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Thermodynamic Formalism and Localization in Lorentz Gases and Hopping Models

C. Appert,[1,3] H. van Beijeren,[1] M. H. Ernst,[1] and J. R. Dorfman[2]

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The thermodynamic formalism expresses chaotic properties of dynamical systems in terms of the Ruelle pressure $\psi(\beta)$. The inverse-temperature-like variable β allows one to scan the structure of the probability distribution in the dynamic phase space. This formalism is applied here to a Lorentz lattice gas, where a particle moving on a lattice of size L^d collides with fixed scatterers placed at random locations. Here we give rigorous arguments that the Ruelle pressure in the limit of infinite systems has two branches joining with a slope discontinuity at $\beta = 1$. The low- and high-β branches correspond to localization of trajectories on respectively the "most chaotic" (highest density) region and the "most deterministic" (lowest density) region, i.e., $\psi(\beta)$ is completely controlled by rare fluctuations in the distribution of scatterers on the lattice, and it does not carry any information on the global structure of the static disorder. As β approaches unity from either side, a localization–delocalization transition leads to a state where trajectories are extended and carry information on transport properties. At finite L the narrow region around $\beta = 1$ where the trajectories are extended scales as $(\ln L)^{-\alpha}$, where α depends on the sign of $1 - \beta$, if $d > 1$, and as $(L \ln L)^{-1}$ if $d = 1$. This result appears to be general for diffusive systems with static disorder, such as random walks in random environments or for the continuous Lorentz gas. Other models of random walks on disordered lattices, showing the same phenomenon, are discussed.

KEY WORDS: Lorentz lattice gases; chaos; thermodynamic formalism; random walks; localization transition.

[1] Instituut voor Theoretische Fysica, University of Utrecht, 3508 TA Utrecht, The Netherlands; e-mail: appert@lps.ens.fr.

[2] Department of Physics and IPST, University of Maryland, College Park, Maryland 20742.

[3] Permanent address: CNRS, LPS, Ecole Normale Supérieure, 75231 Paris Cedex 05, France.

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1. INTRODUCTION

In the past several years a large body of research has focused on the problem of relating the macroscopic behavior of nonequilibrium systems to the underlying chaotic dynamics of the particles of which the system is composed. Some macroscopic transport coefficients appearing in hydrodynamic-like equations have been related to microscopic quantities which characterize the chaotic properties of the system.[1-4] Ruelle, Sinai, and Bowen[5,6] introduced a powerful method to derive most of the interesting chaotic properties of a given system from a free-energy-type function, called the Ruelle or topological pressure. This *thermodynamic formalism* is based on a partition function calculated in a dynamical phase space. For systems governed by discrete, rather than continuous dynamics, one point in the dynamical phase space over t time steps consists of a trajectory $\Omega(t) = \{x_1, x_2, ..., x_t\}$ which is a set of t successive states of the system. The topological pressure $\psi(\beta)$ is defined as the infinite-time limit of the logarithm of the partition function divided by the time t, in a way similar to the definition of the free energy per particle in a canonical ensemble, in the thermodynamic limit. Again, in analogy with the methods of equilibrium statistical mechanics, there is an inverse temperature-like parameter β which allows one to scan the structure of the probability distribution for Ω.

This formalism has been successfully applied to Lorentz gases.[7-10] These are models in which independent light particles are moving among fixed scatterers. They can be considered as elementary models for diffusive transport in fluids and solids. In the continuous case, the effects of disorder in the configuration of scatterers can be taken into account and chaotic properties can be computed in the region of $\beta \approx 1$, as will be discussed in another paper.[11] The model can be simplified further by constraining the light particles to move on a regular lattice, and placing scatterers, with some density, at random locations on the sites of this lattice. Such models are called Lorentz lattice gases (LLGs). For some of these we already calculated the Ruelle pressure around $\beta = 1$ in the framework of a mean-field approximation.[8-10] For one-dimensional open systems on a lattice of size L we obtained the escape rate γ, the Lyapunov exponent λ, and the Kolmogorov–Sinai (KS) entropy, and found good agreement with independent direct numerical estimates of the same quantities.[8] All these quantities depend on the average density of scatterers ρ.

We have previously reported[12] that, for β different from unity, and for systems with static disorder, the Ruelle pressure has unexpected properties as L becomes large enough. In particular, in the thermodynamic limit, $L \to \infty$, it becomes independent of the density of scatterers. The cause of this is that, for large systems, the Ruelle pressure is completely determined by rare localized fluctuations in the configuration of scatterers. This peculiar behavior is expected to be general for all diffusive systems with static disorder, in any dimension. In this paper we develop the *analytical* arguments allowing for such a claim. The numerical counterpart will be presented in a separate paper.[13]

In the next sections we first describe the LLG model in more detail, and then introduce the thermodynamic formalism. Moreover, we will extend the results of ref. 12 to a mixed random walk model, and use it throughout the paper to illustrate the generality of our results. The main line of our calculation is to construct exact upper and lower bounds for the Ruelle pressure, which, as we will show, coincide in the thermodynamic limit, and are determined by rare configurations of scatterers, except in a small region about $\beta = 1$. We refer to this situation as localization of orbits on rare fluctuations of disorder. This means that the dominant contributions to the Ruelle pressure in the limit of large systems originate from orbits (points in the dynamical phase space) where the particle is restricted to move on those rare fluctuations, i.e., for $\beta < 1$, on the largest compact cluster of scatterers, and for $\beta > 1$ on the largest hole. We need, as a side result, the distribution function of the largest cluster size over all configurations, and the crude estimate of ref. 12 will be refined. The analysis of finite-size effects shows that the thermodynamic limit is approached extremely slowly, $\sim (\ln L)^{-\alpha}$, where α depends on the model and on the sign of $1-\beta$. For finite systems, we have estimated the β range around $\beta = 1$ in which the Ruelle pressure is still determined by trajectories extending over the whole system. As β is deviating more and more from unity, the orbits become more and more localized on the largest cluster or in the largest hole of the entire configuration. In one dimension, there is an intermediate state with "weak" localization (see Section 7).

The extension to continuous Lorentz gases is presented in Section 8.

2. LORENTZ LATTICE GASES

A 'light' particle moves ballistically in a finite simple cubic domain $\mathscr{D}$ having periodic or absorbing boundaries and containing $V = L^d$ sites of a d-dimensional cubic lattice. The allowed states of the system $x = \{\mathbf{r}, \mathbf{c}_i\}$ at time t ($t = 0, 1, 2,...$) are specified by the position $\mathbf{r} \in \mathscr{D}$ and the velocity $\mathbf{c}_i$ of the moving particle. The set of possible velocities $\mathbf{c}_i$ ($i = 1, 2,..., b$) connects each site to its b nearest neighbors, where the coordination number b equals $2d$ for a simple hypercubic lattice. A fraction ρ of the sites—chosen at random—is occupied by a scatterer or 'heavy' particle. The quenched configuration of scatterers is specified by the set of Boolean variables $\{\hat{\rho}(\mathbf{r}), \mathbf{r} \in \mathscr{D}\}$, where $\hat{\rho}(\mathbf{r}) = 1$ if site $\mathbf{r}$ is occupied by a scatterer, and $\hat{\rho}(\mathbf{r}) = 0$

if site $\mathbf{r}$ is empty. When the light particle hits a scatterer, it is scattered to one of the lattice directions with a probability that depends on its incident velocity. The scattering laws are further specified by introducing a transmission coefficient p, a reflection coefficient q, and, for hypercubic lattices, a deflection coefficient s, normalized as

$$p + q + 2(d-1)\, s = 1 \tag{1}$$

More formally, W_{ij} with $i, j = \{1, 2,..., b\}$ is the probability that the moving particle with incident velocity $\mathbf{c}_j$ is scattered to the outgoing velocity $\mathbf{c}_i$ with normalization $\sum_i W_{ij} = 1$. For instance, on a square lattice, the transition matrix has the form

$$W_{ij} = \begin{pmatrix} p & s & q & s \\ s & p & s & q \\ q & s & p & s \\ s & q & s & p \end{pmatrix} \tag{2}$$

The scattering at site $\mathbf{r}$ is described by the random transition matrix $\hat{W}_{ij}(\mathbf{r})$, which depends on the configuration of scatterers $\{\hat{\rho}(\mathbf{r}); \mathbf{r} \in \mathscr{D}\}$, and is given by

$$\hat{W}_{ij}(\mathbf{r}) = \hat{\rho}(\mathbf{r})\, W_{ij} + (1 - \hat{\rho}(\mathbf{r}))\, \delta_{ij} \tag{3}$$

At full coverage ($\rho = 1$) the moving particle performs a random walk with correlated jumps, referred to as the persistent random walk (PRW).[14]

The time evolution of this system, in a fixed configuration of scatterers, is described by the Chapman–Kolmogorov equation for the probability $\pi(x, t)$, with $x = \{\mathbf{r}, \mathbf{c}_i\}$, to find the moving particle at time t on site $\mathbf{r}$ with incident velocity $\mathbf{c}_i$, i.e.,

$$\pi(x, t+1) = \sum_y w(x \mid y)\, \pi(y, t) \tag{4}$$

In the case of absorbing boundary conditions, boundary states $y = \{\mathbf{r}', \mathbf{c}_j\}$ referring to a particle entering the domain $\mathscr{D}$ are excluded from the y summation. The transition matrix $w(x \mid y)$ represents the probability to go from state $y = \{\mathbf{r}', \mathbf{c}_j\}$ to state $x = \{\mathbf{r}, \mathbf{c}_i\}$, and is given by

$$w(x \mid y) = \delta(\mathbf{r} - \mathbf{c}_i, \mathbf{r}')\, \hat{W}_{ij}(\mathbf{r}') \tag{5}$$

The basic ideas of this paper are applicable to the much wider class of diffusive models with static disorder, such as hopping models with bond or site disorder,[15] as well as to continuous Lorentz gases (see Section 8). As the most immediate generalization of a LLG, we consider another model of a random walk, called a mixed random walk (MRW), in which a particle moves on a lattice filled by a random mixture of X types of scatterers. This model may be described by X scattering matrices of the form of Eq. (2), i.e., $W_{ij}^{(k)}$ with parameters p_k, q_k, s_k $(1 \leqslant k \leqslant X)$. The model contains the 'ballistic' LLG, described above, as the special case with $X=2$, $p_1 = 1 - q_1 = p$, and $p_2 = 1 - q_2 = 1$ or $W_{ij}^{(2)} = \delta_{ij}$. The scattering at site $\mathbf{r}$ in the MRW model is then described by the random transition matrix

$$\hat{W}_{ij}(\mathbf{r}) = \sum_{k=1}^{X} \hat{\rho}_k(\mathbf{r})\, W_{ij}^{(k)} \tag{6}$$

where $\hat{\rho}_k(\mathbf{r}) = 1$ if site $\mathbf{r}$ is occupied by a scatterer of type k, and zero otherwise.

Boundary conditions may be either periodic (closed system) or absorbing (open system) on the boundaries of domain $\mathscr{D}$, and the transition matrix satisfies the normalization relations

$$\sum_{x} w(x \mid y) \begin{cases} =1 & \text{(closed)} \\ \leqslant 1 & \text{(open)} \end{cases} \tag{7}$$

The inequality sign in (7) for *open* systems refers to the case where $y = \{\mathbf{r}, \mathbf{c}_i\}$ denotes a state at a boundary site $\mathbf{r}$ with nonentering velocity (boundary states with entering velocity do not occur). Indeed, the sum over x excludes states where the particle has escaped from the domain $\mathscr{D}$. Hence the probability for remaining inside the domain decreases when the particle finds itself on a boundary site.

3. THERMODYNAMIC FORMALISM

As stated in the introduction, the starting point for this paper is a partition function defined in the dynamic phase space whose points $\Omega(t)$ represent trajectories of t time steps:

$$Z_L(\beta, t \mid x_0) = \sum_{\Omega} [P(\Omega, t \mid x_0)]^{\beta} \tag{8}$$

where $P(\Omega, t \mid x_0)$ is the probability that the system follows a trajectory $\Omega(t) = \{x_1, x_2, \ldots, x_t\}$, starting from x_0 at $t=0$ in a given system of linear dimension $L = V^{1/d}$. The temperature-like parameter β allows us to scan the structure of the probability distribution P, where large positive and negative

β values select, respectively, the most probable and most improbable trajectories.[6] The concepts used in this section have been discussed in great detail in refs. 3 and 7.

In each specific system the probability $P(\Omega, t \mid x_0)$ for a given trajectory can be expressed in terms of the transition probabilities $w(x \mid y)$:

$$P(\Omega, t \mid x_0) = \prod_{n=1}^{t} w(x_n \mid x_{n-1}) \tag{9}$$

The partition function is determined by the properties of the matrix $w_\beta(x \mid y) \equiv [w(x \mid y)]^\beta$, which is defined by raising each matrix element $w(x \mid y)$ to the power β. For large times the partition function for almost all systems becomes independent of the initial point x_0 (ergodicity; see ref. 10), and is determined by the largest positive eigenvalue $\Lambda_L(\beta)$ of the matrix $w_\beta(x \mid y)$, which for ergodic systems can be shown to be nondegenerate.

There is a slight complication because hypercubic lattices are bipartite, i.e., the moving particle is always on even sites at even times and on odd sites at odd times, or vice versa. The system therefore consists of two independent ergodic components, which should be considered separately, and the matrix $w_\beta(x \mid y)$ is called a periodic matrix of period two.[16] To avoid these complications one may consider the time t to be an even integer multiple of the time step and then consider the matrix $w^2_\beta(x \mid y) = \sum_z w_\beta(x \mid z)\, w_\beta(z \mid y)$, defined between even or between odd sites only, to be the fundamental matrix. Again, the largest eigenvalue $[\Lambda_L(\beta)]^2$ of the matrix $w^2_\beta(x \mid y)$, restricted to one sublattice, is nondegenerate.

In addition, the topological or Ruelle pressure is defined as

$$\psi_L(\beta, \rho) = \lim_{t \to \infty} \frac{1}{t} \langle \ln Z_L(\beta, t \mid x_0) \rangle_\rho \tag{10}$$

where $\langle \cdots \rangle_\rho$ denotes an average over all configurations generated by the prescription that for each lattice site, independently, ρ is the probability that it will be occupied by a scatterer. The topological pressure is independent of x_0 if the system is ergodic, and can be expressed in terms of the largest eigenvalue $\Lambda_L(\beta)$ of the matrix w_β as

$$\psi_L(\beta, \rho) = \langle \ln(\Lambda_L(\beta)) \rangle_\rho \tag{11}$$

where we have taken the infinite-time limit inside the configurational average.

Several chaotic quantities can be derived from this function.[3,7] For example: the sum of all *positive* Lyapunov exponents is $\lambda \equiv \sum_i^{(+)} \lambda_i = -\psi'_L(1)$; the escape rate for open systems is $\gamma = -\psi_L(1)$; the Kolmogorov–

Sinai entropy follows from the generalization of Pesin's theorem to $h_{KS} = \psi_L(1) - \psi'_L(1)$; the topological entropy h_T satisfies $h_T = \psi_L(0)$; the Hausdorff dimension d_H of the repeller (the set of trajectories that never escape) for an open system is the zero point of the Ruelle pressure i.e., $\psi_L(d_H) = 0$. A prime in the above formulas denotes a β derivative.

4. UPPER AND LOWER BOUNDS

In this section the Ruelle pressure will be calculated in the limit of infinite system size, by constructing upper and lower bounds at finite L and analyzing their limiting behavior for large L. Consider first the *Lorentz lattice gas*. For a *closed* system it follows from the definition of $w_\beta(x \mid y)$ and Eq. (3) that

$$\sum_x w_\beta(x \mid y) = \hat{\rho}(\mathbf{r})\, W(\beta) + (1 - \hat{\rho}(\mathbf{r})) \tag{12}$$

with $y = \{\mathbf{r}, \mathbf{c}_i\}$ and

$$\begin{aligned} &W(\beta) \equiv a + b + 2(d-1)\, c \\ &a \equiv p^\beta, \qquad b \equiv q^\beta; \qquad cs^\beta \end{aligned} \tag{13}$$

For *open* systems the equality sign in Eq. (12) is replaced by a "less than" sign in case y is a boundary state. As a general upper bound, valid for both open and closed systems, we obtain

$$\begin{aligned} &\sum_x w_\beta(x \mid y) \leqslant W(\beta) \qquad (\mathbf{r} = \text{scattering site}) \\ &\sum_x w_\beta(x \mid y) \leqslant 1 \qquad\qquad (\mathbf{r} = \text{empty site}) \end{aligned} \tag{14}$$

If $\beta < 1$, this implies that $\sum_x w_\beta(x \mid y) \leqslant W(\beta)$ everywhere, as $W(\beta) \geqslant 1$. This inequality combined with Eqs. (8) and (9) yields

$$Z_L(\beta, t \mid x_0) \leqslant W(\beta)\, Z_L(\beta, t-1 \mid x_0) \leqslant (W(\beta))^t \tag{15}$$

Then the pressure, defined by Eq. (10), satisfies the inequality

$$\psi_L(\beta, \rho) \leqslant \ln W(\beta) \tag{16}$$

If $\beta > 1$, and consequently $W(\beta) \leqslant 1$, the analog of Eq. (15) becomes

$$Z_L(\beta, t \mid x_0) \leqslant 1 \tag{17}$$

and

$$\psi_L(\beta, \rho) \leqslant 0 \tag{18}$$

Equations (16) and (18) provide upper bounds for the Ruelle pressure for all β values.

To construct a lower bound to Z_L we consider clusters of scatterers, i.e., regions where every site is occupied by a scatterer, and select the cluster of largest size M. A cluster is said to have *size M* if the largest inscribed cube, oriented along the lattice directions, has a linear dimension M. If there are several largest clusters of the same size, just choose one arbitrarily. The value of M is well defined for any given configuration of scatterers.

As all terms in the sum (8) are nonnegative, any sum over a subset of trajectories will give an exact lower bound for Z_L. Let $Z_M^{\mathrm{RW}}(\beta, t \mid x_0)$ denote the sum over all trajectories which remain confined for t time steps to the largest inscribed cube of size M (again, if for a given cluster there is more than one inscribed cube of linear size M, choose one arbitrarily); then we have a lower bound:

$$Z_L \geqslant Z_M^{\mathrm{RW}} \tag{19}$$

In fact, Z_M^{RW} is equal to the partition function of a PRW in an open hypercubic domain with M^d sites. According to Eq. (11) this requires the largest eigenvalue $\Lambda_M^{\mathrm{RW}}(\beta)$ of the matrix $w_\beta(x \mid y)$ for the PRW, which can be found in refs. 13 and 17, and reads for sufficiently large M values

$$\Lambda_M^{\mathrm{RW}}(\beta) = W(\beta)\{1 - \Delta(\beta)\, k^2 + \mathcal{O}(k^3)\} \tag{20}$$

where $k^2 = \sum_{\alpha=1}^{d} k_\alpha^2$ and

$$\Delta(\beta) = \left(\frac{1}{2d}\right) \frac{a + (d-1)\, c}{b + (d-1)\, c} \tag{21}$$

Here k is the smallest wave number accessible to the system, i.e., $k = 0$ for a closed system (with periodic boundaries) and $k_\alpha \simeq \pi/M$ ($\alpha = x, y,..., d$) for an open hypercube (with absorbing boundaries). On the basis of Eqs. (11)

and (19) we find the first lower bound on the Ruelle pressure, valid for all β values:

$$\psi_L(\beta, \rho) \geq \langle \ln \Lambda_M^{\mathrm{RW}}(\beta) \rangle_\rho = \ln W(\beta) - \Delta(\beta) \langle d\pi^2/M^2 \rangle_\rho \tag{22}$$

If we can show that the moment $\langle 1/M^2 \rangle$ tends to zero when the system size increases, then this lower bound will tend to the upper bound (16) in the range $\beta < 1$. In the range $\beta > 1$, this lower bound will approach the finite, negative value $\ln W(\beta)$.

We need another lower bound which will tend to the upper bound (18) for $\beta > 1$. In order to find it, we consider for any fixed configuration the longest line segment free of scatterers. Contrary to the largest cluster defined above, the largest empty line segment is always a one-dimensional domain, whatever the dimensionality of the system is. Let $\bar{M}$ be the number of empty sites on this line segment and $\bar{Z}$ the partition sum (8) restricted to trajectories confined to this line segment. In fact, we keep only a single trajectory, which travels continually through the empty region and is reflected by the two scatterers at the end sites. For sufficiently large times the number of reflections is approximately $t/\bar{M}$.

The resulting sum is $\bar{Z} \simeq q^{\beta t/\bar{M}}$ and we have thus a second lower bound for the Ruelle pressure, valid for all β values,

$$\psi_L(\beta, \rho) \geq \beta (\ln q) \langle 1/\bar{M} \rangle_\rho \tag{23}$$

In summary, the following upper and lower bounds apply to all LLG's:

$$\begin{aligned} \ln W(\beta) - \Delta(\beta) \langle d\pi^2/M^2 \rangle_\rho \leq \psi_L(\beta, \rho) \leq \ln W(\beta) \qquad & (\beta < 1) \\ \beta (\ln q) \langle 1/\bar{M} \rangle_\rho \leq \psi_L(\beta, \rho) \leq 0 \qquad & (\beta > 1) \end{aligned} \tag{24}$$

The above bounds can be extended straightforwardly to the mixed random walk (MRW) models, where Eq. (12) becomes

$$\sum_x w_\beta(x \mid y) = \sum_{k=1}^{X} \rho_k(\mathbf{r}) \, W^{(k)}(\beta) \tag{25}$$

with $W^{(k)}(\beta)$, a_k, b_k, and c_k defined in a similar way as in Eq. (13).

The lower bounds Z_M^{RW} and $\bar{Z}_M^{\mathrm{RW}}$ are respectively determined by the largest cube of W^+-scatterers containing M^d scatterers, where W^+ is the type of scatterer for which $\ln W^{(k)}(\beta)$ is largest for a given β. The resulting upper and lower bounds in MRW models can then be summarized as

$$\ln W^+(\beta) - \Delta^+(\beta) \langle d\pi^2/M^2 \rangle_\rho \leq \psi_L(\beta, \rho) \leq \ln W^+(\beta) \tag{26}$$

The bounds for $\beta < 1$ contain the LLG as a special case; the bounds for $\beta > 1$ are different.

5. THERMODYNAMIC LIMIT

The goal of this section is to show that the upper bounds of Section 4 are indeed the asymptotic values for the Ruelle pressure in the limit of infinite systems ($L \to \infty$). To do so, we need to evaluate the inverse moments, $\langle M^{-k} \rangle$ ($k = 1, 2$), entering in Eq. (24), in the limit as $L \to \infty$. This requires the asymptotic behavior of the probability that the largest cluster is of size M.

We first consider the *one-dimensional* case where configurations are generated by distributing scatterers on the lattice sites according to the prescription that the occupation probability for each lattice site is ρ, independently of the other sites. Then the total number of scatterers N may fluctuate around its average value ρL. A crude estimate can be obtained by noticing that the average number of clusters of size m is approximately $L\rho^m(1-\rho)^2$. Indeed the cluster can be centered on L different positions on the lattice (or $L - m$ positions for an open system), it contains m scatterers, and is bordered by two empty sites. For m to be a typical value for the size of the largest cluster, the above expression must be of order unity, which implies that M scales as $\ln L$. For the inverse moments of M this implies $\langle M^{-k} \rangle \sim (\ln L)^{-k}$ for large L. Hence upper and lower bounds in Eqs. (24) approach the same limit.

This argument can be extended directly to higher dimensions. A cluster of size m (this means that the largest inscribed cube has side m) occurs roughly $L^d \rho^{m^d}$ times, where we used that for large m the probability of finding at least one empty site in each of the boundary hyperplanes is very close to unity. For L sufficiently large $L^d \rho^{m^d}$ is of order unity if $m^d \sim \ln L$. Consequently the inverse moments $\langle M^{-k} \rangle \sim (\ln L)^{-k/d}$ for $L \to \infty$.

The L dependence of the inverse moments can be obtained more rigorously by the following observation. We identify the clusters of size m, with $m \gg 1$, as "noninteracting molecules" of *species* m with partial densities $\{n(m) \simeq \rho^{m^d}; m = 1, 2,...\}$. The probability to find a volume of size $V = L^d$ unoccupied by clusters of size $> M$ is then

$$P(M) = \exp\left[-V \sum_{m > M} n(m)\right] \sim \exp[-L^d \rho^{M^d}] \tag{27}$$

Here we replaced the sum in the exponential by the first term, since the size of subsequent terms in the series decreases extremely rapidly. We also replaced $M + 1$ by M, which will induce some correction terms of relative order $(\ln L)^{-1/d}$ in the final expression (30). The probability that the largest cluster is exactly of size M is then $A(M) = P(M) - P(M-1)$, or in the continuum limit,

$$A(M) = P'(M) \sim -dL^d \ln(\rho)\, M^{d-1} \rho^{M^d} P(M) \tag{28}$$

For large L the inverse moments $\langle M^{-k} \rangle = \int_0^\infty dM\, M^{-k} A(M)$ can be evaluated asymptotically by a saddle-point method, as $A(M)$ is sharply peaked around its maximum. The maximum is located at M_0, which is the root of

$$[\ln A(M)]' = -dL^d(\ln \rho)\, M^{d-1} \rho^{M^d} + d \ln(\rho)\, M^{d-1} + (d-1)\, M^{-1} \tag{29}$$

For large M the solution of this equation is determined by the first two terms on the right-hand side (dominant balance argument), yielding

$$M_0 \simeq \left(\frac{d \ln L}{|\ln \rho|} \right)^{1/d} \tag{30}$$

with correction terms of relative order $(\ln L)^{-1/d}$. For large L the inverse moments behave asymptotically as

$$\langle M^{-k} \rangle \sim M_0^{-k} = \left(\frac{d \ln L}{|\ln \rho|} \right)^{-k/d} \tag{31}$$

in agreement with the crude estimate above.

In the preceding paragraphs the probability ρ of occupation of sites by scatterers has been kept fixed. It can be shown that the results (30) and (31) for the L dependence are still correct if one fixes the total number of scatterers N in all configurations.[18]

The above results can also be used to estimate the typical size $\bar{M}$ of the largest empty line segment. The distributions for scatterers and holes are symmetric by exchange of ρ and $1-\rho$. As we are interested in a one-dimensional domain, whatever the dimension d of the lattice, we have to replace M^d by $\bar{M}$. We straightforwardly obtain

$$\langle 1/\bar{M} \rangle = 1/M_0 \simeq -\frac{\ln(1-\rho)}{d \ln L} \tag{32}$$

We conclude therefore that in the thermodynamic limit $L \to \infty$, the moments $\langle M^{-k} \rangle$ vanish and thus the lower bounds of Section 4 converge

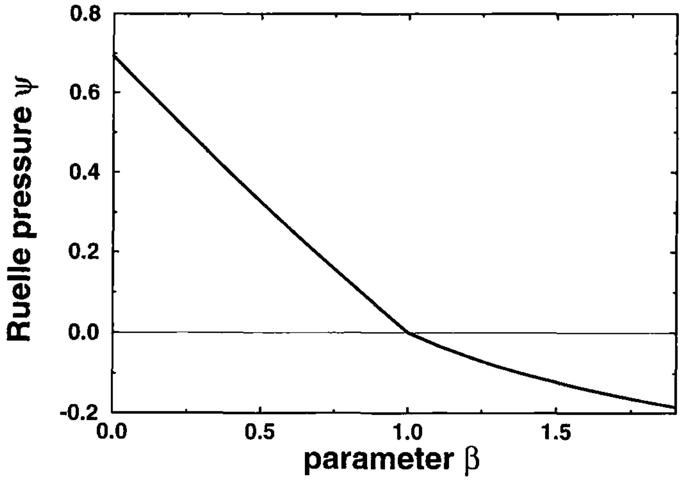

Fig. 1. Ruelle pressure for a MRW in a one-dimensional system of infinite size for $p_1 = 0.9$ and $p_2 = 0.7$. It is independent of the density of scatterers as long as p_1 or p_2 is not 0 or 1. Note the difference from the LLG, where the branch for $\beta > 1$ is $\Psi = 0$.

toward the L-independent upper bounds. This yields for the Ruelle pressure in LLGs in the thermodynamic limit

$$\lim_{L \to \infty} \psi_L(\beta, \rho) = \begin{cases} \ln W(\beta) & (\beta < 1) \\ 0 & (\beta > 1) \end{cases} \tag{33}$$

In the MRW models, the Ruelle pressure is

$$\lim_{L \to \infty} \psi_L(\beta, \rho) = \ln W^+(\beta) \tag{34}$$

as is illustrated in Fig. 1 for MRW models.

6. LOCALIZATION, EXTENSION TO MRWs

In the previous section we showed that the dynamic partition function and the Ruelle pressure of LLGs in thermodynamically large systems are completely determined by the rare fluctuations in the spatial distribution of scatterers. It is worth stressing again here that for the regions $\beta < 1$, $\beta = 1$, and $\beta > 1$, and $L \to \infty$, different sets of trajectories make the dominant contributions to the Ruelle pressure. For $\beta < 1$ the trajectories contributing to the partition function in a given configuration of scatterers are localized on the largest compact cluster of scatterers, i.e., localized in the "most chaotic" or "least deterministic" region. For $\beta > 1$ only a single trajectory contributes, which—on any d-dimensional lattice—is localized on the longest line segment that is free of scatterers, i.e., the relevant trajectory is localized in the "least chaotic" or "most deterministic" region of configuration space.

Therefore, as $L \to \infty$ the Ruelle pressure becomes independent of the configuration (except for atypical configurations such as strictly periodic ones); it is even independent of the density of scatterers (except at $\rho = 0$, where fluctuations no longer exist). It does not carry any information on the structure of the random medium.

Since for β different from unity, relevant trajectories do not explore the whole system but only a small part of it, the "mean-field configuration" with all scatterers more or less equidistant from one another is not at all a typical configuration. On the contrary, it is the one that gives, among all configurations, the minimal value for the Ruelle pressure. On the other hand, the maximal Ruelle pressure is obtained for the configuration where all of the scatterers form a single compact cluster. The average will be somewhere in between. This means that any calculation starting from a mean-field approximation will give very poor results for β values different from unity.[23]

However, at $\beta = 1$, the Ruelle pressure for the LLG and its derivatives with respect to β do depend on the overall density[8] and on more details of the total configuration of scatterers.[15] For *finite L*, this is also true in a small region around $\beta = 1$. There, relevant trajectories are extended or delocalized, and explore large regions of the lattice. This conclusion is based on the reasonably good agreement for escape rates and Lyapunov exponents between the results from computer simulations and mean-field calculations for the LLG.[8]

The same conclusions carry over to the MRW models, where in the thermodynamic limit the trajectories are localized on the largest compact cluster with $W^+(\beta)$-scatterers. At $\beta = 1$, all scatterers have the same $\ln W = 0$ and again trajectories are delocalized on the whole lattice. The structure of the typical mean-field configurations, contributing around $\beta = 1$, has not yet been explored, and mean-field estimates for the Lyapunov exponents in open systems have not yet been derived for MRWs.

Interesting new phenomena can occur near those values of $\beta \neq 1$ where different types of scatterers may have the same value of $\ln W$. For example, this occurs at $\beta = 0$ if all scatterers have the same number of nonzero scattering directions. Then the moving particle cannot distinguish between the different types of scatterers, and the relevant trajectories become again "delocalized" on a large cluster with a random mixture of the different scatterers with the same value of $\ln W(\beta)$. More explicitly, if there are X types of scatterers, it may occur that K $(2 \leqslant K < X)$ of them have the same ln W^+ strictly greater than the ln W for all other types of scatterers. Then the cluster of W^+-scatterers on which the relevant trajectories are localized contains a random mixture of these K types of scatterers.[15]

Suppose now that we consider, for $d>1$, a LLG or a MRW model that shows a percolation transition. In such a case it is important to note that the definition for the cluster size used here is not the number of connected sites, but the size of the largest inscribed hypercube, which typically is much smaller than the system size even for a percolating cluster. Thus the percolation transitions in such models have no effect on our considerations and the results of this paper remain valid.

7. THE DELOCALIZATION REGION

In this section we estimate the size of the delocalization region around $\beta=1$ in LLGs for finite systems. The Hausdorff dimension of the repeller (i.e., the set of trajectories which do not escape from the system after an infinite time) is a root of the Ruelle pressure,

$$\psi_L(d_{\mathrm{H}})=0 \tag{35}$$

For a large system, d_{H} is close to unity.[7] Using the facts that $\psi_L(1)=-\gamma\simeq Dd\pi^2/L^2$ for a hypercubic domain in d dimensions, where D is the diffusion coefficient, and $\psi'_L(1)=-\sum_{\lambda_i>0}\lambda_i\simeq-\lambda_\infty$, where λ_∞ represents the sum of positive Lyapunov exponents in the infinite-L limit, we find that the Hausdorff dimension d_{H} for a large hypercubic domain is, in first approximation,

$$d_{\mathrm{H}}\simeq 1-\left(\frac{D}{\lambda_\infty}\right)\frac{d\pi^2}{L^2} \tag{36}$$

where D and λ_∞ depend on the density of scatterers. Therefore, as the structure of the repeller is a fundamental feature of the system, the crossover region should extend at least over a β range of order $1/L^2$. On the other hand, we have concluded that for $L\to\infty$ and for β different from unity, the Ruelle pressure becomes independent of the global structure of the disorder, as the relevant trajectories become localized in regions of the lattice where rare fluctuations of high or low density of scatterers occur. This was demonstrated in previous sections in the limit of infinite systems. Therefore as long as the mean-field value of the Ruelle pressure or of the largest eigenvalue is smaller than the lower bound, the states of the system are localized. In fact, numerical results[13] support our intuition that the effect of localization can be estimated fairly well for any, large but finite system by taking the lower bounds in Eqs. (24) as estimates of the Ruelle pressure for $\beta < 1$ or > 1. Hence, for a given L crossover from localized to extended states occurs as we approach $\beta = 1$ from either side, when the mean-field value equals the lower bound.

To obtain an estimate of these crossover values, we compare the Ruelle pressure of the mean-field configuration with the estimate for the Ruelle pressure based on the lower bounds [see Eq. (22)]. It is equivalent to comparing the eigenvalues of the matrix w_β associated with a localized and with a delocalized eigenstate.

The second one is obtained for the "mean-field" configuration in LLGs from the PRW expression (20) by a rescaling argument.[8, 13] It reads

$$\Lambda_L^{\mathrm{MF}}(\beta) = (W(\beta))^\rho \, (1 - \rho\Delta(\beta)\, d(\pi/\rho L)^2) + \mathcal{O}(1/L^3) \tag{37}$$

with $W(\beta)$ and Δ defined in Eqs. (13) and (21).

For $\beta < 1$ localization takes certainly place if the lower bound on the Ruelle pressure is larger than the mean-field value, i.e.,

$$\ln W(\beta) - \Delta(\beta)\, d\pi^2/M_0^2 > \ln(W(\beta))^\rho + \mathcal{O}(1/L^2) \tag{38}$$

where the left-hand side is the lower bound given in Eq. (22) with $\langle M^{-2}\rangle \simeq M_0^{-2}$ on account of (31). The right-hand side is the mean-field value given by Eq. (37). By expanding both sides in powers of $\varepsilon \equiv 1 - \beta$, we find that the Ruelle pressure is determined by localized trajectories only if

$$\varepsilon > \varepsilon_- \equiv \frac{d\pi^2\, \Delta(1)}{\delta(1-\rho)\, M_0^2} \simeq \frac{d\pi^2\, \Delta(1)}{\delta(1-\rho)} \left[\frac{|\ln \rho|}{d \ln L}\right]^{2/d} \tag{39}$$

where $\delta = |p \ln p + q \ln q + 2(d-1)\, s \ln s| > 0$. We note that $d_{\mathrm{H}} = 1 - \varepsilon$ in Eq. (36) is indeed within the delocalized region, as was to be expected.

However, the crossover between localized and delocalized states may involve some intermediate states. In principle one might have a "weak localization" in a region of size M_1 (with $\ln L \ll M_1 \ll L$), where the local density $\rho + \Delta\rho$ is slightly larger than ρ, but where $\Delta\rho$ is large enough so that trajectories remaining confined to this region dominate the Ruelle pressure. To estimate the largest density fluctuation to be found in a region of size M_1 we first note that the probability for a density fluctuation $\Delta\rho$ in such a region can be estimated as $\exp(\mu\, \Delta\rho M_1^d)$, with μ the chemical potential of the scatterers (considered as lattice gas particles). Since the number of different regions of this size is on the order of L^d for M_1 in the above range, the largest density fluctuation occurring in one of these regions follows from the requirement $L^d \exp(\mu\, \Delta\rho M_1^d) \approx 1$, or

$$-\mu\, \Delta\rho M_1^d \sim \ln L^d \tag{40}$$

In a manner similar to (38) we compare the mean-field value $\psi_L^{\mathrm{MF}} \simeq \ln(W(\beta))^\rho$ with the mean-field estimate of the Ruelle pressure corresponding to trajectories confined in a region of average density $\rho + \Delta\rho$,

$$\psi_{M_1}^{\mathrm{MF}} \simeq \ln \left\{ [W(\beta)]^{\rho+\Delta\rho} \left[1 - \Delta(\beta) \frac{d\pi^2}{(\rho+\Delta\rho) M_1^2} \right] \right\} \tag{41}$$

Expressing $\Delta\rho$ in terms of M_1 according to (40) and expanding the difference $\psi_{M_1}^{\mathrm{MF}} - \psi_L^{\mathrm{MF}}$ to lowest order in ε yields a condition for "weak localization" in the most dense region of size M_1, namely

$$\psi_{M_1}^{\mathrm{MF}} - \psi_L^{\mathrm{MF}} \simeq \varepsilon \frac{\delta d \ln L}{M_1^d} - \frac{d\Delta(1)\pi^2}{\rho M_1^2} > 0 \tag{42}$$

By taking the estimate of the delocalization region in (39) one immediately sees that for $\varepsilon \ll (\ln L)^{-2/d}$, this inequality can only be satisfied in $d = 1$. Localization will occur on a region of size M_1 maximizing the difference (42) in Ruelle pressures. Differentiating (42) with respect to M_1 gives an M_1 that is proportional to $1/(\varepsilon \ln L)$. As long as this is $\ll L$, weak localization will occur. As soon as $\varepsilon \sim \varepsilon_{w} \equiv 2\Delta\pi^2/(\rho\,\delta L \ln L)$ the confinement region of the dominant trajectories becomes comparable to the full system and weak localization is no longer a meaningful concept. Hence, in one dimension one can distinguish in addition the weak localization regime $\varepsilon_{w} < \varepsilon < \varepsilon_-$. The region of full delocalization is narrowed down to $1 - \beta < \varepsilon_{w}$.

For $\beta > 1$ and $d > 1$, the crossover value can be determined by comparing the mean-field estimate with the lower bound (23) for the Ruelle pressure in the LLG, combined with Eq. (31), i.e.,

$$\beta \ln q/M_0 > \ln(W(\beta))^\rho + \mathcal{O}(1/L^2) \tag{43}$$

By expanding in powers of $\beta - 1 \equiv \varepsilon'$ we find localization for

$$\varepsilon' > \varepsilon'_+ \equiv \left(\frac{|\ln q|}{\rho\delta} \right) \frac{1}{M_0} \simeq \left(\frac{|\ln q|}{d\rho\delta} \right) \frac{|\ln(1-\rho)|}{\ln L} \tag{44}$$

For $d = 1$ one can show again, by using arguments similar to those above, that there is a region of weak localization where the density is slightly lower than average. This region occurs for β values given by $C'/(L \ln L) < \beta - 1 < \varepsilon'_+$, where C' is a positive constant.

In summary, the Ruelle pressure in LLG models is determined by extended or delocalized states if β is in the interval $\{1 - a_-/(\ln L)^{2/d}, 1 + a_+/(\ln L)^{1/d}\}$ for $d > 1$, and in the interval $\{1 - C/(L \ln L), 1 + C'/(L \ln L)\}$ for $d = 1$, where $a_\pm$, C, and C' are some positive constants.

8. EXTENSION TO CONTINUOUS SYSTEMS

Our considerations can be extended to the case of continuous Lorentz gases with static disorder. For $\beta < 1$, we expect the moving particle to be localized in a region of space with a high density of scatterers, while for $\beta > 1$ it should be localized in a large region where the density of scatterers is zero. To provide some qualitative explanations of this observation, we consider a Lorentz gas with hard spherical scatterers, the so-called non-overlapping Lorentz gas. Extension to overlapping scatterers or soft scatterers is possible, but will not be considered here. In the nonoverlapping Lorentz gas and $\beta < 1$ the Ruelle pressure approaches in the thermodynamic limit that of a closely packed system of hard spheres of diameter a. To understand this it suffices to bound the dynamical partition function by the contribution of all trajectories confined to a hypercubic volume of size M^d containing the centers of $\mathcal{N} \equiv \rho M^d$ scatterers. The probability of finding such a volume in the system can be estimated conservatively to be at least proportional to

$$\frac{V}{a^d} \frac{Q(N - \mathcal{N}, V - M^d)}{Q(N, V)} Q(\mathcal{N}, M^d) \tag{45}$$

By expanding the logarithm of the ratio of configurational partition functions in powers of the volume M^d of the hypercube (using $\mathcal{N} = \rho M^d$)—as the hypercube is a small subsystem of the total system with (N, V)—and noting on the other hand that the partition function $Q(\mathcal{N}, M^d)$ of the hypercube increases exponentially in M^d, we conclude that the probability in (45) is proportional to $(V/a^d) \exp(-\alpha M^d)$ with α some constant.

For any average density below the close-packing density this can be made of order unity by choosing M^d proportional to $\ln(V/a^d)$, which implies that for increasing V arbitrarily large volumes with a density arbitrarily close to the close-packing density can be found.

It is not clear what happens to the Ruelle pressure when all of the particles can move, as in fluids, for example, although it seems obvious that for $\beta > 1$, trajectories where the particles rarely collide will dominate the Ruelle pressure.

9. CONCLUSION

We conclude this paper with a number of remarks:

1. In this paper we have discussed the Ruelle pressure for diffusive models with static disorder. Our results indicate that for large systems and

for all but a small range of values of the inverse temperature-like parameter β, the Ruelle pressure is determined by rare fluctuations in the configuration of scatterers, and consequently carries no physical information on the chaotic scattering of the moving particle during its motion through the frozen-in disorder. Only in a narrow region around $\beta = 1$ does the thermodynamic formalism yield physically relevant information on the chaotic scattering in diffusive systems with static disorder. The extension to continuous systems outlined in ref. 12 has been made explicit here without having to use the usual tools of kinetic theory. The localization phenomena in the Ruelle pressure are in fact most similar to the asymptotic behavior (stretched exponential decay) of the survival probability of a random walk in a random array of absorbing traps. The survival probability is solely determined by the extremely rare fluctuation that the random walk finds itself in the largest region free of traps.[19]

In different areas of statistical physics analogous phenomena occur, where the large-time or the small-frequency/energy asymptotics are controlled by extremely rare spatial fluctuations, such as in Lifshitz tails,[20] Griffith's singularities,[21] and directed polymers.[22]

2. It has been shown numerically in one dimension[13] that for finite systems and outside the crossover region the lower bound found for the Ruelle pressure is also a good estimate for the pressure itself, indicating that localization on the largest cluster indeed occurs. We conjecture that in higher dimensions it is the largest *convex* cluster inscribed in a set of connected scattering sites that will determine the Ruelle pressure.

3. To allow the dynamical partition function to scan the full structure of our diffusive models with static disorder, time should be sufficiently large that the moving particle can explore the entire volume of the system. Consequently, $t \gg L^2$, which determines the physically relevant order of limits. In determining the Ruelle pressure in Eq. (8) one takes first the limit $t \to \infty$ for fixed L, and next allows L to tend to ∞. Therefore, for a fixed system size L, the trajectory has an infinite time to explore the system and to find the largest cluster, where it will then stay localized with a high probability. An interesting open problem remains to explore both the time and size dependence of the dynamical partition function, Eq. (8), to see how the various features discussed here are approached in the limit of infinite time, but finite size; to study diffusive behavior when the time is kept finite and the size of the lattice is allowed to become infinite; and to study the behavior of the dynamical partition function when both L and t approach infinity in some coupled manner.

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