesimal deviations between nearby trajectories in phase space). In section III we introduce the radius of curvature tensor and its inverse, relate the KS-entropy to the time average of the trace of the inverse radius of curvature tensor and investigate the dynamics of these tensors both during free flight and at collisions. In IV we present two approximate calculations of the average distribution of the eigenvalues of the inverse radius of curvature tensor. In section V we compare the results of these calculations to those of numerical simulations and we also compare the resulting value for the coefficient $B$ in Eq. (1) to those obtained in simulations and in previous calculations. Finally, in section VI we present our conclusions.

II. LYAPUNOV EXPONENTS AND DYNAMICS OF HARD SPHERES IN TANGENT SPACE

This section is an abbreviated version of similar sections in Refs. [20, 21]. It appears here to make this paper more self-contained. For more details the reader may also consult Ref. [14]. Consider a system with an $N$-dimensional phase space $\Gamma$. At time $t = 0$ the system is at an initial point $\gamma_0$ in this space. It evolves with time, according to $\gamma(\gamma_0, t)$. If the initial conditions are perturbed infinitesimally, by $\delta\gamma_0$, the system evolves along an infinitesimally different path $\gamma + \delta\gamma$, which can be specified by

$$\delta\gamma(\gamma_0, t) = M_{\gamma_0}(t) \cdot \delta\gamma_0 ,$$

with the matrix $M_{\gamma_0}(t)$ defined by

$$M_{\gamma_0}(t) = \frac{d^2\gamma(\gamma_0, t)}{dt^2} .$$

The Lyapunov exponents are the possible average rates of growth or shrinkage of such perturbations, i.e.,

$$\lambda_i = \lim_{t \to \infty} \frac{1}{t} \ln |\mu_i(t)| ,$$

where $\mu_i(t)$ is the $i$-th eigenvalue of $M_{\gamma_0}(t)$. For ergodic systems, the Lyapunov exponents are expected to be the same for almost all initial conditions. For each exponent there is a corresponding eigenvector of $M_{\gamma_0}(t)$.

For a classical system of hard spheres without internal degrees of freedom, the phase space and tangent space may be represented by the positions and velocities of all particles and their infinitesimal deviations,

$$\gamma_i = (r_i, v_i) ,$$

$$\delta\gamma_i = (\delta r_i, \delta v_i) ,$$

where $i$ runs over all particles and $\gamma_i$ and $\delta\gamma_i$ are the contributions of particle $i$ to $\gamma$ and $\delta\gamma$.

In the case of a purely Hamiltonian system, such as the one under consideration here, hard spheres with only the hard particle interaction, the dynamics of the system are completely invariant under time reversal. Together with Liouville’s theorem, which states that phase space volumes are invariant under the flow, this leads to the conjugate pairing rule [23, 24], i.e. for every positive Lyapunov exponent there is a negative exponent of equal absolute value. In systems which are time reversal invariant, but do not satisfy Liouville’s theorem, the conditions for and the form of the conjugate pairing rule are somewhat different [14].

The system under consideration here has only hard-core interactions. Consequently, the evolution in phase space consists of an alternating sequence of free flights and collisions.

During free flights the particles do not interact and the positions change linearly with the velocities. The components of the tangent-space vector accordingly transform to

$$\left( \begin{array}{c} \delta r_i' \\ \delta v_i' \end{array} \right) = \left( \begin{array}{cc} 1 & (t - t_0)1 \\ 0 & 1 \end{array} \right) \cdot \left( \begin{array}{c} \delta r_i \\ \delta v_i \end{array} \right) ,$$

in which $1$ is the $d \times d$ identity matrix.

At a collision between particles $i$ and $j$ momentum is exchanged between the colliding particles along the collision normal, $\hat{\sigma} = (r_i - r_j)/a$, as shown in Fig. 1. The other particles do not interact. For convenience we switch to relative and center of mass coordinates, $\delta r_{ij} = \delta r_i - \delta r_j$, $\delta R_{ij} = (\delta r_i + \delta r_j)/2$, $\delta v_{ij} = \delta v_i - \delta v_j$, and $\delta V_{ij} = (\delta v_i + \delta v_j)/2$. We find [16, 25]

$$\delta r_{ij}' = \delta r_{ij} - 25 \cdot \delta r_{ij} ,$$

$$\delta R_{ij}' = \delta R_{ij} ,$$

$$\delta v_{ij}' = \delta v_{ij} - 25 \cdot \delta v_{ij} - 2Q \cdot \delta r_{ij} ,$$

$$\delta V_{ij}' = \delta V_{ij} ,$$

in which $S$ and $Q$ are the $d \times d$ matrices

$$S = \hat{\sigma} \cdot \hat{\sigma} ,$$

$$Q = \frac{[(\hat{\sigma} \cdot v_{ij}) 1 + \hat{\sigma} v_{ij}] \cdot [(\hat{\sigma} \cdot v_{ij}) 1 - v_{ij} \hat{\sigma}]}{a(\hat{\sigma} \cdot v_{ij})} ,$$

FIG. 1. Two particles at a collision in relative coordinates. The collision normal $\hat{\sigma}$ is the unit vector pointing from the center of one particle to the center of the other.
where \( \mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j \). Here the notation \( \mathbf{a} \cdot \mathbf{b} \) denotes the standard tensor product of vectors \( \mathbf{a} \) and \( \mathbf{b} \). Note that \( Q \) transforms vectors that are orthogonal to \( \mathbf{v}_{ij} \) into vectors that are orthogonal to \( \mathbf{v}'_{ij} \). The vector \( \mathbf{v}_{ij} \) is a right zero eigenvector of \( Q \), and \( \mathbf{v}'_{ij} \) a left zero eigenvector. Equations (7) through (13) determine \( M_{ij}(t) \).

### III. RADIUS OF CURVATURE TENSOR

Of particular interest for the Kolmogorov-Sinai entropy is the radius of curvature tensor, as the former is equal to the time average of the trace of the latter’s inverse. Let \( \delta r \) and \( \delta \mathbf{v} \) represent the full \( dN \) dimensional position respectively velocity perturbations of all particles. The inverse radius of curvature tensor, \( \mathcal{T}(t) \) is defined \[3,8,11,22,26\] as the inverse of the radius of curvature matrix \[27\]. It satisfies

\[
\delta \mathbf{v}(t) = \mathcal{T}(t) \cdot \delta \mathbf{r}(t) ,
\]

resulting from some, almost arbitrary initial \( \mathcal{T}(0) \) \[28\].

#### A. KS-entropy and inverse ROC-tensor

To establish the relationship between the KS entropy and the trace of the inverse radius of curvature tensor we consider the time evolution over long times of the projection onto \( \delta \mathbf{r} \) space of the infinitesimal volume evolving from an initial volume in tangent space spanned by \( \delta \mathbf{r}(0) \) and \( \delta \mathbf{v}(0) \). Since the projections of all Lyapunov eigenvectors with positive exponents onto \( \delta \mathbf{r} \) space are linearly independent, the size of this projected volume will grow roughly as the exponent of the sum of the positive Lyapunov exponents. A more precise statement is

\[
\lim_{t \to \infty} \frac{1}{t} \ln \frac{\text{vol} \delta \mathbf{r}(t)}{\text{vol} \delta \mathbf{r}(0)} = \sum_{\lambda_i > 0} \lambda_i .
\]

Here \( \text{vol} \delta \mathbf{r}(t) \) denotes the volume of the projection onto \( \delta \mathbf{r} \) space of the evolving infinitesimal volume in tangent space. Additionally, we have the identity

\[
\delta \mathbf{v}(t) = \frac{d \delta \mathbf{r}(t)}{dt} ,
\]

which holds, except at the instants of collisions \( t_i \), when \( \delta \mathbf{r} \) is reflected in a volume-preserving unitary transformation \( U_i \). Together with Eq. (14), one obtains

\[
\text{vol} \delta \mathbf{r}(t) = \text{vol} \left( \prod_i U_i \lim_{\Delta t \to 0} \prod_{n=t_{i-1}/\Delta t}^{t_i/\Delta t-1} (1 + \mathcal{T}(n \Delta t) \Delta t) \delta \mathbf{r}(0) \right)
\]

\[
= \prod_i \det U_i \lim_{\Delta t \to 0} \prod_{n=t_{i-1}/\Delta t}^{t_i/\Delta t-1} \det(1 + \mathcal{T}(n \Delta t) \Delta t) ,
\]

where the first product is over the sequence of all collisions and we employ the convention \( \prod_{i=1}^{n} a_i = a_n \cdots a_1 \). This leads to

\[
\lim_{t \to \infty} \frac{1}{t} \ln \frac{\text{vol} \delta \mathbf{r}(t)}{\text{vol} \delta \mathbf{r}(0)} = \langle \text{Tr} \mathcal{T} \rangle .
\]

By comparing Eqs. (15) and (18) one obtains the desired identity \[20\]

\[
h_{KS} = \langle \text{Tr} \mathcal{T} \rangle .
\]

Within the framework of this article, this identity is very central. It relates the trace of the inverse radius of curvature tensor directly to the Kolmogorov-Sinai entropy, which we wish to calculate.

The rest of this paper is therefore dedicated to the description of the eigenvalues of the inverse radius of curvature tensor. We will consider their dynamics and derive approximate equations for the time evolution of their distribution. Using these we will calculate the changes in the distribution of the eigenvalues due to both free streaming and collisions. From this we obtain approximations for the stationary distribution of eigenvalues.

This calculation is simplified appreciably by restriction to low densities. We may assume then that in each collision the elements of the precollisional inverse ROC tensor involving either of the colliding particles are small, due to their decrease during the free flight preceding the collision. This assumption is violated only in collisions where one of the colliding particles had collided shortly before. The fraction of all collisions where this is the case decreases linearly with density.

In the next section two simple approximation schemes will be presented, based on the dynamics describing the changes in the distribution of eigenvalues of the inverse ROC tensor resulting from collisions.

#### B. Dynamics of the inverse radius of curvature tensor

At a given collision, between particles labelled \( i \) and \( j \), let \( S \) and \( Q \) be the \( dN \times dN \) dimensional matrices which perform the transformations of \( 2S \) and \( -2Q \) on the relative components in tangent space of the colliding particles and act as zero on all other independent components of \( \delta \mathbf{v} \) or \( \delta \mathbf{r} \), as is described in Eqs. \[8,11\]. Note that \( Q \cdot (I - S) \), where \( I \) is the \( dN \times dN \) identity matrix, has \( d - 1 \) nonzero eigenvalues and is symmetric. One of the non-zero eigenvalues of \( Q \cdot (I - S) \) is equal to

\[
\xi_0 = -\frac{2v_{ij}}{\sigma \hat{v}_{ij} \cdot \sigma} ,
\]

with \( \hat{v}_{ij} \) the unit vector in the direction of \( v_{ij} \). The corresponding eigenvector has components in the subspaces belonging to the colliding particles of \( e_i = -e_j = \).
non-zero eigenvalues are given by
\[ \xi_0 = -\frac{2\nu_{ij} \cdot \hat{\sigma}}{a}, \quad (21) \]
with eigenvector with components \( e_i = -e_j \) normal to both \( \nu_{ij} \) and \( \hat{\sigma} \) and again \( e_k = 0 \). The dynamics of the inverse radius of curvature tensor at a collision can be derived by expressing \( \delta v' \) in terms of \( \delta r' \),
\[ \delta v' = (I - S) \cdot \delta v + Q \cdot \delta r \\ = \left[(I - S) \cdot T \cdot (I - S)^{-1} + Q \cdot (I - S)^{-1}\right] \delta r'. \quad (23) \]
With \( (I - S)^{-1} = (I - S), \) we find for the inverse radius of curvature tensor after the collision,
\[ T' = (I - S) \cdot T \cdot (I - S) + Q \cdot (I - S). \quad (24) \]
The dynamics during free flight follow from \( \xi \) as
\[ T(t + dt) = [T(t)^{-1} + Idt]^{-1} \quad (25) \]
The eigenvectors of \( T \) do not change during a free flight, so its time evolution may be specified by the evolution of its eigenvalues \( \xi \). From Eq. (25) one finds these satisfy
\[ \xi'(t) = -\xi(t)^2. \quad (26) \]
with solution
\[ \xi(t) = \frac{1}{\xi^{-1}(0) + t}. \quad (27) \]
Note that this may be simplified by considering the dynamics of the radius of curvature tensor, \( T^{-1} \). For this operator, the drift velocity becomes a constant, \( 1 \), irrespective of the eigenvalue and the choice of time unit. However, in this case Eq. (24) becomes more complicated.

C. Eigenvalue distribution at low densities

At low densities the mean free-flight time is given by
\[ \tau = 1/\nu = \frac{a\Gamma(\xi)}{\nu_0 2n^* \pi^{3/2}}. \quad (28) \]
with \( \nu_0 = (kB T/m)^{1/2} \) the thermal velocity and \( n^* = n a^d \). The probability of a particle colliding within a free flight time of order \( a/\nu_0 \) (this is the typical order of \( \xi^{-1}(0) \)) is of order \( n^* \) and these events, to first approximation, may be neglected.

Let us denote a spanning set of the subspace spanned by the eigenvectors with non-zero eigenvalues of \( Q \cdot (I - S) \) for a specific collision as \( e_1 \) through \( e_{d-1} \). Because \( Q \cdot (I - S) \) is symmetric, these vectors are both right and left eigenvectors. The corresponding eigenvalues to linear order in \( n^* \) are given by
\[ \xi = e_i \cdot [(I - S) \cdot T \cdot (I - S) + Q \cdot (I - S)] \cdot e_i, \quad (29) \]
\[ \approx e_i \cdot [Q \cdot (I - S)] \cdot e_i, \quad (30) \]
since the elements of \( T \) between these eigenvectors on average are of order \( n^* \) compared to the elements of \( Q \cdot (I - S) \).

Under the approximation of Eq. (30) the vectors \( e_i \) only depend on the collision parameters \( v_{ij} \) and \( \hat{\sigma} \), as specified below Eqs. (20) and (21). The remaining eigenvalues of \( T \), to leading order in \( n^* \), can be identified as the eigenvalues of the projection \( PTP \) of the matrix \( T \) onto the \( dN - d + 1 \) dimensional space orthogonal to the \( d - 1 \) eigenvectors \( e_i \), as follows from standard perturbation theory. Hence it follows that they are interspersed between the precollisional eigenvalues. This is worked out in Appendix A.

These eigenvalues are distributed in roughly the same way as the eigenvalues of the full matrix \( T \). But, as the eigenvalues of \( PTP \) lie in between those of \( T \), the distribution of these eigenvalues is slightly narrower than that of the eigenvalues of \( T \). For more details on this see Appendix B.

In the next section, we present two approximation schemes. In the first scheme, the narrowing will be ignored and the approximation will be made that the distribution of eigenvalues of \( PTP \) is the same as that of \( T \). The resulting equation for the distribution of eigenvalues can be solved analytically. Its solution is expressed in terms of the distribution \( f_0(\xi_0) \) of the non-zero eigenvalues of \( Q \cdot (I - S) \).

In the second scheme, a somewhat more refined approximation is made, in which we assume that each eigenvector that is changed significantly by the collision, but not created in it, can be written as a linear combination of exactly 2 precollisional eigenvectors. Why this is an improvement will be argued in the discussion, where we will also briefly discuss possibilities for further improvements.

IV. THE DISTRIBUTION OF EIGENVALUES OF THE INVERSE RADIUS OF CURVATURE TENSOR

A. First approximation scheme

Now that the dynamics of the eigenvalues of the inverse radius of curvature tensor are specified, we may write down approximate time-evolution equations for the distribution of these eigenvalues, \( f(\xi,t) \), which is normalized to unity. Let \( f_0(\xi) \) be the distribution of nonzero eigenvalues of \( Q \cdot (I - S) \), which follows from Eqs. (21) and (22) and the distribution of the collision parameters \( v_{ij} \) and \( \hat{\sigma} \). We equally normalize it to unity. The simplest approximation for the rate of change of the distribution of
eigenvalues of the inverse radius of curvature tensor is the one announced at the end of the previous section: after a collision, the new distribution of eigenvalues is the same as the old one, except for the contributions from the nonzero eigenvalues of $Q \cdot (I - S)$. Combining this with the rate of change resulting from free streaming one obtains

$$
\frac{d}{dt} f(\xi, t) = \frac{\nu(d-1)}{2d} \left[ f_0(\xi) - f(\xi, t) \right] + \frac{\partial}{\partial \xi} [\xi^2 f(\xi, t)] ,
$$

(31)

where the single-particle collision frequency is given at low density by Eq. (23). The first term on the right-hand side is due to collisions. The first part of it is the gain. The second part is the loss. Its form here is based on our approximation that the shape of the distribution of remaining eigenvalues is not changed in a collision. The final term is due to the drift during free flight.

For time going to infinity, the distribution of eigenvalues becomes stationary. In other words, the left hand side of Eq. (31) becomes zero. Eq. (31) then may be rewritten in a more convenient form, as

$$
f_0(\xi) = f_{\text{stat}}(\xi) - c[\xi^2 \frac{\partial}{\partial \xi} f_{\text{stat}}(\xi) + 2\xi f_{\text{stat}}(\xi)] ,
$$

(32)

where

$$
c = \frac{2d}{(d-1)\nu} .
$$

(33)

Solutions to this equation are of the form

$$
f_{\text{stat}}(\xi) = \int_\xi^\infty d\xi_0 f_0(\xi_0) \frac{1}{c\xi^2} \exp \left( \frac{\xi - \xi_0}{c\xi_0} \right) .
$$

(34)

Notice that for $\xi$ small, as a consequence of Eq. (20), this reduces to $f_{\text{stat}}(\xi) = \frac{\nu}{(d-1)\xi^2} \exp \left( \frac{-\xi}{\nu} \right) .

From Eq. (19) it follows that the KS entropy may be obtained directly from the first moment of $f_{\text{stat}}(\xi)$. From Eq. (34) we find that

$$
h_{\text{KS}} = \frac{Nd}{e} \int_0^\infty d\xi_0 f_0(\xi_0) \frac{1}{c\xi^2} \exp \left( \frac{\xi}{c\xi_0} \right) \Gamma \left( 0, 1 \frac{\xi}{c\xi_0} \right) ,
$$

(35)

where $\Gamma(\cdot)$ denotes the incomplete gamma function, defined by

$$
\Gamma(x, y) = \int_y^\infty dt t^{x-1} e^{-t} = e^{-y} \int_0^\infty dt (t + y)^{x-1} e^{-t}
$$

(36)

At low densities the collision frequency is low, so that $c$ is very large and the product $\exp(1/(c\xi_0)) \Gamma(0, 1/(c\xi_0))$, up to corrections of $O(n^2)$, is equal to $\ln(c\xi_0) - \gamma$, where $\gamma = 0.577216$ is Euler’s constant. The Kolmogorov-Sinai entropy then becomes

$$
h_{\text{KS}} \approx \frac{Nd\nu(d-1)}{2} \left\{ \ln \frac{\xi_0}{\nu} + \ln \left[ 2d \frac{\nu}{(d-1)} \right] - \gamma \right\}. 
$$

(37)

We note that here the brackets, instead of a time average denote an average over the probability distribution for the new eigenvalues at a collision, in this case $f_0$. This can be expressed in terms of the joint probability distribution of the collision parameters as

$$
\langle g(\xi_0) \rangle = \int_0^\infty d\xi_0 f_0(\xi_0) g(\xi_0)
$$

$$
= \sqrt{\frac{3m}{\pi d-1}} \int dv_i dv_j d\sigma \theta(-\hat{v}_{ij} \cdot \hat{\sigma}) |(v_i - v_j) \cdot \hat{\sigma}| \phi_M(v_i) \phi_M(v_j)
$$

$$
= 1 \left\{ \frac{1}{d-1} \left[ g \left( \frac{2v_{ij}}{a \hat{v}_{ij} \cdot \hat{\sigma}} \right) + (d-2)g \left( \frac{-2v_{ij}}{a \hat{\sigma}} \right) \right] \right\} ,
$$

(38)

where Eqs. (20) and (21) have been substituted and $\phi_M(v)$ is the Maxwell distribution,

$$
\phi_M(v) = \frac{2\pi k_B T}{m} \left( \frac{2\pi k_B T}{m} \right)^{-d/2} \exp \left( -\frac{m|v|^2}{2k_B T} \right) .
$$

(39)

The function $\theta(x)$ is the unit step function, which vanishes for $x < 0$ and equals unity for $x \geq 0$. In general, time averages of functions of $\xi$ may be expressed as averages over $f_{\text{stat}}$.

In Sec. V the results from Eq. (37) will be discussed and compared with results from molecular dynamics simulations.

B. Second approximation scheme

In the previous subsection, the distribution of eigenvalues after a collision was assumed to be the same as the one before, except for the non-zero eigenvalues of $Q \cdot (I - S)$. In Appendix A it is shown that in reality these eigenvalues are determined by the equation

$$
\sum_i \frac{c_i^2}{\xi - \xi_i} = 0,
$$

(40)

at least in the case of $d = 2$, when $Q \cdot (I - S)$ has a single non-zero eigenvector $\psi_i$, which can be expressed in terms of pre-collisional eigenvectors $\psi_i$ of $T$ with eigenvalues $\xi_i$, as $e = \sum_i c_i \psi_i$. From Eq. (10) one sees that precisely one new eigenvalue $\xi$ originates between each subsequent pair of pre-collisional ones.

We can divide the $c_i$ into two categories, appreciable and almost vanishing. In a pragmatic way, this distinction can be made by considering as appreciable the set of largest $c_i$ that sum to all but a small fraction of unity (for instance 0.01). The other $c_i$, then, are almost vanishing. Due to the locality of the interactions, one may argue that, in the limit of a large system, the number of appreciable $c_i$ is small compared to $N$ in most cases.

For eigenvectors with very small values of $c_i$ a new eigenvalue is found very close to an old one, typically to
the right of \( \psi \) almost vanishing. The square is approximately the solution of Eq. (40) with only the eigenvalues with appreciable \( c_i^2 \), indicated with bold crosses, contributing. The circles almost coincide with precollisional eigenvalues with almost vanishing \( c_i^2 \).

The number of eigenvectors contributing appreciably to Eq. (10) varies from collision to collision, but it always is at least 2, because the two colliding particles cannot have collided before without intermediate collisions with other particles. The actual distribution of the number of contributing eigenvectors and the distribution of the values of the corresponding original eigenvectors always retain the property that new eigenvalues are interspersed between the old ones. This is illustrated in figure 2.

The crosses denote precollisional eigenvalues, the circles and squares postcollisional ones. The bold and the regular crosses denote eigenvalues corresponding to eigenvectors with an appreciable respectively almost vanishing \( c_i^2 \). The circles and square denote new eigenvalues. The eigenvalue indicated by the square is approximately the solution of Eq. (40) with the corresponding eigenvectors and the distribution of the other particles. The actual distribution of the number of eigenvectors contributing appreciably to Eq. (40) varies from collision to collision, but it always is at least 2, because the two colliding particles cannot have collided before without intermediate collisions with other particles. The actual distribution of the number of contributing eigenvectors and the distribution of the values of the corresponding original eigenvectors are not easy to determine. In this subsection we make two simplifying assumptions: firstly that the number of contributing eigenvectors always is just 2 and, secondly that their coefficients \( c_1 \) and \( c_2 \) are distributed isotropically, irrespective of the eigenvalues \( \xi_1 \) and \( \xi_2 \). This means that these coefficients can be represented as \( c_1 = \cos \phi \) and \( c_2 = \sin \phi \), with \( \phi \) distributed uniformly on the unit circle. This assumption implies that the distribution of the corresponding original eigenvalues \( \xi_1 \) and \( \xi_2 \) is the same as the (as yet unknown) overall distribution of eigenvalues of the inverse radius of curvature tensor. Obviously, these assumptions are at best approximately correct, but in our discussion we will make plausible why, on the basis of these assumptions, a better approximation can be obtained for the eigenvalue distribution than the one given in Eq. (54).

At a collision, the two eigenvalues \( \xi_1 \) and \( \xi_2 \) disappear and are replaced by a new eigenvalue, \( \xi_0 \), related to \( Q \cdot (I - S) \), and the mixed eigenvalue

\[
\xi = \xi_1 e_2^2 + \xi_2 e_1^2,
\]

as follows from Eq. (11). The eigenvector belonging to this mixed eigenvalue is a linear combination of the two old eigenvectors, orthogonalized to the non-zero eigenvectors of \( Q \cdot (I - S) \). Under these approximations the collision term in Eq. (51) is modified, leading to

\[
\frac{d}{dt} f(\xi, t) = \frac{\tilde{\nu}(d - 1)}{2d} \left[ f_0(\xi) + f_{\text{coll}}[f](\xi, t) - 2f(\xi, t) \right] + \frac{\partial}{\partial \xi} [\xi^2 f(\xi, t)] ,
\]

where \( f_{\text{coll}}[f](\xi, t) \) represents the distribution of the new mixed eigenvalue after the collision, as a functional of \( f(\xi, t) \), the distribution before the collision.

Under the assumptions described above this distribution can be written as

\[
f_{\text{coll}}[f](\xi, t) = \int \int d\xi' d\xi'' f(\xi', t) f(\xi'', t) h(\xi|\xi', \xi'') \]

Here \( h(\xi|\xi', \xi'') \) is the distribution of the new eigenvalue \( \xi \) between the eigenvalues \( \xi' \) and \( \xi'' \). The function \( h \) assumes the form

\[
h(\xi|\xi', \xi'') = \frac{1}{\pi \sqrt{(\xi - \xi')(\xi'' - \xi)}} .
\]

From this an equation similar to Eq. (22) can be derived. One finds

\[
f_0(\xi) = 2f_{\text{stat}}(\xi) - f_{\text{coll}}[f_{\text{stat}}](\xi) - c[\xi^2 \frac{\partial}{\partial \xi} f_{\text{stat}}(\xi) + 2\xi f_{\text{stat}}(\xi)] ,
\]

This equation can easily be solved numerically and from its solution a second prediction of \( h_{KS} \) can be obtained. These results are discussed in the next section.

V. RESULTS AND DISCUSSION

In the previous sections we have developed two closely related analytical schemes that enable us to calculate approximations for the stationary distribution of eigenvalues of the inverse radius of curvature tensor. From this distribution we may obtain expressions for the leading order terms in the density expansion of the KS entropy of a gas of hard disks or spheres. In particular, the predictions resulting from Eq. (54) and numerical solutions of Eq. (45) may be compared to the results of Refs. [11, 21] and results from molecular dynamics simulations. In Ref. [11] Van Beijeren et al. proposed as approximation for the KS-entropy

\[
h_{KS}^{(0)} \approx \frac{N \tilde{\nu}(d - 1)}{2} \ln \xi_0 + \ln \left( \frac{\tau_1 + \tau_2}{2} \right) ,
\]

with \( \tau_i \) the free flight time of particle \( i \) since the previous collision. Putting this in the form of Eq. (11) leads to \( A = (d - 1)/2 \) and, after numerical integration,

\[
B^{(0)} \approx \begin{cases} 0.209 & \text{if } d = 2 \\ -0.583 & \text{if } d = 3 \end{cases}
\]

From molecular dynamics simulations Posch and coworkers [11, 33] found the following results for the Kolmogorov-Sinai entropy at low densities:...
Comparing the results of Eq. (57) to those of Ref. 11, Eq. (10), we find that $A$ is the same, but for $B$ one obtains corrections to Eq. (17) of the form

$$\Delta B = \ln \left( \frac{2d}{d-1} \right) - \gamma - \left\langle \ln \left[ \frac{\rho(\tau_i + \tau_j)}{2} \right] \right\rangle .$$

(49)

Dorfman et al. already expected corrections of $\ln 4 \approx 1.386$ for $d = 2$ and $\ln 3 \approx 1.098$ for $d = 3$ [34], corresponding to the first term in Eq. (49).

In Ref. [21], elements of the radius of curvature matrix were estimated by considering the stretching of the tangent phase space during a sequence of two collisions with free flights, it was estimated that

$$B^{\text{PW}} = \begin{cases} 1.47 \pm 0.11 & \text{if } d = 2 \\ 0.35 \pm 0.08 & \text{if } d = 3 \end{cases}$$

(50)

We have evaluated the averages in Eq. (49) by integrating over the joint distribution of the collision parameters [see Eq. (58)]. The values for the parameter $B$ resulting from the first approximation scheme follow as

$$B^{(1)} = \begin{cases} 2 - \frac{3}{2} \gamma + \ln 2 - \frac{1}{2} \ln \pi \approx 1.255 & \text{if } d = 2 \\ \frac{1}{2} - \frac{3}{2} \gamma + \ln 3 - \frac{1}{2} \ln \pi \approx 0.160 & \text{if } d = 3 \end{cases}$$

(51)

These results are in reasonable agreement with the results from the molecular dynamics simulations [33], given in Eq. (48).

More accurate results can be obtained from the second approximation scheme by numerically solving Eq. (15). The solution for $f_{\text{stat}}(\xi)$ for $d = 2, n = 0.001$ is displayed in Fig. 4. From this, one finds an additional correction to $B$ of

$$\Delta B = 0.086 ,$$

(52)

regardless of dimensionality. This leads to a final result for the constant $B$ of

$$B^{(2)} \approx \begin{cases} 1.341 & \text{if } d = 2 \\ 0.247 & \text{if } d = 3 \end{cases}$$

(53)

This is in good agreement with the results from the molecular dynamics simulations, and in particular also in better agreement than the results of Ref. [21], Eq. (50).

A. Comparing approximation schemes

We now argue why the distribution of inverse radius of curvature tensor eigenvalues obtained from the two-eigenvalue approximation resulting into Eq. (42) can be expected to be better than the simpler approximation, Eq. (41), resulting from assuming the distribution of interspersed new eigenvalues to be the same as that of the precollisional eigenvalues. Consider the first two moments of these distributions. In the simple approximation these are not changed from their precollisional values. Therefore, as mentioned already, the spectrum does not exhibit any narrowing in collisions, as it should according to the arguments presented before, which are supported by the calculations presented in Appendix B.

In the two-eigenvalue approximation, two eigenvalues $\xi_1$ and $\xi_2$ are sampled independently from the stationary distribution and replaced by one interspersed eigenvalue with the value $\xi' = \xi_1 c_2^2 + \xi_2 c_1^2$, according to Eq. (41). The other interspersed eigenvalues retain their precollisional values. The coefficients $c_1$ and $c_2$ are sampled as $c_1 = \cos \phi$ and $c_2 = \sin \phi$, with $\phi$ distributed uniformly on the unit circle. Hence the average value of $\xi'$ is the same as that of the precollisional eigenvalues, as should be the case (see Appendix B). From Eq. (41) and the assumed distribution of the $c_i$ one also easily finds the collisional changes of the second moments. In Appendix B it is shown that, to leading order in $1/n$ the average of the second moment is reduced at a collision by a factor $1 - (1 - A)/n$, with $A$ a constant with a value between zero and unity. This constant, defined in the Appendix through $\sum_{i=1}^{n} \left( c_i^4 (\xi_i - \langle \xi \rangle)^2 \right) = A/n \left( \sum_{i=1}^{n} (\xi_i - \langle \xi \rangle)^2 \right)$, can be calculated in the two-eigenvalue approximation from the assumed distribution of $c_1$ and $c_2$ as $A_2 = \frac{3}{4}$. Since in most cases the new eigenvector will be composed of more than 2 precollisional eigenvectors, $A_2$ will be an upper bound to the actual $A$. Hence the two-eigenvalue approximation does lead to a narrowing of the spectrum, but it underestimates its extent. This is especially true in the region where $f(\xi)$ reaches its maximum, since there the eigenfunctions of the ROC tensor tend to be carried by many particles, as one can see from Figs. 3 and 4.

The results may be improved, in principle, by considering larger sets of eigenvectors for spanning the $\epsilon_i$. However, to do this in a sensible way one would need the distribution of the $c_i$, preferably as a function of all $\xi_i$. So far no theory has been developed for this and it seems no simple task to do so. One could of course study this distribution numerically, but that would bring one close already to a full numerical study of the eigenvalue spectrum of the inverse radius of curvature tensor.

In Fig. 3 we plot numerical results for the average number of particles contributing to an eigenvalue as function of $\xi$, in a system of 64 two-dimensional par-
particles in a square box with periodic boundary conditions. For $\xi$ larger than the collision frequency most eigenvectors are carried by two particles, indicating that these are new eigenvectors $\epsilon_i$. For smaller $\xi$ there is a rapid increase in the average number of particles carrying an eigenvector, followed by a sharp drop below $\xi \approx 0.25 \nu \approx 0.9 \times 10^{-2} (k_B T/m)^{1/2}/a$. The eigenvectors corresponding to smaller eigenvalues have drifted for a long time, during which in most cases the particles contributing to them have collided many times. These eigenvectors are therefore typically carried by more particles. But, remarkably, for very low eigenvalues the number of particles carrying the eigenvector becomes very close to 1. This is related to the existence of particles that have not collided for several mean free times. As a result of subsequent projections normal to new eigenvectors the weight of such a particle in the remaining eigenvector can increase from the original value 1/2 to values close to unity. The contribution of these eigenvectors to the KS-entropy is very small.

We cannot directly translate the data of Fig. 3 to an estimate of the number of eigenvectors contributing significantly to a newly generated eigenvector $\epsilon_i$. It is clear though that there is a strong correlation. Since the new $\epsilon_i$ are always carried by just the two colliding particles, the components along them of eigenvalues carried by several particles necessarily have to be small. Hence, many of these are required to reconstruct any given $\epsilon_i$.

Another, more technical approach was based on a calculation of the distribution of elements of the radius of curvature [21 53]. The results in the present paper are more accurate than the results of that calculation, and were obtained in a more elegant way. On the other hand, it is not directly clear to us how to further improve the accuracy of the calculation presented here, nor if the distribution of eigenvalues of the radius of curvature could be used to calculate specific Lyapunov exponents of the system, as can be done with the distribution of the elements of the radius of curvature [22].

**B. Distribution of eigenvalues from simulation**

In our present calculation of the Kolmogorov-Sinai entropy of a dilute hard-sphere gas the central quantity to be computed is the stationary distribution of eigenvalues of the inverse radius of curvature tensor. It is interesting to compare the calculated distribution to results from computer simulations. We have performed MD simulations for a system of hard disks, in which we calculated
the radius of curvature tensor from the numerical values of $\delta r$ and $\delta v$ by making use of Eq. (14) and diagonalized it at regular time intervals. The results of these simulations are displayed in Fig. 4 along with the theoretical predictions. For a large range of eigenvalues, the calculations follow the simulations closely, including at very high $\xi$. At the lowest values of the range studied, there appear some differences.

It can be seen from Fig. 4 that the small eigenvalues have a more peaked, hence narrower distribution than was found from the calculations. This is due to the fact that only linear combinations of two eigenvectors were considered for $\epsilon_2$. In fact, as can be seen from Fig. 6 eigenvectors near the peak are generally carried by more particles and their contribution to $\epsilon_2$, which is carried by only two particles therefore will have a small coefficient $c_2$. As argued above, the larger the number of particles carrying an eigenvector, the smaller the value of $A$ and the stronger the narrowing. And Eq. (40) reveals that for given $\xi$ the dynamics are dominated by nearby eigenvalues and their $c_i$. As can be seen from Fig. 4 the distribution calculated using linear combinations of two eigenvectors not only predicts the KS-entropy better than the approximation based on no change in the spectrum of interspersed eigenvalues, but it also follows the simulation results more closely for intermediate eigenvalues.

VI. CONCLUSIONS

In this paper we have calculated the Kolmogorov-Sinai entropy of systems consisting of hard disks or spheres from the stationary distribution of the eigenvalues of the inverse radius of curvature tensor. The dynamics of these eigenvalues consist of free streaming and collisional effects. The latter are a combination of the generation of new eigenvalues, with a well-defined distribution, and a slight narrowing of the spectrum of remaining eigenvalues with respect to the precollisional spectrum. Already a simple approximation, which ignores this narrowing and assumes the spectrum to remain unchanged at collisions on average, reproduces the numerically observed spectrum quite well, with a fairly accurate prediction of the KS entropy. A slightly more refined approximation, assuming the new eigenvectors consist of just two precollisional ones, both sampled randomly from the full distribution, does predict a narrowing of the spectrum at collisions, though it underestimates its extent. This approximation gives quite accurate results for the KS entropy and it reproduces the eigenvalue spectrum of the inverse radius of curvature tensor better than the simplest approximation. The remaining underestimation of the narrowing is strongest and most clearly visible at small eigenvalues.

In order to improve on the estimates developed here one needs more knowledge on the decomposition of the new eigenvectors created at a collision into precollisional eigenvectors. This is highly nontrivial, however.

It should be noted that, though the specific dynamics of the inverse radius of curvature tensor are different for other high-dimensional systems, such as the high-dimensional Lorentz gas (12) (which has uniformly convex scatterers), their overall behavior is generic for all systems consisting of many particles.

An attractive approach seems describing the dynamics of the eigenvalues of the inverse radius of curvature tensor by means of a Fokker-Planck equation. In order to do so one needs expressions for the local drift and diffusion of the eigenvalues due to collisions. For this again more knowledge is needed of the way new eigenvectors are composed of old ones. Furthermore, the Fokker-Planck equation is a good approximation for systems where the dynamics consist of small jumps, while in the present case also large jumps happen. However, these mostly will occur for large values of $\xi$, where the dynamics is dominated by the drift. Therefore the Fokker-Planck equation may still be a good approximation.

Finally, the expressions derived here for the dynamics of the inverse radius of curvature tensor, and the equations for the distribution of its eigenvalues, Eqs. (31) and (12), can also be used for systems in a stationary non-equilibrium state. In such a state, the distributions of velocities and collision parameters are different and one has to take this into account when calculating the averages or the source terms in Eqs. (31) and (12).

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Appendix A: Eigenvalues of a submatrix

Let $P_i$ through $P_{d-1}$ be the projection operators which project out the $d-1$ orthogonal unit vectors $\epsilon_1$ through $\epsilon_{d-1}$. We are interested in the (distribution of) nonzero eigenvalues of submatrix $PTP$ of a symmetric matrix $T$, with $P = P_1 \cdots P_{d-1}$. We shall determine these by considering the nonzero eigenvalues $\xi'_i$ of $\tilde{T}' = P_x T P_x$, and their corresponding eigenvectors $\eta_i$. The eigenvalues of $PTP$ can now be determined by applying this procedure $d-1$ times projecting subsequently normal to each of the $d-1$ non-vanishing eigenvalues of $(I - S) \cdot Q$. Thus one obtains matrices $\tilde{T}$ with a decreasing number of nonzero eigenvalues.

Let $\psi_1$ through $\psi_z$ be the $z$ normalized eigenvectors of a matrix $\tilde{T}$ with corresponding eigenvalues $\xi_1$. Let us write the unit vector that is to be projected out, $\epsilon_z$, and
an eigenvector $\eta$ of $\tilde{T}'$ with eigenvalue $\xi'$ in terms of the
eigenvectors of $T$,
\[ \epsilon_x = \sum_i c_i \psi_i, \quad (A1) \]
\[ \eta = \sum_i \beta_i \psi_i, \quad (A2) \]
with
\[ \sum_i c_i^2 = \sum_i \beta_i^2 = 1. \quad (A3) \]
As $\eta$ has no component along $\epsilon_x$, we may write
\[ \xi' \eta = \xi' \sum_i \beta_i \psi_i \]
\[ = \tilde{T}' \eta = \mathcal{P}_x \tilde{T} \eta = \mathcal{P}_x \sum_i \beta_i \xi_i \psi_i \]
\[ = \sum_i (\beta_i \xi_i - \mu c_i) \psi_i, \quad (A6) \]
with $\mu$ a constant such that
\[ \epsilon_x \cdot \xi' \eta = \sum_i c_i (\beta_i \xi_i - \mu c_i) = 0. \quad (A7) \]
By taking the inner product of Eq. (A6) with a given $\psi_i$ one finds that,
\[ \beta_i = -\frac{\mu c_i}{\xi' - \xi_i}. \quad (A8) \]
By substituting Eq. (A8) into Eq. (A7), and dividing by $\mu$ and $\xi'$, we find that
\[ \sum_i \frac{c_i^2}{\xi_i - \xi'} = 0. \quad (A9) \]
From this equation it follows directly that between each subsequent pair $\xi_i$ and $\xi_{i+1}$ there must be precisely one solution for $\xi'$.

**Appendix B: Narrowing of eigenvalue spectrum**

In order to investigate the narrowing of the spectrum of eigenvalues as result of a collision we rewrite Eq. (A9), multiplying it by $-\prod (\xi' - \xi_i)$ and find
\[ \xi'^{n-1} - \sum_i (1 - c_i^2) \xi_i \xi'^{n-2} + \sum_{i<j} (1 - c_i^2 - c_j^2) \xi_i \xi_j \xi'^{n-3} \]
\[ + \ldots = 0, \quad (B1) \]
where we have made use of Eq. (A3). By comparing the coefficient of $(\xi')^{n-2}$ to the coefficient in the eigenvalue equation for $\xi'$, one immediately obtains
\[ \sum_{i=1}^{n-1} c_i^2 = \sum_{i=1}^n (1 - c_i^2) \xi_i. \quad (B2) \]
In section III we have found that the eigenvectors $\epsilon_z$ consist of equal and opposite components on two arbitrarily determined (colliding) particles along a unit vector that is distributed isotropically in d-dimensional space. From this it follows immediately that the average of $c_i^2$ over many collisions has to be equal to $1/n$. If in Eq. (B2) we replace $c_i^2$ by this average we find that the mean value of the interspersed eigenvalues on average is the same as that of the precollisional ones. Note that Eqs. (A11) and (12) both satisfy this property.

Similarly, from the coefficient of $(\xi')^{n-2}$ one obtains the identity
\[ \sum_{i<j} c_i^2 c_j^2 \xi_i \xi_j = \sum_{i<j} (1 - c_i^2 - c_j^2) \xi_i \xi_j. \quad (B3) \]
Combining this with Eq. (B2) one finds the identity
\[ \sum_{i=1}^{n-1} \langle (\xi'_i - \langle \xi \rangle)^2 \rangle = \frac{1}{n^2} \left( \sum_{i=1}^n (\xi_i - \langle \xi \rangle)^2 \right)^2 + \left( 1 - \frac{2}{n} - \frac{1}{n^2} \right) \sum_{i=1}^n \langle (\xi_i - \langle \xi \rangle)^2 \rangle + \sum_{i=1}^n \langle c_i^4 (\xi_i - \langle \xi \rangle)^2 \rangle. \quad (B4) \]

Here the brackets indicate an average over many subsequent collisions. We used the identity
\[ \langle c_i^2 c_j^2 \xi_i \xi_j \rangle = \frac{1}{n^2} \langle \xi_i \xi_j \rangle \quad i \neq j, \quad (B5) \]
and we introduced the symbol $\langle \xi \rangle$ defined by
\[ \langle \xi \rangle = \frac{1}{n} \left( \sum_{i=1}^n \xi_i \right), \quad (B6) \]
To leading order in $1/n$ the terms proportional to $1/n^2$ in Eq. (B5) may be ignored. We introduce the constant $A$ defined through
\[ \sum_{i=1}^n \langle (\xi_i - \langle \xi \rangle)^2 \rangle = \frac{A}{n} \sum_{i=1}^n \langle (\xi_i - \langle \xi \rangle)^2 \rangle. \quad (B7) \]
Note that $A$ is smaller than 1, since $c_i^4 < c_i^2$ and $c_i^2 > 1$. To leading order in $1/n$ combination of Eqs. (B4) and (B7) leads to the reduction factor mentioned in section III A. Obviously, the smaller $A$, the stronger the nar-
narrowing. This should apply also locally, implying stronger narrowing in regions where the eigenvectors tend to be carried by more particles.

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