Lyapunov exponents and the extensivity of dimensional loss for systems in thermal gradients

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An explicit relation between the dimensional loss (ΔD), entropy production, and transport is established under thermal gradients, relating the microscopic and macroscopic behaviors of the system. The extensivity of ΔD in systems with bulk behavior follows from the relation. The maximum Lyapunov exponents in thermal equilibrium and ΔD in nonequilibrium depend on the choice of heat baths, while their product is unique and macroscopic. Finite-size corrections are also computed and all results are verified numerically.

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I. INTRODUCTION

Fractal structures in phase space have become the focus of attention in the understanding of the relationship between microscopic dynamics and macroscopic nonequilibrium physics [1]. In the escape-rate formalism, the properties of a fractal repellor are known to govern the transport [2]. In contrast, in boundary-driven nonequilibrium steady states, the stationary distribution is generally fractal, but the precise connection to transport is not fully understood [1]. This reduction in dimension, ΔD, has been argued to be related to transport [3–5], although the only precise understanding arises in the weak field limit of the Lorentz gas [3]. The presence of fractals has been used to demonstrate how the second law of thermodynamics is consistent with time-reversal invariant, deterministic dynamics [6].

Dimensional loss is ubiquitous, present in dynamical, boundary-driven nonequilibrium steady-state microscopic simulations systems. Such systems include those in a thermal gradient set up through boundary heat baths, or those being sheared through moving walls. In all these cases, the accessible states in phase space contract onto a fractal set when transport is present. The difference between the equilibrium phase space volume and that in a given nonequilibrium steady state seems intimately connected to the transport process. In such dynamical approaches, the resulting transport requires the underlying phase space fractal to be present, and the corresponding loss of dimension which characterizes the fractal leads to the natural questions as to whether it is physically realizable macroscopically.

In this article, we derive a relation between the chaotic microscopic behavior of the system and the macroscopic transport properties. This relation clarifies properties regarding the *extensivity* of ΔD. Namely, what is the scaling behavior of ΔD with respect to the system size and what is the precise meaning of "extensivity" in boundary-driven systems? If the behavior can be demonstrated to be extensive, then one can understand how the results obtained in finite-size system simulations carry over to the bulk limit. This would then suggest how the dimensional loss in macroscopic nonequilibrium steady states is in principle observable. We try to elucidate these points for systems under thermal gradients.

II. RELATIONS BETWEEN DIMENSIONAL LOSS, LYAPUNOV EXPONENTS AND TRANSPORT

Many of the issues relating to ΔD require the understanding of the Lyapunov spectrum of the nonequilibrium system, whose analytic properties are known only in certain special cases [7]. Here, for ΔD, we use the Kaplan-Yorke dimension which is known to be consistent with other definitions of the attractor dimension for physically reasonable dynamical systems [1]. The precise definition of ΔD appears below. We study general Hamiltonians coupled to two heat baths at different temperatures at opposite sides of the system, generating heat flow. In Fig. 1 we illustrate some of the general features of boundary thermostatted systems.

We focus on dynamical thermostats of the Nosé-Hoover-type and its variants, which constitute one of the standard approaches to the study of physical systems out of equilibrium and are well studied. We will see that the type of heat baths chosen affect ΔD and the Lyapunov exponents, for the same boundary temperatures; in thermal equilibrium, two different boundary conditions can strongly modify the maximum exponent as well as the entire spectrum. Nevertheless, meaningful thermodynamic information can be extracted. In

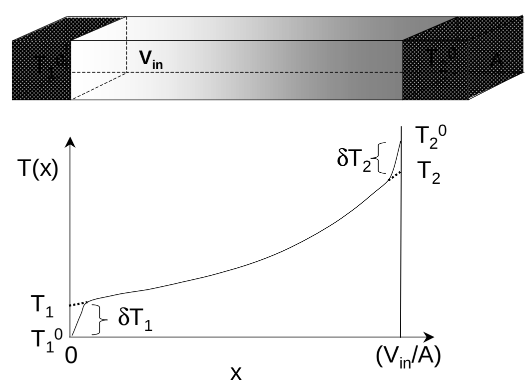

FIG. 1. (Top) Diagram of a system thermostatted (with finite regions) at both ends with internal system volume V_{in} and cross section A. The shading indicates the temperature variation within. (Bottom) The relation between the boundary temperatures T_i^0 ($i=1,2$), the actual temperatures just inside the system T_i, and the boundary temperature jumps δT_i. T_i are obtained by extrapolating the interior temperature profile $T(x)$ to the boundaries. Near equilibrium, $\delta T_1 = \delta T_2$.

this context, we investigate the meaning and the origins of extensivity of ΔD in systems with bulk behavior, including finite-size corrections, and relate them to transport. Our results are then verified numerically. We systematically study the system not only close to but also far from equilibrium, as well as the dependence on the heat baths themselves. While the extensivity of dimensional loss has been disputed due to the incompatibility with local equilibrium [3], we will see that this is not an issue.

ΔD has been studied previously for color conduction [3,8,9], sheared fluids [4,5,10] and thermal conduction [4], numerically. Analytic computations have understandably been restricted to small or idealized systems [3,7,11]. The physical properties are far from trivial; even whether ΔD generally arises has been an issue [12]. Extensivity of ΔD under thermal gradients has been analyzed [4], but the relation to transport and entropy production was not elucidated previously. Extensivity has been investigated in sheared fluids [5,9] and for color conductivity [8,9]. Study of the dependence on the number and types of thermostats or systematic analysis far from equilibrium have not been performed before.

Consider a system of volume V_{in}, with cross-sectional area A placed in contact with two heat baths at both ends having temperatures (T_1^0, T_2^0), as in Fig. 1. By *system*, we refer to the degrees of freedom not in direct contact with the bath, while *bath* refers to all thermostats and thermostatted degrees of freedom. The system and the bath give rise to D first order equations of motion. The Lyapunov spectrum $\{\lambda_j | \lambda_{max} \equiv \lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_D \equiv \lambda_{min}\}$ distills the microscopic properties of the system and the bath, describing how the classical trajectories diverge or converge over time in phase space. The Kaplan-Yorke fractal dimension D_{KY} is computed from the full spectrum as

$$\Delta D = D - D_{KY} = D - K + \frac{\sum_{j=1}^{K} \lambda_j}{\lambda_{K+1}}, \quad \sum_{j=1}^{K-1} \lambda_j \geqslant 0 > \sum_{j=1}^{K} \lambda_j, \tag{1}$$

ΔD is strictly positive in nonequilibrium, and $\Delta D = 0$ in equilibrium systems [1].

Since D_{KY} is a global quantity, we consider its expansion in terms of the heat flow in the system, J, which we shall now analytically derive near equilibrium. We show that

$$\frac{\Delta D}{V_{in}} = C_D J^2. \tag{2}$$

This relation shows precisely in what sense these systems are extensive, specifying how the dimensional loss scales with the system size. Here, C_D is a constant of proportionality whose explicit relation to other physical quantities is derived and given in Eq. (5). We note that for a given set of temperature boundary conditions, J is constant within the system because there are no heat sinks nor reservoirs inside. A few comments are in order. First, naively one might have thought it more natural to use ∇T instead of J. However, such an expression will be ambiguous since ∇T is in general *not* constant within the system, whereas J is, as explained above. Second, V_{in} denotes the (interior) volume of the system, which does not include the thermostatted boundaries. This is intuitively satisfying in that the thermal gradient exists solely in the interior of the system and the dimensional loss can be represented using the variables pertaining to it. It is important to note that the boundary thermostats can have fewer or even more degrees of freedom than the internal system, and its dependence will enter in a rather subtle manner, to be clarified below. Third, the system can have boundary jumps in temperature, δT, shown generically in Fig. 1 (bottom). These describe how the interior temperature profile $T(x)$, smoothly extrapolated to the boundaries, differs from the temperatures at the boundaries controlled by the heat baths. These have been quantitatively studied and we will also include these effects in the following analysis [14].

Let us systematically investigate how the extensivity of ΔD arises. The phase space contracts because the system is in nonequilibrium. This fact is reflected explicitly in a physical property of Nosé-Hoover thermostats and demons: The contraction rate onto the attractor, $-\sum_{j=1}^{D} \lambda_j$, is also the rate of entropy production, $\dot{S}$ [1,8]. We can use this to obtain a thermodynamic relation [13]

$$\sum_{j=1}^{D} \lambda_j = -\dot{S} = AJ\left(\frac{1}{T_1^0} - \frac{1}{T_2^0}\right), \tag{3}$$

As we approach equilibrium, J approaches 0 so that we can expand in powers of J as

$$\sum_{j=1}^{D} \lambda_j = \frac{V_{in} J^2}{\kappa T^2}\left(1 + \frac{2\alpha\kappa}{V_{in}}\right) + O(J^4), \tag{4}$$

where κ is the thermal conductivity and T represents the average temperature. In Eq. (4), we have included the effects of boundary temperature jumps that behave as $\delta T = \alpha J$ when the jumps are not too big [14]. α, which arises as a model-dependent finite-size correction, measures the efficacy of the heat baths (stochastic or deterministic), and can have significant effects as will be shown. Note that Eq. (3) holds both close to and far from equilibrium and is independent of the type and number of thermostats used.

The maximum Lyapunov exponent in the nonequilibrium system, λ_{max}, can be expanded around the thermal equilibrium value as $\lambda_{max} = \lambda_{max}^{eq} + O(J^2)$. Extensivity of ΔD depends on λ_{max}^{eq} being *independent* of V_{in} for large enough systems, although it can depend on T (we will see that this is the case; see Fig. 6 and further discussion below). In principle, it can also depend on the thermostats used and does, as we will see below. Close to equilibrium, the above behavior of $\sum_{j=1}^{D} \lambda_j$ and λ_{max}^{eq}, when combined, explain the extensivity of ΔD in Eq. (2). In this limit, the extensivity of ΔD arises from extensivity of $\sum_{j=1}^{D} \lambda_j$ and intensivity of λ_{max}^{eq}.

Possible thermostat dependence of λ_{max}^{eq} can give rise similar dependence of ΔD. Using the definition of D_{KY}, C_D can be derived in the $J \to 0$ limit:

$$C_D = \frac{1}{\kappa \lambda_{max}^{eq} T^2} \left(1 + \frac{2\alpha\kappa}{V_{in}} \right) \xrightarrow{V_{in} \to \infty} \frac{1}{\kappa \lambda_{max}^{eq} T^2} \qquad (5)$$

which relates macroscopic transport and entropy production to the microscopic ΔD. A subtlety needs to be mentioned: We find in model systems below that λ_{max}^{eq} is consistent with having a finite, large-volume limit but have not proven this statement analytically. In fact, this difficult issue is open and there have been somewhat conflicting results on the existence of the thermodynamic limit of λ_{max}^{eq} [15]. From our argument, we see that the extensive nature of ΔD requires that λ_{max}^{eq} have a thermodynamic limit or vice versa.

Computing ΔD requires the full Lyapunov spectrum, which becomes rapidly impractical for increasing system size. Close to equilibrium, this difficulty can be overcome as follows [5,8]. Define $\Delta D_{max}, \Delta D_{min}$ as

$$\Delta D_{max} \equiv -\frac{\sum_{j=1}^{D} \lambda_j}{\lambda_{max}}, \quad \Delta D_{min} \equiv \frac{\sum_{j=1}^{D} \lambda_j}{\lambda_{min}}, \qquad (6)$$

where $\lambda_{max}, \lambda_{min}$ are the maximum and minimum exponents. When $\Delta D \leqslant 1$, $\Delta D_{min} = \Delta D$ holds *exactly*. For systems with bulk transport properties, $\nabla T/T \sim A/V_{in}$ and $\Delta D/D \sim (A/V_{in})^2$ so that $\Delta D/D$ is always small for large systems and ΔD itself is small in one dimension. [For systems without a bulk limit, such as the one-dimensional (1D) FPU model, the dependence of $\nabla T/T$ can be anomalous, as well as display crossover behavior in temperature [16].] Since $\lambda_{min} = -\lambda_{max}$ in equilibrium, ΔD_{max} should also be a good approximation to ΔD, close to equilibrium. $\sum_{j=1}^{D} \lambda_j$ can be computed from the equations of motion alone and λ_{max} can be computed from evolving in addition one tangent vector, so these estimates are relatively simple to compute, and bound the behavior of ΔD.

III. ϕ^4 THEORY—A CONCRETE EXAMPLE

While the above theory is valid in any dimension, we now apply it to the 1D ϕ^4 theory described by the following Hamiltonian:

$$H = \sum_{x=1}^{L} \left[\frac{\pi_x^2}{2} + \frac{(\nabla \phi_x)^2}{2} + \frac{\phi_x^4}{4} \right]. \qquad (7)$$

Here, L is the total size of the system, including the thermostatted regions. We choose the ϕ^4 theory because it is a classic statistical model that naturally appears in broad physical contexts. Also, the statistical properties of the theory have been studied previously, including thermal transport which has bulk behavior [13,17]. We model the heat baths dynamically by applying Nosé-Hoover (NH) thermostats or their generalizations (demons) at the boundaries. The demons impose the finite temperature boundary conditions statistically as we integrate the equations of motion *deterministically*. The coupling strength of the demons do not affect the results below as long as the demons act effectively as thermostats. More details regarding the thermostats can be found in Ref. [13]. The interior includes the dynamics only of the ϕ^4 theory. Temperature is defined using the ideal gas thermometer, $T(x) = \langle \pi_x^2 \rangle$. The number of (heat-bath) boundary sites thermostatted on each end, N_B, will be varied. We employed one set of thermostats per thermostatted site. We ran the simulations using the fourth-order Runge-Kutta method to integrate the equations of motion with time steps of 10^{-3}–0.05 for 10^6–10^9 steps. We paid attention to understanding its convergence properties and also checked that the results do not change with the step size. To obtain the complete Lyapunov spectrum, we used the method explained in Refs. [18,8].

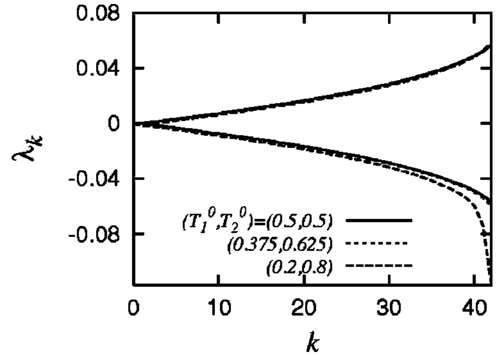

FIG. 2. Three sets of complete Lyapunov spectra for the ϕ^4 theory ($L = 41$) in equilibrium and nonequilibrium centered around $T = 0.5$. (The boundary temperatures are shown in the legend.) The exponents have been joined by lines.

Some examples of the Lyapunov spectrum for the ϕ^4 theory are shown in Fig. 2. We see that the spectrum is symmetric with under $\lambda \leftrightarrow -\lambda$ in equilibrium as it should be. In nonequilibrium, the spectrum has no analogous symmetry since the system is inhomogeneous [1]. Let us now look at the dependence of ΔD, ΔD_{max}, and ΔD_{min} with respect to J (Fig. 3). Each value of J represents a different temperature boundary condition. We see that close enough to equilibrium, all three quantities agree and display J^2 behavior as in Eqs. (2) and (5). Remarkably, even far from equilibrium and well into the nonlinear regime, ΔD has a robust J^2 behavior, but not $\Delta D_{max,min}$. We further note that the boundary tempera-

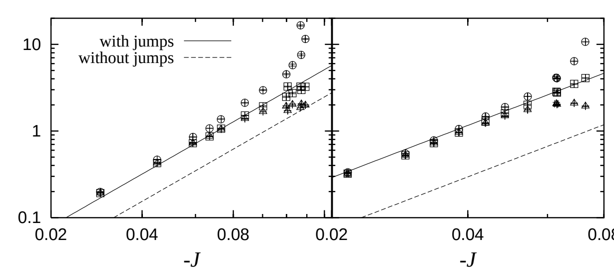

FIG. 3. ΔD(□), ΔD_{max} (○), and ΔD_{min} (△) against $-J$ in $L = 11$ (left) and $L = 41$ (right) at $T = 0.5$ for the $N_B = 1$ case. J^2 behavior with and without finite size corrections are also shown. ΔD displays J^2 behavior even for large $-J$ and Eq. (2) is readily verified for these systems. The need to include boundary jump corrections is evident as well.

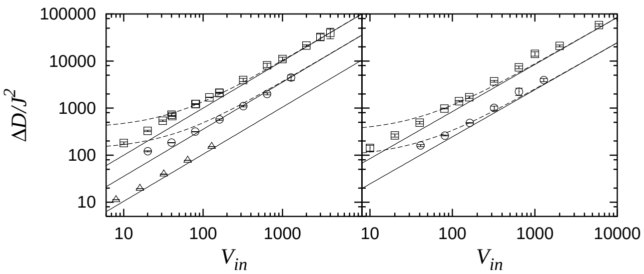

FIG. 4. (left) $\Delta D/J^2$ against V_{in} for $N_B=1$ (□), and $N_B=40$ (○), with NH thermostats (left) and demons (right) at $T=0.5$. $V_{in}/(\kappa\lambda_{max}^{eq}T^2)$ (solid) and $V_{in}/(\kappa\lambda_{max}^{eq}T^2)(1+2\alpha\kappa/V_{in})$ (dashes) are plotted. Application of the formulas to the data of Ref. [4] (△) also works very well (data and formulas rescaled by 5000 for plotting).

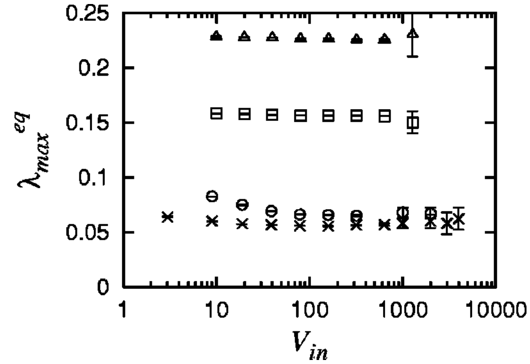

FIG. 6. System size dependence of λ_{max}^{eq} at $T=0.5$ for NH thermostats $N_B=1$ (×) and $N_B=40$ (□) and demons $N_B=1$ (○) and $N_B=40$ (△). We see that λ_{max} tend to constant values, within error.

ture jumps have a significant effect, the effect being larger for smaller T. This is because the mean free path of the excitations are larger for smaller T in the ϕ^4 theory [13]. For instance, using $\kappa=2.83(4)T^{-1.35(2)}$ and $\alpha=2.6(1)$, $2\alpha\kappa=300{,}6$ for $T=0.1{,}2$, respectively.

For each L, N_B, and T, we vary the temperature boundary conditions using the thermostats and obtain different values of J at the same average temperature T. Analyzing this data as in Fig. 3, we extract the proportionality constant $\Delta D/J^2$ for a particular value of L, N_B, and T. Further combining this data for various $V_{in}(=L-2N_B+1)$ and N_B, we find that relations (2) and (5) describe the results well over a few orders in magnitude as shown in Fig. 4. Here, both Nosé-Hoover thermostats and demons are used, and the size of the baths is varied from 1 to 40 sites on each side. The agreement of Eqs. (2)–(5) with the simulation is quite good. We have also included the data of Ref. [4] which used *stochastic* thermostats, and see that the formulas work quite well, demonstrating the robustness of relation (2).

A few subtleties can now be resolved. First, we can and have made the distinction between the total volume (which includes the thermostatted region) and V_{in} in Eq. (2), since we have performed analyses with $N_B=1$–40 sites. Second, C_D can and does depend on the type of thermostats used (demons or NH) and its number N_B as well as on T. C_D has similar behavior both for NH thermostats and demons, with the former being larger, and both decreasing with N_B. Furthermore, somewhat surprisingly, when we increase N_B by one, thereby *increasing* the total number of degrees of freedom by 6 (8) in the NH thermostat (demons) case, C_D *decreases* and so does ΔD for the same J. So the general trend, somewhat remarkably, is that as we increase the number of thermostats, the dimensional loss decreases for the same J. The reason for this will be clarified below.

We study examples of the behavior of $\Sigma_{j=1}^{D}\lambda_j$ in Fig. 5. We see that the entropy production relation Eq. (3) works well near and far from equilibrium, and that the quadratic behavior with respect to J can be observed close to equilibrium. This is true, *independently* of the type of thermostats used. As discussed above, λ_{max}^{eq} is independent of the system size for large volumes, as can be seen in Fig. 6. On the other hand, λ_{max}^{eq} can and does depend on the type of thermostats used as well as T (Figs. 6 and 7), explaining the thermostat dependence of C_D seen in Fig. 4. This might seem surprising at first in an equilibrium system. However, physical quantities, especially microscopic ones, can depend on the thermostats and they do in general. The larger λ_{max}^{eq} for demons and its increase with N_B are physically sensible since the existence of more thermostats lead to more chaotic behavior.

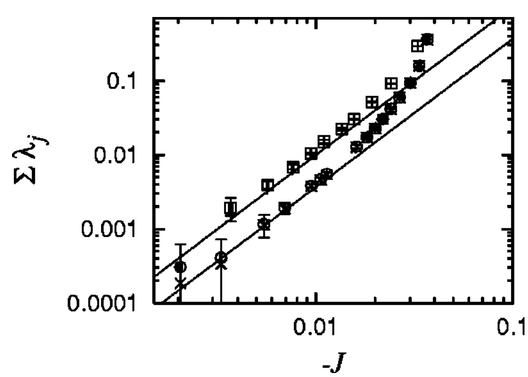

FIG. 5. $\Sigma_{j=1}^{D}\lambda_j$ and $J(1/T_1^0-1/T_2^0)$ against $-J$, for $T=0.5$ (□,+), $T=2$ (○,×), and their quadratic behavior Eq. (3) near equilibrium (solid) for the $L=162, N_B=1$ case. The quantities agree excellently.

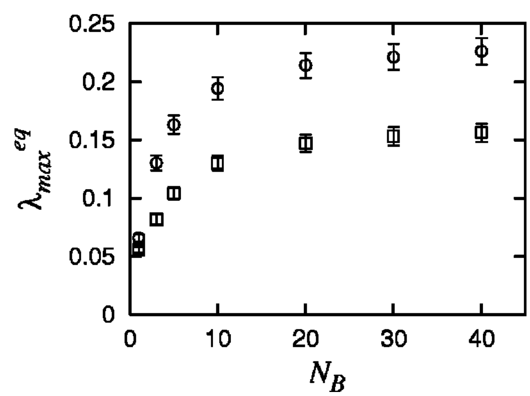

FIG. 7. The dependence of the λ_{max}^{eq} on N_B at $T=0.5$ for NH thermostats (□) and demons (○). This demonstrates that λ_{max}^{eq} is strongly heat-bath dependent, and is not uniquely determined by the local equilibrium conditions.

This is not obvious *a priori*, but increasing chaoticity decreases ΔD for the same T,J through Eq. (5).

IV. ESTIMATES FOR DIMENSIONAL LOSS

It is possible to establish the general conditions under which the loss of dimension is not more than one degree of freedom, $\Delta D \leqslant 1$. It is convenient to define the external environment through the ratio $r \equiv \Delta T/T$, where T is the central temperature and ΔT is the difference in the boundary temperatures. With this definition, $r \leqslant 2$, always, and $\nabla T \simeq rT/V_{in}$. Then, from Eqs. (2) and (5) we derive a simple estimate for how large the system must be in order to satisfy this dimensional loss condition:

$$\Delta D \leqslant 1 \Leftrightarrow V_{in} \geqslant \frac{\kappa(\nabla T)^2}{\lambda_{max}^{eq} T^2} \simeq r^2 \frac{\kappa}{\lambda_{max}^{eq}}. \tag{8}$$

Let us analyze $T=0.5$ case more concretely; the condition is most stringent for $N_B=1$ (NH) case, when λ_{max}^{eq} is the smallest. So we obtain the condition $V_{in}/r^2 \gtrsim 130$ for $\Delta D \leqslant 1$ and for large lattices, $V_{in} \gtrsim 400$, it should be satisfied for any gradient, which is consistent with our results. While we did not consider here the nonlinearity of the profiles, the boundary temperature jumps, and the nonlinearity of the response [14,19], we are in some sense close to equilibrium when $\Delta D \leqslant 1$ so that the rough arguments suffice for the purpose at hand.

For the case of small dimensional loss, specifically $\Delta D \leqslant 1$, we can ask how large the difference is between the actual dimensional loss ΔD and the upper-bound estimate ΔD_{max}. In this case, we need to consider $\lambda_{max} + \lambda_{min}$, which is zero in equilibrium since the Lyapunov spectrum is symmetric with respect to sign inversion [1]. As we move away from equilibrium, the behavior can be described by $\lambda_{max}/\lambda_{min} + 1 = C_\lambda J^2 + O(J^4)$. Then, for $\Delta D \leqslant 1$,

$$\frac{\Delta D_{max} - \Delta D}{\Delta D} \simeq C_\lambda J^2 \leqslant \frac{C_\lambda}{V_{in} C_D}. \tag{9}$$

For $N_B=1$, $T=0.5$, we have found through numerical simulations that $C_\lambda = 13L^{0.5}$, so that

$$\frac{(\Delta D_{max} - \Delta D)}{\Delta D} \lesssim 0.1 \left(\frac{V_{in}}{100} \right)^{-0.5}. \tag{10}$$

The statistical errors in the numerical computation of ΔD are typically at a few percent level, so when $\Delta D \leqslant 1$, we can see from this inequality that the difference between ΔD and ΔD_{max} is at most comparable to these errors, except for small systems. In Fig. 3, it can indeed be seen that for $\Delta D \leqslant 1$, ΔD_{max} agrees with ΔD within error. We further note that ΔD_{max} is a better approximation when the system size is larger so that $\Delta D/D$ is smaller, as seen in Fig. 3. Similar analysis can be applied at different T.

Perhaps a practical comment is appropriate: Computing ΔD from D_{KY} is a numerically intensive task for moderate sized systems, quickly becoming prohibitive for large systems since the necessary effort grows as $\sim D^2$. In contrast, the effort of computing ΔD_{max} grows only as $\sim 2D$, which is quite affordable for larger systems. These computations can complement each other, as was done here. Larger systems inevitably tend to be closer to equilibrium so that ΔD tend to be small and ΔD_{max} are good approximations to ΔD. One can further refine the computation by including the next largest Lyapunov exponent and so on, if need be. On the other hand, for small systems, ΔD_{max} in general is *not* a good approximation to ΔD but then the complete Lyapunov spectrum is obtainable so that ΔD can be computed without approximation.

V. SUMMARY AND DISCUSSION

We have derived the scaling properties of ΔD in systems with bulk behavior under thermal gradients in Eq. (2), thereby establishing precisely in what sense these systems are extensive, for a common class of dynamical thermostats. This extensivity explicitly relates the microscopic nature of phase space to the macroscopic transport properties as in Eq. (5) through entropy production. Previously, it was emphasized that the extensivity of ΔD is not compatible with local equilibrium so that it is questionable [3]. It is now known that systems such as ϕ^4 theory in $d=1$–3 display violations of local equilibrium under thermal gradients in a similar manner, as $\sim J^2$ [19]. This resolves the apparent conflict since the violations of local equilibrium emerge in a similar manner, and in conjunction with dimensional loss.

We further explicitly verified using numerical simulations that ΔD in ϕ^4 theory behaves extensively under various thermal gradients for $L \lesssim 10^4$ and its relation to transport. Relations (2), (3), and (5), however, are more general. We saw that the relations applied well to Ref. [4] which used *stochastic* thermostats in a different model. An application to dilute gas using the standard estimates of λ_{max} [1] yields

$$C_D \simeq \frac{2}{\rho v^2 \ln(4l/d)} \tag{11}$$

where ρ is the density, v is the average particle velocity, l is the mean free path, and d is the particle diameter. Then for $\boldsymbol{\nabla} T/T \sim 0.01\ \mathrm{m}^{-1}$, $\Delta D \sim 10^8\ (V_{in}/\mathrm{m}^3)$ at room temperature—quite large, yet far smaller than the total number of degrees of freedom.

We find the results satisfying from the physics point of view: Since ΔD pertains to the whole system, it includes the temperature profile which is curved in general, boundary temperature jumps and the various types of thermostats. Yet, ΔD can be related to macroscopic transport with the thermostat dependence cleanly separated into λ_{max}. Furthermore, ΔD has extensive behavior with respect to the internal volume wherein the system is manifestly in nonequilibrium. We have seen that λ_{max}^{eq} is not unique: In global thermal equilibrium, different choices of heat baths can lead to very different values. The result is that dimensional loss is not unique either, only the product $\Delta D\lambda_{max}^{eq}$ behaves macroscopically and can be related to thermodynamic quantities.

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