

A Note on the Ruelle Pressure for a Dilute Disordered Sinai Billiard

Henk van Beijeren

Institute for Theoretical Physics

Utrecht University

Leuvenlaan 4, 3584 CE Utrecht, The Netherlands

and

Centre d' Etudes des Phénomènes Non-linéaires et des Systèmes Complexes

Université Libre de Bruxelles

Campus de la Plaine, Boulevard du Triomphe, 1050 Bruxelles, Belgium

J. R. Dorfman

Institute for Physical Science and Technology and Department of Physics

University of Maryland

College Park, MD 20742, USA

(February 8, 2008)

The topological pressure is evaluated for a dilute random Lorentz gas, in the approximation that takes into account only uncorrelated collisions between the moving particle and fixed, hard sphere scatterers. The pressure is obtained analytically as a function of the temperature-like parameter, β , and of the density of scatterers, n . The effects of correlated collisions on the topological pressure can be described qualitatively, at least, and they significantly modify the results obtained by considering only uncorrelated collision sequences. As a consequence, for large systems, the range of β -values over which our expressions for the topological pressure are valid becomes very small, approaching zero, in most cases, as the inverse of the logarithm of system size.

I. INTRODUCTION

One of the most important developments in dynamical systems theory over the past several decades is the discovery by Sinai, Ruelle, and Bowen, that Gibbs ensembles have as central a role to play in the description of hyperbolic dynamical systems, as they do in statistical thermodynamics [1–3]. The dynamical analog of the Gibbs formalism for statistical thermodynamics is usually referred to as the *thermodynamic formalism* [2,4]. One of the central quantities in the application of Gibbs ensembles to dynamical systems is the so-called topological pressure, or Ruelle pressure, which is the analog, apart from a sign, of the Helmholtz free energy per particle of a thermodynamic system, in the thermodynamic limit. This correspondence is made clear by its definition in terms of a dynamical partition function, where the pressure is defined in essentially the same way as the free energy per particle, with time t playing the role of system size.

In the dynamical case, the analog of the thermodynamic limit is the infinite time limit ¹. Like the free energy, as a function of temperature, volume and particle number, generates the full equilibrium thermodynamics of a many particle system, the topological pressure and its derivatives with respect to a temperature like parameter, provide useful information about the dynamical properties of the system under study. Kolmogorov-Sinai and topological entropies per unit time can be expressed in terms of this pressure and its derivatives, as can escape rates, and Hausdorff dimensions of fractal structures and measures [4,5].

Despite the beauty of the theory and the power of the theorems that have been proven about the dynamical Gibbs ensembles, there are few examples of deterministic dynamical systems where the topological pressure can be evaluated by analytical methods, other than simple maps, such as baker maps and toral automorphisms [6]. The present authors, together with Appert and Ernst calculated the topological pressure for a more complicated dynamical system, a Lorentz lattice gas [7,8]. Here a moving particle hops from one site to a neighboring site on a lattice, at each time step. Some of the lattice sites are occupied by scatterers, such that if the particle encounters a scatterer, it may change the direction of its motion at the next step, with some given probability. If the particle lands on a site that does not have a scatterer, it continues moving in the same direction at the next time step. While this model can be reformulated as a deterministic dynamical system, it was possible to evaluate the topological pressure by treating the system as a stochastic one, and using the thermodynamic formalism as it applies to stochastic systems [4]. In the large system limit the topological pressure turns out to be determined by either large dense clusters of scatterers (for the inverse temperature like parameter $\beta < 1$), or large vacant regions (for $\beta > 1$), that form in a quenched distribution of scatterers on the lattice. This phenomenon is very analogous to the one responsible for *Lifshitz tails* in disordered systems showing critical phenomena [9–11].

The purpose of this note is to provide a similar analysis of the topological pressure for a very useful model for studies in the kinetic theory of gases, the Lorentz gas. This model served as the inspiration for the Lorentz lattice gas described above, but is a continuum model. It is constructed by placing fixed scatterers in d spatial dimensions, and allowing a particle to move in this system of scatterers, colliding with them, and moving freely between collisions. When the scatterers are placed on a regular lattice this model is known as the Sinai billiard [12], which has served as a paradigm in the theory of dynamical systems for several decades now. It is one of the few nontrivial dynamical systems that are really close to realistic physical systems and yet allow for rigorous proofs of many important properties, including the existence of a finite diffusion coefficient [13]. For the application of kinetic theory methods, however, it is simpler to consider disordered systems, where the scatterers are located at random positions in space. Further simplifications occur when the density of scatterers is low, so that the average distance between them is much larger than their radii. In this case the average time for return of the moving particle to a scatterer with which it

¹In addition one may consider the limit of infinite system size for the topological pressure as well. As we will see this leads to new complications which do not occur in the Gibbsian formalism of equilibrium statistical mechanics

has previously collided becomes very long and therefore the effects of correlations between collisions, to a first approximation, may be ignored in many applications. The moving particle makes specular elastic collisions with the scatterers, and travels freely between collisions. At low density of scatterers, in large but not too large systems (we will become more specific about this in section IV) with periodic boundary conditions (the simplest choice; in fact the precise nature of the boundaries does not matter so much, as long as they are elastic) it is very reasonable to assume that subsequent collisions of the light particle may be considered as independent random flights, sampled from the equilibrium distribution of random flights in the dilute d -dimensional Lorentz gas. This will be the basis for our calculations in section II, where we will describe the model in more detail and define the dynamical partition function and the topological pressure. Then we show that the contributions from the supposedly uncorrelated collision sequences can be accounted for in a relatively simple way, in the spirit of Sinai's analysis of billiard ball models. The following section shows how the topological pressure can then be evaluated in terms of the poles of a zeta function, called the Ruelle zeta function. We discuss the properties of this pressure and evaluate the relevant dynamical properties of the Lorentz gas in this approximation.

For large systems it is to be expected that the topological pressure will be determined by large clusters of scatterers or large vacant regions, as in the case of the Lorentz lattice gas. This will be investigated in section IV, where we will make some specific estimates for the topological pressure in large systems both for $\beta > 1$ and for $\beta < 1$. These are based on plausible assumptions about the types of closed orbits (for $\beta > 1$) or dense regions (for $\beta < 1$) that will dominate under these conditions. The paper concludes with a discussion of similar large system properties to be expected in systems of many moving particles, with some remarks on possible relations between the topological pressure for $\beta > 1$ and scars in the corresponding quantum mechanical models.

II. THE DYNAMICAL PARTITION FUNCTION FOR THE RANDOM LORENTZ GAS

We consider an infinitely extended system of fixed hard-sphere scatterers of radius a , placed at random with number density n and without overlapping, in a space of d dimensions. A point particle, of mass m , moves with speed v in this array of scatterers making specular, elastic collisions with the scatterers, and traveling freely between collisions. This system, the random Lorentz gas, is therefore a Hamiltonian system, with the usual symplectic properties. We consider here the case of low density, specified by the condition that the radius of a scatterer is small compared to the average distance between two scatterers, *i. e.* $na^d \ll 1$. For the two and three dimensional version of this model the Lyapunov exponents and Kolmogorov-Sinai (KS) entropies have been calculated, with the use of kinetic theory methods, appropriate for low densities of the scatterers [14,15]. Here we apply the same methods for the calculation of the topological pressure.

The topological pressure is given in terms of a dynamical partition function, $Z(\beta, t)$, defined, as a function of an inverse-temperature-like parameter β and time t , by

$$Z(\beta, t) = \int d\mu(\vec{r}, \vec{v}) [\Lambda(\vec{r}, \vec{v}, t)]^{(1-\beta)}. \quad (1)$$

Here the integration is over the equilibrium measure, $\mu(\vec{r}, \vec{v})$, for the phase space of the moving particle. The position and velocity of the particle are denoted by \vec{r}, \vec{v} , respectively, where \vec{r} ranges over the configuration space region available to the moving particle, not occupied by scatterers, and \vec{v} ranges over all possible directions of the velocity, while the magnitude of the velocity remains constant. The quantity $\Lambda(\vec{r}, \vec{v}, t)$ is the “stretching” factor for a phase space trajectory of the particle starting at \vec{r}, \vec{v} and extending over a time t . The stretching factor is the factor by which the projection of an infinitesimal phase space volume onto the unstable directions will expand over a time t . For *very long times* the stretching factor is given in terms of local positive Lyapunov exponents, $\lambda_i(\vec{r}, \vec{v})$ by

$$\Lambda(\vec{r}, \vec{v}, t) \approx e^{t \sum_i \lambda_i(\vec{r}, \vec{v})}, \quad (2)$$

where the subscript i labels the distinct unstable manifolds in phase space for the moving particle. The number of these unstable manifolds is given in terms of the spatial dimension as $d-1$, since there are two neutral directions in phase space, and equal numbers of unstable and stable manifolds. Finally, β can be used to determine various dynamical properties of the system. The topological pressure, or Ruelle pressure, $P(\beta)$ is expressed in terms of the dynamical partition function by

$$P(\beta) = \lim_{t \rightarrow \infty} \frac{1}{t} \ln Z(\beta, t), \quad (3)$$

which establishes the formal connection between the topological pressure in dynamics and the negative of the Helmholtz free energy in statistical thermodynamics.

The structure of the dynamical partition function, given by Eq. (1) suggests the procedure for its calculation for a Lorentz gas. One classifies the regions of phase space according to the number of collisions the moving particle will suffer in time t starting from a point in that region. Thus we would need to calculate the contributions to $Z(\beta, t)$ from regions with no collisions, one collision, and so on. For each such region we then need to calculate the associated stretching factors. These stretching factors have been given for the dilute, random Lorentz gas by Van Beijeren, Latz, and Dorfman, as products of stretching factors, $\Lambda_i^{(d)}$ for each collision of the moving particle. They depend on the dimension, d , of the system and are easily obtained, for low densities (long free flight times), by methods described in [14,15], ass

$$\Lambda_i^{(d)}(\tau_i, \theta_i) = \left[\frac{2v\tau_i}{a} \right]^{(d-1)} |\cos \theta_i|^{(d-3)} \quad (4)$$

Here τ_i is the free time between the collision denoted by the subscript i , and the previous collision of the moving particle, and θ_i is the angle of incidence at collision i . It will be convenient here to express this angle in terms of the inner product of the incident velocity \vec{v} and $\hat{\sigma}_i$, the unit vector from the center of the scatterer to the point of incidence at collision i , as $v \cos \theta_i = |\vec{v} \cdot \hat{\sigma}_i|$, with the incident velocity and unit vector oriented so that $\vec{v} \cdot \hat{\sigma}_i \leq 0$. The time between one collision of the moving particle and the next is sampled from the normalized equilibrium distribution of free times, $p(\tau)$, given for low densities, by

$$p(\tau) = \nu e^{-\nu\tau}, \quad (5)$$

where ν is the low density value of the average collision frequency, given for d -dimensional dilute, random Lorentz gases by

$$\nu = 2nva^{d-1} \frac{\pi^{\frac{d-1}{2}}}{(d-1)\Gamma(\frac{d-1}{2})}. \quad (6)$$

Using this expression, we can write the total stretching factor for a sequence of \mathcal{N} collisions of the moving particle as

$$\Lambda(\vec{r}, \vec{v}, \mathcal{N}) = \prod_1^{\mathcal{N}} \Lambda_i^{(d)}(\tau_i, \theta_i). \quad (7)$$

The total time, T between the initial instant, and the final collision is $T = \tau_1 + \dots + \tau_{\mathcal{N}}$.

For low densities we can provide an expression for the average value of the stretching factor for a sequence of \mathcal{N} uncorrelated collisions taking place within a time interval t where the first collision takes place at time τ_1 and the last at time T . This average includes the probability that \mathcal{N} collisions will take place within a time t , so these averages will directly determine the dynamical partition function. The average value of the stretching factor is given by

$$\begin{aligned} \langle [\Lambda(\vec{r}, \vec{v}, \mathcal{N})]^{(1-\beta)} \rangle_t &= \nu \left(\frac{\nu}{J_d}\right)^{\mathcal{N}} \int_0^\infty d\tau_1 \cdots \int_0^\infty d\tau_{\mathcal{N}+1} \int' d\hat{\sigma}_1, \dots, d\hat{\sigma}_{\mathcal{N}} \prod_1^{\mathcal{N}} \cos \theta_i \times \\ &\left[\prod_{i=1}^{\mathcal{N}} \Lambda_i^{(d)}(\tau_i, \theta_i) \right]^{(1-\beta)} e^{-\nu(\tau_1 + \dots + \tau_{\mathcal{N}} + \tau_{\mathcal{N}+1})} \left[\Theta\left(t - \sum_1^{\mathcal{N}} \tau_i\right) - \Theta\left(t - \sum_1^{\mathcal{N}+1} \tau_i\right) \right]. \end{aligned} \quad (8)$$

Here $\Theta(x)$ is the usual Heaviside function. The Heaviside functions and the additional time integral, over $\tau_{\mathcal{N}+1}$, are included in this expression to require that precisely \mathcal{N} collisions take place over time t . The averaging includes averages over all possible free times between two collisions, using Eq. (5), as well as integrations over the possible directions of incidence at each collision. The prime on the integrations over solid angles indicates that only half of the total solid angle is to be included corresponding to the requirement that $\vec{v} \cdot \hat{\sigma} \leq 0$, at each collision. The angular factors of $\cos \theta_i$ properly account for the volumes of collision cylinders when one calculates the rate at which collisions take place with angle of incidence, θ_i , and J_d is a normalization constant used in the averaging and is given, for d -dimensions, by

$$J_d = \frac{2\pi^{\frac{d-1}{2}}}{(d-1)\Gamma(\frac{d-1}{2})}. \quad (9)$$

The dynamical partition function for the Lorentz gas at low density can be expressed in terms of these average values by summing over contributions from all uncorrelated collision sequences as

$$Z(\beta, t) = \sum_{\mathcal{N}=0}^{\infty} \langle [\Lambda(\vec{r}, \vec{v}, \mathcal{N})]^{1-\beta} \rangle_t. \quad (10)$$

The term for $\mathcal{N} = 0$, will be set equal to $\nu \exp[-\nu t]$, corresponding to the dynamical partition function for a particle with no collisions in the time interval $(0, t)$ and a stretching factor of unity.

III. THE ZETA FUNCTION

Although the integrals in each term in Eq. (10) are not difficult, the calculation of the topological pressure is greatly simplified by introducing a zeta function [2], adapted to continuous time dynamics, obtained by taking the Laplace transform on Eq. (10). One finds, using Eq. (4), that

$$\begin{aligned} \mathcal{Z}^{(d)}(z) &= \int_0^\infty dt e^{-zt} Z(\beta, t) = \\ &= \frac{1}{\nu + z} \left\{ 1 - G(d, \beta) \frac{d-1}{2} \frac{\nu}{(z + \nu)^{(d+\beta-d\beta)}} \left(\frac{2\nu}{a} \right)^{(d-1)(1-\beta)} \right\}^{-1} \end{aligned} \quad (11)$$

where

$$G(d, \beta) = \frac{\Gamma(\frac{d-1}{2})\Gamma(\frac{d-1+\beta(3-d)}{2})\Gamma(d + \beta - d\beta)}{\Gamma(d - 1 + \frac{\beta(3-d)}{2})}. \quad (12)$$

The pole of the zeta function which is closest to the origin is the topological pressure. This follows simply from the observation that if the dynamical partition behaves, for asymptotically large t as $\exp[tP(\beta)]$, the zeta function will have a pole at $z = P(\beta)$. It is an elementary calculation to find this pole, which is given by

$$P_{mf}^{(d)}(\beta) = \left[\nu \frac{d-1}{2} \left(\frac{2\nu}{a} \right)^{(d-1)(1-\beta)} G(d, \beta) \right]^{\frac{1}{d+\beta-d\beta}} - \nu. \quad (13)$$

Here the subscript mf indicates that these are ‘‘mean field’’ results, obtained by ignoring correlations between successive collisions. As we shall see in the next sections, these results are valid only in a small region about $\beta = 1$ for large systems.

We can now use these results for the pressure to check if they agree with known results and to determine the values for other dynamical quantities. The topological pressure for $\beta = 1$, should vanish for a closed system, and one easily sees from Eq. (13), using simple identities for gamma functions, that this expression satisfies this condition. Further, the KS entropy can be determined from the topological pressure by taking a derivative with respect to β and setting $\beta = 1$, as

$$h_{KS} = - \left. \frac{dP(\beta)}{d\beta} \right|_{\beta=1} \quad (14)$$

Simple calculations show that this condition is satisfied as well, leading, for $d = 2, 3$ to the results found by Van Beijeren, Latz, and Dorfman [14,15]:

$$h_{KS}^{(2)} = 2nav(1 - \gamma - \ln(2na^2)); \quad (15)$$

$$h_{KS}^{(3)} = 2na^2v\pi(\ln 2 - \gamma - \ln(na^3\pi)). \quad (16)$$

Here γ is Euler’s constant.

New results can be obtained from the pressure by setting $\beta = 0$. The value of the pressure at this point is the topological entropy per unit time, and we thus obtain the mean field value

$$h_{top}^{(d)} = \left[nv^d (d-1) (4\pi)^{\frac{d-1}{2}} \Gamma\left(\frac{d-1}{2}\right) \right]^{\frac{1}{d}} - \nu, \quad (17)$$

where we have inserted expression Eq. (6) for the collision frequency in the first term on the right hand side of Eq. (17). It is interesting to note that these topological entropies depend upon the $1/d$ -th power of the density of the scatterers, and have a finite, non-zero limit as the size of the scatterers vanishes. This latter result is consistent with rigorous results of Burago, Ferleger, and Kononenko [16] who provided estimates for the topological entropy of the periodic Sinai billiard in d -dimensions. They were able to prove that for this system, the topological entropy has a finite non-zero limit as the radius of the scatterers vanishes, and that in this limit, when variables are used in which both the density and the velocity equal unity, the topological pressure is a non-decreasing function of the number of dimensions, bounded from below by $\ln(2d-1)$. One easily checks that these properties are also satisfied by the disordered Lorentz gas. For large d in fact one finds an increase proportional to \sqrt{d} rather than $\ln d$. However, please note that with increasing system size, for fixed radius a , the present expressions for the topological pressure of the disordered Lorentz gas, for β -values well below unity, soon have to be replaced by values resulting from orbits restricted to regions with high scatterer density. Therefore the validity of Eq. (17) is restricted to a maximal system size, depending in turn on the density of scatterers. We will come back to this in our discussion.

IV. LARGE SYSTEMS

For chaotic systems the dynamical instability typically gives rise to an exponential increase with time of the stretching factor $\Lambda(\vec{r}, \vec{v}, t)$. For a given time, the actual rate of increase will depend on the initial values of \vec{r} and \vec{v} . For $\beta > 1$ regions of slow increase will be weighted most heavily. Therefore such regions may dominate the dynamical partition function, even if the probability of the moving particle to stay inside it decays exponentially with time. Our claim is that for specific realizations of the disordered Lorentz gas the orbits dominating the dynamical partition function for long times at $\beta > 1$ are orbits concentrated around the least unstable periodic orbit (LUPO) of the system, that is, the periodic orbit with the smallest exponential increase of its stretching factor. We have no rigorous proof for this statement, but we think it is extremely plausible. And in any case, the resulting values for the topological pressure do establish strict lower bounds to the actual values.

For $\beta < 1$ the dynamical partition function will tend to be dominated by orbits in regions with a higher than average stretching factor. In analogy with the case $\beta > 1$, one might expect that, for $\beta < 1$, the dominating region will consist of orbits concentrated around the most unstable periodic orbit ². For $\beta < 0$ this is indeed the case, for large enough

²We observe from Eq. (4) that the stretching factor of an orbit may be large for $d = 2$, and

systems, but for β between 0 and 1 this is not true. The reason is that this set of orbits picks up a weight factor $1/\Lambda(\vec{r}, \vec{v}, t)$ for its long term survival probability, hence one sees from Eq. (1) that for β between 0 and 1 periodic orbits with a large stretching factor get small weight in the dynamical partition function. Instead one has to look for the spatial region with the optimal combination of low escape rate and high average stretching factor for orbits confined to it. Here one recognizes a strong analogy to the Donsker-Varadhan arguments [11] for stretched exponential decay in diffusion among fixed traps.

In the remainder of this section we separately discuss the cases $\beta > 1$ and $\beta < 1$ in greater detail.

A. The topological pressure for $\beta > 1$

The least unstable periodic orbit is, roughly speaking, the orbit with the smallest number of collisions per unit time. In almost all cases this will simply be an orbit with the light particle bouncing back and forth between the same two scatterers, as illustrated in Fig. 1. In exceptional cases though, the LUPO may involve more than two scatterers.

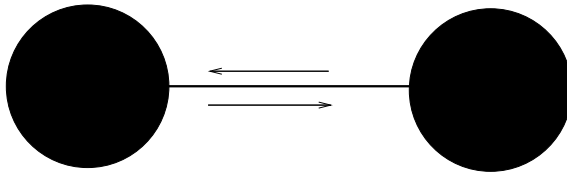


FIG. 1. A typical unstable periodic orbit. The light particle bounces back and forth between the same two scatterers.

Assuming that indeed the LUPO involves just two scatterers and, for simplicity, that the density of scatterers is low, we easily find an approximation for the distribution of the length of the free, periodic path between the two scatterers. Let $P(l)$ denote the probability that the system nowhere contains a periodic path of the type sketched above with a free path length exceeding l . For a large system, with N scatterers in a volume V , this probability, in two dimensions, satisfies an equation which is approximately

$$\frac{dP(l)}{dl} = \pi n(l + 2a)N e^{-2nal} P(l), \quad (18)$$

which is obtained by the following reasoning: suppose the system has no periodic paths with a free path length exceeding l . The chance for this is $P(l)$. To obtain the probability for

for grazing collisions where $\theta \approx \pi/2$. However for a disordered Lorentz gas it is not possible to find long orbits mainly consisting of nearly grazing collisions, and the typical contribution to the topological pressure for $\beta < 1$ will come from orbits of the type discussed here.

a largest periodic path between l and $l - dl$ one has to multiply this with the probability of having two scatterers at a distance between $l + 2a$ and $l + 2a - dl$, which is roughly $N^2 2\pi(l + 2a)dl/(2V)$, times the probability, $\exp(-2nal)$, that the periodic orbit between those scatterers is free from other scatterers. Integrating this equation and taking the derivative of $P(l)$ with respect to l , one finds the probability distribution $p(l)$ for the length of the LUPO as

$$p(l) = \pi n N(l + 2a) e^{-2nal} \exp \left\{ -\frac{\pi N}{2a} \left(l + 2a + \frac{1}{2na} \right) e^{-2nal} \right\}. \quad (19)$$

For large N this distribution is sharply peaked around a value l_0 satisfying

$$l_0 = \frac{\log \frac{\pi N(l_0 + 2a)}{2a}}{2na} \quad d = 2. \quad (20)$$

The width of the distribution is of $O(1)$, and therefore of $O(1/\log N)$ relative to l_0 . In three dimensions a completely analogous calculation leads to

$$P(l) = \exp \left\{ -2N \left(\frac{(l + 2a)^2}{a^2} + \frac{2(l + a)}{\pi n a^4} + \frac{2}{\pi^2 n^2 a^6} \right) e^{-\pi n a^2 l} \right\}. \quad (21)$$

From this one finds the maximum l_0 in the distribution of the length of the LUPO satisfies the equation

$$l_0 = \frac{\log \frac{2(l_0 + 2a)^2 N}{a^2}}{\pi n a^2} \quad d = 3. \quad (22)$$

Again, one finds that the distribution is sharply peaked around a value proportional to $\log N$, with fluctuations of $O(1)$. Here too the results could easily be extended to arbitrary dimensionality d , but we did not work this out.

For a given scatterer configuration the topological pressure resulting from the orbits near the LUPO follows from the value of l_0 , as

$$P_{po}^{(d)}(\beta) = -\beta \frac{(d-1)v}{l_0} \log \frac{2l_0}{a}, \quad (23)$$

where we used Eq. (4), with $\tau_i = l_0/v$ and $\phi_i = 0$, and the fact that the long time survival probability near an unstable periodic orbit of stretching factor $\Lambda(t)$ is given by $1/\Lambda(t)$.

For given β and l_0 the topological pressure is found as the larger of the expressions (13) and (23). Since the former are proportional to $\beta - 1$ and the latter roughly to $\beta/\log N$, there is a sharp phase transition at a β -value satisfying $\beta - 1 \sim 1/\log N$. In the terminology of ordinary thermodynamics this is a *first order phase transition*, as the first derivative of the topological pressure with respect to β is discontinuous at this transition. This implies, however, that the range of β -values > 1 for which the topological pressure gives information about the bulk properties of the system is very limited for large systems; specifically it is of order $1/\log N$. For larger β -values the topological pressure rather gives information about the smallest escape rate of orbits from the neighborhoods of unstable periodic orbits. This obviously is of great importance for the asymptotic rate of decay to equilibrium, which

cannot be larger than this smallest escape rate. It can easily be smaller, if the asymptotic rate of mixing is smaller than the smallest escape rate or, even worse, if the system does not decay to equilibrium at all. Notice that the smallest escape rate may be zero, corresponding either to algebraic escape or to finite probability of not escaping at all (in which case one should not speak of *unstable* periodic orbits any more). But one should also notice that the pockets in phase space corresponding to the neighborhoods of unstable periodic orbits often cover such minute fractions of the total available phase space volume, that for the physics of the system they are of no practical importance. We will come back to this briefly in our discussion.

B. The topological pressure for $0 < \beta < 1$

For $0 < \beta < 1$ the factor $1/\Lambda(t)$ in the weighting of the near periodic orbits suppresses the contributions of strongly diverging periodic orbits to the topological pressure, as we noted already. Instead, we have to look for compact regions with high collision rate and slow escape. In two dimensions, with scatterers not allowed to overlap each other, the regions best satisfying these criteria obviously are enclosures of three scatterers almost touching each other, as illustrated in Fig. 2. Again, we have no rigorous proof of this, but the statement seems even more obvious than the one about the LUPO's.

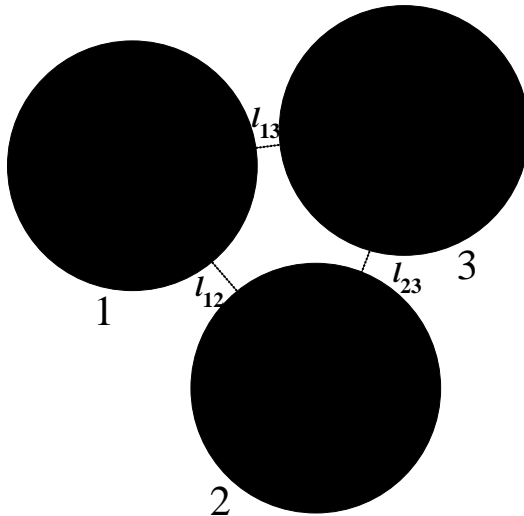


FIG. 2. A region enclosed by three disks. The escape rate of a light particle from this region is small and the collision frequency with the surrounding scatterers is high. The total escape length l is the sum of l_{12} , l_{13} and l_{23} .

The escape rate from such a trapping region may be expressed to a very good approximation as [17]

$$\nu_{tr} = \frac{vl_{esc}}{\pi O}, \quad (24)$$

with $O \approx (\sqrt{3} - \frac{1}{2}\pi)a^2$ the surface area of the trapping region and the escape length l_{esc} , the sum of the distances between the pairs of surrounding spheres.

In large systems there will be many of such trapping regions and the one with the smallest l_{esc} will determine the topological pressure when β is sufficiently smaller than 1. Let us call this value l_1 . We define $Q(l)$ as the probability that none of the trapping regions has an escape length $< l$ and notice that it approximately satisfies the equation

$$\frac{dQ(l)}{dl} = -\frac{1}{6}\sqrt{3}\pi al^2 n^2 N \chi_3 Q(l), \quad (25)$$

with χ_3 the triplet correlation function for three scatterers, all touching each other. The solution to this equation is

$$Q(l) = \exp\left(-\frac{\sqrt{3}\pi al^3 n^2 N \chi_3}{18}\right), \quad (26)$$

from which the distribution of l_1 is obtained as $q(l_1) = -dQ(l_1)/dl_1$. The maximum of this distribution is not sharp, but for our purpose, it is only important that this maximum scales as a function of $l_1/(N^{1/3}a)$. Consequently, as a function of N the escape rate ν_{tr} scales in the same way, even though its specific value depends on the scatterer configuration at hand.

The topological pressure in this case may be expressed as

$$P_{tr}^{(2)}(\beta) = (1 - \beta)\lambda_{cp}^{SB} - \nu_{tr}, \quad (27)$$

with λ_{cp}^{SB} the positive Lyapunov exponent of a triangular Sinai billiard at close packing. From Ref. [18] we quote the value $\lambda_{cp}^{SB} \approx 3.6v/a$. Comparing (27) and (13) we note that the range of β -values over which the mean-field value usually dominates that of the most trapping region satisfies

$$\beta > 1 - \frac{\nu_{tr}}{\lambda_{cp}^{SB} - h_{KS}^{(2)}}, \quad (28)$$

where $h_{KS}^{(2)}$ is given by Eq. (16). Thus, the validity of the mean field result is restricted in this case to a region of β values slightly below unity, with size of $O(N^{-1/3})$. Here, too, the phase transition that occurs when the most trapping region becomes dominant will be of first order.

The three dimensional case (again, for simplicity we won't consider arbitrary d) is more subtle because, with non-overlapping scatterers, there are no trapping regions from which escape only is possible through very narrow channels. Instead, a large topological pressure will result from the presence of a fairly large compact volume with a higher than average scatterer density. Thus, such high density regions will determine the topological pressure, even in three dimensions, away from a small region near $\beta = 1$. In order to obtain useful estimates of the size of this region, we consider compact volumes of radius R , typically of spherical shape, though this particular shape is not essential to our argument. The escape rate from such a region will be of the form $\nu(R) \sim D/R^2$, with D the diffusion coefficient. Here we use the fact that the distribution of moving particles in the disordered Lorentz gas satisfies a diffusion equation on large time and length scales. The largest density fluctuation found

in such a region in a system of total volume R^3 will typically be $\sim n^{1/2}R^{-3/2} \log^{1/2}(N/nR^3)$. This follows from the Gaussian nature of density fluctuations in large regions, with standard deviation $\sim n/(R^3)$, and the observation that the number of independent volumes of radius R is proportional to N/nR^3 . Therefore the excess topological pressure resulting from trajectories restricted to a region of radius R with maximal density fluctuation is obtained by means of a simple Taylor expansion of the topological pressure about its mean field value in powers of the density deviation. The resulting correction to the mean field pressure will then be roughly of the form

$$\Delta P_{tr}^{(3)}(\beta) = C_1(1 - \beta) \frac{n^{1/2}}{R^{3/2}} \frac{\partial c_{mf}^{(3)}}{\partial n} \left(\log \frac{N}{nR^3} \right)^{1/2} - \frac{C_2 D}{R^2}, \quad (29)$$

with C_1 and C_2 constants of order unity and the subscript tr indicating that these corrections are due to trapping regions. Furthermore,

$$c_{mf}^{(3)} \equiv \frac{P_{mf}^{(3)}(\beta)}{1 - \beta}.$$

The expression (29) takes its largest value, $\sim (1 - \beta)^4 (\log N)^2$, for R roughly proportional to $(1 - \beta)^{-2} (\log N)^{-1}$. In order for this largest value of $\Delta P_{tr}^{(3)}$ to be a small correction to $P_{mf}^{(3)}(\beta)$, the parameter β must satisfy the condition $1 - \beta \ll (\log N)^{-2/3}$. Furthermore, for $\Delta P_{tr}^{(3)}(\beta)$ to be negative for all allowable values of R one needs $1 - \beta < CN^{-1/6}$, with C some constant.

On the basis of this analysis one can expect that also the phase transition from $P_{mf}^{(3)}$ to $P_{tr}^{(3)}$ will be first order, but only very, very weakly so. If β is increased within the range $1 - \beta \sim N^{-1/6}$ one finds that for β very close to 1, the expression (29) is negative definite within the allowable range of R -values. It first becomes positive, at a value of $R/V^{1/3}$ where the expression on the right hand side of Eq. (29) attains a maximum, for some specific β , which then marks the phase transition. Since at this transition R jumps to a value $\ll V^{1/3}$ it is a first order transition indeed. However, the resulting change in the topological pressure is so small, for β in the range between $1 - \beta \sim N^{-1/6}$ and $1 - \beta \sim (\log N)^{-2/3}$, that in fact the transition will appear to be continuous. Furthermore one should keep in mind that the scenario sketched here for the determination of the topological pressure is very heuristic. There may be additional contributions to the dynamical partition function, which we have overlooked, but are in fact dominant for certain ranges of β -values.

Further, we want to remark that Eq. (29) should be used with care for $1 - \beta$ strongly exceeding $(\log N)^{-2/3}$. For the diffusion approximation for the escape rate to be valid R should be much larger than both the size of the scatterers, a , and the mean free path between collisions. Further, for the Taylor expansion of the topological pressure to be valid, the expression multiplying $\partial c_{mf}^{(3)}/\partial n$ on the right hand side of Eq. (29) should be $\ll 1$. Nevertheless, in this range of β -values we can be sure that for large systems the topological pressure is dominated by contributions from one of the trapping regions.

It is also useful to note that even for $\beta > 1$ there is a small region that is dominated by trajectories trapped in compact regions, this time in regions of *lower than average* density. Combining the arguments presented before, one finds that this region is determined roughly

by conditions of the form $C_3 N^{-1/6} < \beta - 1 < C_4 (\log N)^{-3/4}$, with C_3 and C_4 constants of order unity. However, throughout this region the relative corrections to $P_{mf}^{(3)}$ are small.

V. DISCUSSION

In summary, we have obtained explicit, mean-field type expressions for the topological, or Ruelle pressure of a dilute disordered Lorentz gas, leading to Kolmogorov-Sinai entropies in agreement with the results of previous calculations. However, we also found that for large systems the range of the inverse-temperature like parameter β of Ruelle's thermodynamic formalism over which these expressions are valid, is restricted to a very small region around $\beta = 1$. For $\beta > 1 + O(1/\log N)$, with N the number of scatterers in the system, the topological pressure is determined by the decay rate of orbits from the region in phase space surrounding the least unstable periodic orbit, and for $\beta < 1 - O(N^{-1/3})$ in two dimensions, and for $\beta < 1 - O((\log N)^{-2/3})$ in three dimensions it is determined by orbits that remain trapped in areas enclosed by three disks, or in fairly large regions of higher than average scatterer density, respectively. In fact these restrictions do not only apply to dilute systems. They will hold for any system with particles moving among a disordered array of fixed scatterers.

The periodic orbit results are of interest because they give information related to the asymptotic long time decay to equilibrium. Similarly the trapped region results contain information about the fastest rate of information loss that may be observed for long times, but the way in which different regions are weighted, especially how their escape rates are taken into account, depends on the choice of β .

Another context where the least unstable periodic orbits play a crucial role is in the description of *scars*, i.e. eigenfunctions in quantum systems that are concentrated in the neighborhoods of periodic orbits of the corresponding classical system [19]. An important difference is that in this case the classical orbit need not have a minimal length (or more precisely, a stretching factor that is sufficiently smaller than the average bulk stretching factor) to be observable as a scar. Nevertheless, our findings suggest that the topological pressure for $\beta > 1$ may be used as a tool for finding the most prominent scar in the quantum mechanical counterpart of a classically chaotic system.

Two of the most interesting questions to be asked are: In how far can the results obtained here be generalized to systems of interacting moving particles? and: In how far will similar conclusions hold in such cases? For simple gases at low densities we believe that we can calculate the leading order mean field approximation to the topological pressure along the lines sketched in the present paper, by combining these with the methods of [20]. Again, for $\beta < 1$ we expect dominance of near periodic orbits. In fact, for hard spheres the situation is even slightly worse than in the Lorentz gas. With periodic or simple reflecting boundary conditions one may easily construct periodic orbits without any collisions, simply by assigning equal velocities to all particles (or, if one insists on zero total momentum, velocity \vec{v} to half of the particles, in one half of the box, and $-\vec{v}$ to the other half, in the other half of the volume). The neighborhoods of these orbits will give rise to a strictly vanishing topological pressure for all $\beta > 1$. Even with irregularly shaped boundaries and not too many particles, one may construct orbits without inter-particle collisions by lining

up all the particles in a long row, or “duck march”, along the same single particle trajectory in phase space, chosen such that there are no near-intersections with a short time lag. There may be a stretching factor > 1 for such an orbit, but that is entirely due to the collisions with the boundaries and therefore will be anomalously small compared to the stretching factors for typical initial conditions. One must say that it looks unsatisfactory when the topological pressure of a system of many interacting particles is determined exclusively by a very rare process in which the only collisions occurring are with the boundaries. This obviously is a case where the long time asymptotics of the equations of motion in tangent space is completely irrelevant from the physics point of view. It is a clear example illustrating once more why the large system limit is both so hard and so interesting.

For $\beta < 1$ our conclusion that the topological pressure soon becomes dominated by orbits constrained to a denser than average part of space, does not carry over in this way to systems of many interacting particles. There are no stationary regions in such systems that will maintain a higher than average density forever. On the other hand, this phenomenon is a strong warning that similar behavior might very well occur in fluid systems. For example, if the phase space of a many particle system contains metastable regions with local stretching factors that are larger than the average stretching factor of a “typical” equilibrium region, the topological pressure for $\beta < 1 - \epsilon$ most likely will be determined by orbits constrained to one of these metastable regions. In such a case again, the topological pressure contains no information on the equilibrium properties of the system, but it is a fascinating idea that a study of the β -dependence of the topological pressure may reveal properties of the metastable states of a system. A concrete example where such dominance may be expected, in our opinion is provided by hard spheres at densities beyond solidification. For such densities there are many glassy states, as is known for example from experiments on colloidal systems [21]. It is very likely that the collision frequency in these glassy states is higher than in the crystalline state, and the corresponding stretching factor will be higher.

We also remark that it may be very helpful to use the Ruelle zeta-function not only for extracting the topological pressure from its pole, but also for studying its full z -dependence in more detail. For small, but not too small, z one might expect this function to exhibit the behavior of “typical stretching factors” in the bulk system. A possibility would be to examine various scalings of z with system size and to consider the behavior of the zeta-function in terms of its dependence upon the scaled parameter in the infinite system limit, much in the spirit of hydrodynamic scaling.

We also want to add some words of caution regarding the topological entropy, in other words the topological pressure for $\beta = 0$. For not even very large systems this value of β is far beyond the region in which the topological pressure is determined by bulk averages. Therefore, in disordered systems, the topological entropy, rather than revealing how the explored area in phase space of a typical trajectory bundle increases with time, will merely provide information, in most cases, about very atypical trajectory bundles, restricted to some small subspace of phase space.

Finally, we plan to extend the work reported here, not only to dilute gases of moving particles, but also to Lorentz gas systems with open boundaries and/or with driving fields combined with Gaussian thermostats.

ACKNOWLEDGMENTS

We are very pleased and honored to dedicate this paper to David Ruelle and Yasha Sinai, whose fundamental and fruitful contributions to the fields of dynamical systems theory and statistical mechanics, we greatly admire and heavily use. The authors thank the referee for calling their attention to the work of Burago, Ferleger, and Kononenko on the topological pressure of billiard systems, and for other helpful remarks. HvB acknowledges support by the National Fund for Scientific Research (F. N. R. S. Belgium) and by the Mathematical Physics program of FOM and NWO/GBE. JRD acknowledges support from the National Science Foundation (USA) under grant NSF-PHY-98-20824.

- [1] Ya. G. Sinai, Gibbs measures in Ergodic theory, *Russ. Math. Surveys* **27**, 21, (1972).
- [2] D. Ruelle, *Thermodynamic formalism*, Addison-Wesley Publishing Co., New York, (1978).
- [3] R. Bowen, *Equilibrium states and the ergodic theory of Anosov diffeomorphisms*, Lecture Notes in Mathematics, Vol. 470, Springer Verlag, Berlin, (1975).
- [4] P. Gaspard, *Chaos, scattering, and statistical mechanics* (Cambridge University Press, Cambridge UK, 1998).
- [5] C. Beck and F. Schlögl, *Thermodynamics of chaotic systems*, Cambridge University Press (Cambridge 1993).
- [6] A. Katok and B. Hasselblatt, *Introduction to the modern theory of dynamical systems*, Cambridge Univ. Press, Cambridge, (1995).
- [7] C. Appert, H. van Beijeren, M. H. Ernst and J. R. Dorfman, The thermodynamic formalism in the thermodynamic limit: diffusive systems with static disorder, *Phys. Rev.* **E54**, R1013 (1996).
- [8] C. Appert, H. van Beijeren, M. H. Ernst and J. R. Dorfman, Thermodynamic formalism and localization in Lorentz gases and hopping models, *J. Stat. Phys.* **87**, 1253 (1997).
- [9] I. M. Lifshitz, Energy spectrum of disordered systems, *Adv. Phys.* **13**, 483 (1964).
- [10] R. Griffiths, Nonanalytic behavior above the critical point in a random Ising ferromagnet, *Phys. Rev. Lett.* **23**, 17 (1969).
- [11] M. Donsker and S. R. S. Varadhan, Asymptotics for the Wiener sausage, *Commun. Pure Appl. Math.* **28**, 525 (1975); *ibid* **32**, 721 (1979).
- [12] Ya. G. Sinai, Dynamical systems with elastic reflections, *Russ. Math. Surveys*, **25**, 137 (1970).
- [13] N. I. Chernov, Decay of correlations and dispersing billiards, *J. Stat. Phys.* **94**, 513, (1999).
- [14] H. van Beijeren and J. R. Dorfman, Lyapunov exponents and KS entropy for the Lorentz gas at low densities, *Phys. Rev. Lett.* **74**, 4412 (1995).
- [15] H. van Beijeren, A. Latz and J. R. Dorfman, Chaotic properties of dilute two- and three-dimensional random Lorentz gases I: Equilibrium systems, *Phys. Rev.* **E57**, 4077 (1998).
- [16] D. Burago, S. Ferleger, and, A. Kononenko, Topological entropy of semi-dispersing billiards, *Ergodic Theory Dynam. Systems* **18**, 791, (1998).
- [17] J. Machta and R. Zwanzig, Diffusion in a periodic Lorentz gas, *Phys. Rev. Lett.* **50**, 1959 (1983).

- [18] P. Gaspard and F. Baras, Chaotic scattering and diffusion in the Lorentz gas, *Phys. Rev.* **E51**, 5332 (1995).
- [19] E. J. Heller, Bound state eigenfunctions of classically chaotic Hamiltonian systems: Scars of periodic orbits, *Phys. Rev. Lett.* **53**, 1515 (1984).
- [20] H. van Beijeren, J. R. Dorfman, H. A. Posch and Ch. Dellago, Kolmogorov-Sinai entropy for dilute gases in equilibrium, *Phys. Rev.* **E56**, 5272 (1997).
- [21] P. N. Pusey and W. van Meegen, Observation of a glass transition in suspensions of spherical colloidal particles, *Phys. Rev. Lett.* **59**, 2083, (1987).