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Hamiltonian formulation of the Gaussian isokinetic thermostat

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We show that the Gaussian isokinetic thermostat used in nonequilibrium molecular-dynamics calculations can be derived from a Hamiltonian. An alternative variational approach involves geodesic motion in a curved space. We consider the implications of this result for the nonequilibrium Lorentz gas and thermostated systems in general. [S1063-651X(96)09209-4]

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I. INTRODUCTION

Nonequilibrium steady states involve a flow of energy through the system. For example, consider a conductor in an electric field. The energy supplied by the field must be removed to enable the system to approach a steady state. More precisely, the state of the system must be constrained to a compact region of phase space [1]. This may be obtained in one of two ways: An idealized heat bath may be included at the boundary or throughout the system. Stochastic methods are difficult to treat analytically, making it difficult to ensure that the thermostating effects have been modeled accurately, so most approaches in use today include some deterministic modification of either the boundary conditions, the equations of motion, or both.

Probably the most significant boundary approach has been the escape rate method of Gaspard and co-workers [2,3]. Here transport processes are modeled as deterministic systems with chaotic scattering. Transport coefficients are obtained in terms of the escape rate, which can then be related to the Lyapunov exponents and Kol'mogorov-Sinai entropy, which are microscopic properties of the underlying chaotic dynamics. An advantage of this approach has been that the dynamics is unchanged, thus Hamiltonian, and hence well understood. A disadvantage is that homogeneity has been lost, making simulation and interpretation more difficult.

Alternatively, the equations of motion may be modified by the addition of a ''thermostating'' term. This has the advantage of retaining homogeneity and gives the correct linear response [4]. There are a number of types of thermostat. The ones referred to in this paper are the Gaussian isokinetic (GIK), Gaussian isoenergetic (GIE), Nosé-Hoover isokinetic (NHIK), and Nosé-Hoover isoenergetic (NHIE) thermostats. All of these give the same averages and time correlation functions in the thermodynamic limit [5].

The NHIK thermostat is described at the beginning of Sec. II. The Gaussian thermostats are based on Gauss's principle of least constraint [6], as described in Chap. 3 of Ref. [4]. We want to modify the equations of motion so that the energy of the system remains bounded, despite the influence of an external force. This can be done by constraining the kinetic energy of the system to be constant, as in the GIK thermostat, or including both kinetic energy and internal potential energy, but not the potential energy associated with the external force, as in the GIE thermostat. Gauss's principle gives a prescription for doing this so that the force of constraint is a minimum along the trajectory.

The usual (Lagrangian and Hamiltonian) descriptions of classical mechanics are formulated in terms of variational principles, which allow a compact representation of the system by a single function, simplify perturbation theory, and make a connection with quantum mechanics. Gauss's principle is more general in that it gives the same results for systems with holonomic constraints, but does not have the same advantages as the Lagrangian and Hamiltonian approaches, so it has not had the same popularity.

Here we write down a Hamiltonian formulation of the GIK thermostat. This permits a large number of statements to be made about these systems, pertaining to conservation of phase volume, the symplectic structure of phase space, and so on. Related to this is a formulation in terms of geodesic motion in a curved space, which allows us to write down a variational formulation of the GIK equations. This has application in computing orbits of the system. The Hamiltonian approach also permits correspondences to be made between a GIK thermostat and other, nonthermostated, systems. Finally, it allows the possibility of a quantum description of these systems, which is discussed at the end of this paper. In short, it allows the GIK dynamics to be treated on a similar footing as more conventional dynamical systems, such as that used in the escape rate approach referred to above, while still retaining the advantages of homogeneity.

An obvious question that may be raised at this point is how the phase volume conservation of a Hamiltonian system is to be reconciled with the fact that thermostats cause phase-space contraction on the average. This is very important because it is related to the rate of entropy production of the nonequilibrium system. This contraction leads to steady distributions that are multifractal on phase space [7,8], although the support may have the same dimension as phase space [8]. The apparent contradiction is resolved by noting the distinction between *mechanical* and *canonical* momenta, familiar from the motion of a charged particle in a magnetic field [9]. Phase-space volume is conserved when written in terms of canonical momenta $\boldsymbol{\pi}$, but this need not be proportional to the velocity $\mathbf{v}$, which is used to define physically measurable parameters, such as the current.

There are a number of nonequilibrium molecular dynamics algorithms available for the various transport coefficients, described in Chap. 6 of Ref. [4]. All of these require a thermostating method of some kind. Of these, the SLLOD algorithm for determining the shear viscosity and the heat conduction algorithm are not (known to be) Hamiltonian systems before the thermostat is included in the equations of motion. The DOLLS algorithm (also for shear viscosity) is derived from a Hamiltonian, but does not give the correct response beyond linear order. It would be interesting to see whether either the Nosé or Gaussian thermostated dynamics for the DOLLS algorithm is derivable from a Hamiltonian; we defer this question to a future paper.

The self-diffusion coefficient may be evaluated by the color conductivity algorithm, which we are now going to describe. There are N particles interacting via a short-range potential Φ_{int} and subject to periodic boundary conditions. In addition, half of them have a positive ''color'' charge c and half have the opposite charge $-c$, which interacts with an external color field F, but not with each other. The Hamiltonian for this (unthermostated) system is

$$H_C=\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m_i}+\Phi_{\mathrm{int}}(\mathbf{q})-\sum_{i=1}^{N}c_iz_iF. \tag{1}$$

The response is the color current density

$$J_x=\frac{1}{V}\sum_{i=1}^{N}c_i\dot{z}_i. \tag{2}$$

It is clear that the designation ''internal'' and ''external'' is not really necessary at this stage; the last term in the Hamiltonian is of the same form as the second term and may be grouped together with it as a single potential. If we impose an isokinetic thermostat (described later) this remains the case, but an isoenergetic thermostat distinguishes between the two, conserving the sum of the kinetic energy and Φ_{int}.

If there are only two particles with equal masses and the center of mass fixed in the center of the box, the relative motion becomes that of a single-point particle in a periodic potential, subject to an external field. If the potential is that of a hard sphere, the problem is the same as the periodic nonequilibrium Lorentz gas [10–12], although usually the periodic array of hard spheres is taken to be hexagonal rather than the square lattice obtained using the usual periodic boundary conditions. The Lorentz gas is a model of electrical conduction and has been studied as a low-dimensional example of a nonequilibrium system.

The remainder of this paper is organized as follows. First we will formulate a one-parameter family of Hamiltonians that generate the dynamics of the GIK thermostat and show that it is equivalent to geodesic motion in a curved space. Then this approach will be applied to the nonequilibrium Lorentz gas, giving an alternative method of refining the periodic orbits. Finally, we will discuss this result in relation to different thermostats and the possibility of formulating a quantum theory.

II. HAMILTONIAN FORMALISM

There is one previous Hamiltonian formulation of a thermostated system, due to Nosé [13,14], the NHIK thermostat. The Hamiltonian for N particles moving in a potential Φ (which may contain both interactions between the particles and external fields) is

$$H_N(\mathbf{q},s;\boldsymbol{\pi},p_s)=\sum_{i=1}^{N}\frac{\boldsymbol{\pi}_i^2}{2ms^2}+\Phi(\mathbf{q})+\frac{p_s^2}{2Q}+(3N+1)k_BT\ln s, \tag{3}$$

where s is an additional degree of freedom, corresponding to an external reservoir, and Q is an arbitrary constant corresponding to the ''mass'' of the reservoir. The time variable that appears in the Hamilton equations of motion will be denoted by λ and does not correspond to real time. A connection is made with physically measured quantities by introducing a time $dt=d\lambda/s$ and momentum $\mathbf{p}_i=\boldsymbol{\pi}_i/s$, which are the physically measured time and momentum. Hoover [15] showed that by using these variables, it is possible to remove s and p_s from the equations of motion, which then become

$$\frac{d\mathbf{q}_i}{dt}=\frac{\mathbf{p}_i}{m}, \tag{4}$$

$$\frac{d\mathbf{p}_i}{dt}=\mathbf{F}_i-\zeta\mathbf{p}_i, \tag{5}$$

$$\frac{d\zeta}{dt}=\frac{1}{\tau^2}\left(\frac{K}{K_0}-1\right). \tag{6}$$

Here $\zeta=p_s/Q$ is the coefficient of a frictionlike force that plays a role similar to α, which appears in Gaussian thermostats (below). τ is a relaxation time that is related to Q, K is the total kinetic energy, and K_0 is the kinetic energy corresponding to the given temperature, that is, $(3N+1)k_BT/2$. The thermostat operates by increasing ζ whenever the kinetic energy rises too high, thus damping the motion. See Ref. [16] for more details of the calculation and its application to statistical mechanics. The NHIE thermostat can be defined by analogy with these equations [5]. The main points to note are that the Hamiltonian is associated with a nonphysical time scale and a scaled momentum and that the Nosé-Hoover thermostats correspond to the canonical ensemble of equilibrium statistical mechanics, in that the total kinetic energy fluctuates around a mean determined by the temperature of a heat reservoir.

Gaussian thermostats enforce the constancy of the energy directly in the equations of motion and thus correspond to the microcanonical ensemble of equilibrium statistical mechanics. They are derived from Gauss's principle of least constraint, as described in the Introduction. The equations take the form

$$\frac{d\mathbf{q}_i}{dt}=\frac{\mathbf{p}_i}{m_i}, \tag{7}$$

$$\frac{d\mathbf{p}_i}{dt}=\mathbf{F}_i-\alpha\mathbf{p}_i, \tag{8}$$

where $\mathbf{F}$ is the total force, given by a sum of interparticle forces $\mathbf{F}_{\mathrm{int}}$ and the external driving field $\mathbf{F}_{\mathrm{ext}}$. The thermostating multiplier α is determined by the condition that the energy is fixed identically as a consequence of the equations of motion. For the isokinetic thermostat the kinetic energy is fixed; for the isoenergetic thermostat the sum of the kinetic and internal potential energy is fixed. The value of α for the GIK thermostat is

$$\alpha=\frac{\Sigma_{i=1}^{N}\mathbf{F}_i\cdot\mathbf{p}_i}{\Sigma_{i=1}^{N}\mathbf{p}_i\cdot\mathbf{p}_i}. \tag{9}$$

The expression for α in the GIE case is the same, with the total force $\mathbf{F}$ replaced by the external force $\mathbf{F}_{\text{ext}}$.

These equations may be simplified by using $\mathbf{q}_i'=\mathbf{q}_i\sqrt{m_i}$, $\mathbf{p}_i'=\mathbf{p}_i/\sqrt{m_i}$, and $\mathbf{F}_i'=\mathbf{F}_i/\sqrt{m_i}$ to remove the mass from the equations. The potential energy Φ and thermostating multiplier α are unchanged by this transformation. In addition, for the case of a GIK thermostat *only*, we write $P^2=\Sigma_{i=1}^{N}\mathbf{p}'^2$, which is twice the kinetic energy, and hence a constant of the motion; then $t'=tP$, $\mathbf{p}_i''=\mathbf{p}_i'/P$, $\mathbf{F}_i''=\mathbf{F}_i'/P^2$, $\Phi'=\Phi/P^2$, and $\alpha'=\alpha/P$. Remove the primes from all the symbols and the equations become

$$\frac{d\mathbf{q}_i}{dt}=\mathbf{p}_i, \tag{10}$$

$$\frac{d\mathbf{p}_i}{dt}=\mathbf{F}_i-\alpha\mathbf{p}_i, \tag{11}$$

$$\alpha=\sum_{i=1}^{N}\mathbf{F}_i\cdot\mathbf{p}_i. \tag{12}$$

In these variables, the total kinetic energy is normalized to 1/2.

Now we come to the most important result of this paper: a one-parameter family of Hamiltonians that generate these equations:

$$H_\beta(\mathbf{q},\boldsymbol{\pi})=\frac{1}{2}e^{(\beta+1)\Phi}\sum_{i=1}^{N}\boldsymbol{\pi}_i^2-\frac{1}{2}e^{(\beta-1)\Phi}. \tag{13}$$

As before, Φ is the potential corresponding to the total force $\mathbf{F}$. Just as with the Nosé Hamiltonian (3), the physically measured time t and momentum $\mathbf{p}$ do not appear directly in the Hamiltonian; they are related to the Hamiltonian time λ and canonical momentum $\boldsymbol{\pi}$ by $dt=e^{\beta\Phi}d\lambda$ and $\mathbf{p}_i=e^{\Phi}\boldsymbol{\pi}$. These Hamiltonians are somewhat simpler than the Nosé Hamiltonian, especially in the special cases outlined below, and do not contain any extraneous variables. The conserved value of the Hamiltonian is zero and leads directly to the isokinetic constraint.

The phase-space contraction factor in the canonical variables is, of course, unity. Thus, for the simplest case ($\beta=0$) in which $\lambda=t$, the (constant) phase-space element is

$$\begin{aligned}\Gamma&=d^{3N}q\,d^{3N}\pi\,\delta(H-E)\\&=2e^{(3N-1)\Phi}d^{3N}q\,d^{3N}p\,\delta\left(\sum_i\mathbf{p}_i^2-1\right),\end{aligned}$$

with $E=0$. From this the physical phase-space compression factor is seen to be $e^{(3N-1)\Delta\Phi}$, which is easily shown to be the value obtained directly from the equations of motion, $\exp[-\int(3N-1)\alpha dt]$.

The value of β is completely arbitrary and does not affect the equations of motion; however, there are three particular values of β in which the canonical variables have a simple interpretation. The Hamiltonians with different β are not related by any of the usual types of canonical transformation since the time variables differ in each case.

When $\beta=-1$, the Hamiltonian reduces to the familiar form of kinetic plus potential energy. The thermostated equations are thus equivalent to a potential problem with zero total energy. Alternatively, any system of particles with purely attractive forces and zero total energy can be represented in terms of GIK thermostated dynamics. When $\beta=0$, the canonical and physical times are equivalent, so this is the most natural form in which to derive the thermostatted dynamics.

When $\beta=1$, the Hamiltonian takes a form equivalent to that of a geodesic in a curved space with metric $g_{\mu\nu}$, that is [17],

$$H_g(\mathbf{q},\boldsymbol{\pi})=\frac{1}{2}g^{\mu\nu}(\mathbf{q})\pi_\mu\pi_\nu, \tag{14}$$

where there is summation over repeated indices. Comparing this with $H_{\beta=1}$ and ignoring the constant, we see that GIK dynamics is equivalent to geodesic motion on configuration space with a metric given by

$$ds^2=e^{-2\Phi}\sum_{i=1}^{N}d\mathbf{q}_i^2. \tag{15}$$

In particular, the trajectory followed between two points in configuration space has extremal length with respect to the above metric. That is, given any two points in configuration space, the trajectory followed by the system is a minimum value of $\int ds$ among all trajectories from one point to the other. Occasionally it may be only a local minimum or even (for sufficiently pathological Φ) a maximum. We have also incidentally proved that the dynamics is time reversible, as there is no preferred direction along a geodesic.

Thus we have shown that the GIK thermostat is intimately related to more conventional dynamical systems, augmenting the link that has already been made between quadratic Hamiltonians and geodesic motion in a curved manifold [18].

III. THE LORENTZ GAS

The above discussion has been very general, applying to the color conductivity algorithm with any number of particles and any potential. Now we will apply it to the nonequilibrium Lorentz gas [10–12], which has only one particle and a particular (hard sphere) interaction, but still exhibits most of the features of larger nonequilibrium systems and in particular is chaotic. The result is a more intuitive understanding of the principles outlined above and alternative techniques for numerical and possibly experimental investigation of the nonequilibrium Lorentz gas. The $\beta-1$ form of the Hamiltonian for the Lorentz gas has been exhibited previously [19].

We begin with a study of the variational principle derived at the end of Sec. II. Consider a single particle moving in

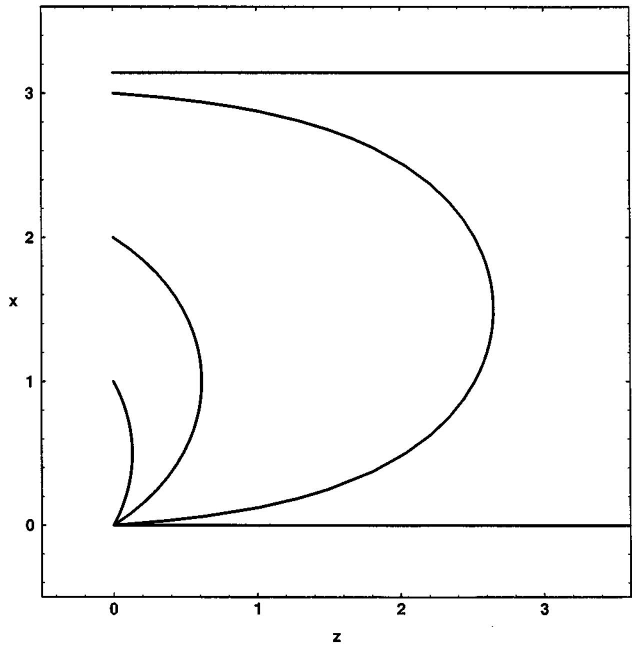

FIG. 1. Trajectories for the Lorentz gas at $\epsilon=1$ and a Δx between the end points of 1, 2, 3, and π.

three dimensions under the influence of a constant field $\mathbf{F}=-\epsilon\hat{\mathbf{z}}$. The potential is $\Phi=\epsilon z$. The GIK equations of motion (10)–(12), which in this case are identical to the GIE equations, can be solved analytically, leading to

$$\phi=\phi_0, \tag{16}$$

$$\tan\frac{\theta}{2}=\tan\frac{\theta_0}{2}\exp\frac{t-t_0}{\epsilon}, \tag{17}$$

$$x=x_0+\frac{\theta-\theta_0}{\epsilon}\cos\phi_0, \tag{18}$$

$$y=y_0+\frac{\theta-\theta_0}{\epsilon}\sin\phi_0, \tag{19}$$

$$z=z_0+\frac{1}{\epsilon}\ln\frac{\sin\theta}{\sin\theta_0}, \tag{20}$$

where a subscript zero indicates the initial value and $p_x=\sin\theta\cos\phi$, $p_y=\sin\theta\sin\phi$, and $p_z=\cos\theta$. The metric defined in Sec. II is

$$ds^2=e^{-2\epsilon z}(dx^2+dy^2+dz^2). \tag{21}$$

It does not depend on either x or y, so $\pi_x=e^{-\epsilon z}p_x$ is a constant of the motion (and similarly $e^{-\epsilon z}p_y$). This is not at all obvious from the equations of motion. Consider the trajectory between two points that differ by a separation in the x direction. This is shown in Fig. 1 for the case $\epsilon=1$. The intermediate points have larger values of z because lengths as defined by Eq. (21) are smaller for larger values of z. If, however, the separation of the two points is larger than π/ϵ, Eq. (18) shows that no trajectory exists between the two points, as the initial and final values of θ can differ by at most π. What has happened is that the total length of the path from a point to infinity along the z direction is finite and is equal to $e^{-\epsilon z}/\epsilon$. If the two end points are too far apart, the shortest path between the two points consists of two straight lines projecting from the points in the z direction.

The actual value of the length between any two points may be calculated analytically as a function of the initial and final coordinates, as follows.

(i) Solve Eqs. (18) and (19) for ϕ_0 and $\theta-\theta_0$.

(ii) Write Eq. (20) in terms of θ_0 and solve for θ_0 and hence θ.

(iii) Note that the length element reduces to

$$ds=e^{-\epsilon z}\sqrt{dx^2+dy^2+dz^2}=\frac{e^{-\epsilon z}}{\epsilon}\frac{\sin\theta_0}{\sin^2\theta}d\theta; \tag{22}$$

thus the total length is $e^{-\epsilon z}\sin\theta_0(\cot\theta_0-\cot\theta)/\epsilon$.

This approach may be applied to the calculation of the periodic orbits of the Lorentz gas. In addition to the free equations of motion described above, the particle undergoes elastic collisions with a periodic array of spherical scatterers. There is also a Lorentz gas where the scatterers are placed randomly [20]. For the periodic case, it is often useful to enumerate and locate the periodic orbits, which are used to calculate averages over the steady-state distribution, which is multifractal, owing to the contraction in phase space [11,12].

Suppose we have an approximate periodic orbit, obtained by integrating the system for a long time and selecting a part that almost returns to the same location after a small number of collisions. If there is a true periodic orbit close to the approximate one, the trajectory will be such that the length is minimized (locally), subject to the condition that the particle collides with the spheres in a sequence particular to that periodic orbit. There is one slight complication: a periodic orbit may not return to the initial sphere, but will continue making the same sequence of collisions, differing from the first by a translation. If this translation has a component in the z direction, the total path length of the second iteration of the orbit is not equal to the first and it is not clear exactly what should be minimized.

Let us denote the path length between two points, obtained by the above procedure, as $l(\Delta x,\Delta y,\Delta z,z_0)$. From this we can define the path length from sphere A to sphere B as $d(B,A)$, where there is implicit dependence on the two angles ϑ and φ needed to define the position on the spheres. d can be calculated from these angles, together with the translation vector, and the value of z of one of the spheres.

Now, given the end points of a trajectory on spheres A and C, the location on B can be determined by the condition that $d(B,A)+d(C,B)$ is a minimum and hence

$$\frac{\partial}{\partial\vartheta_B}[d(B,A)+d(C,B)]=\frac{\partial}{\partial\varphi_B}[d(B,A)+d(C,B)]=0\,. \tag{23}$$

There is a similar equation for the angles corresponding to C in terms of $d(C,B)+d(D,C)$ and so on, until the last point on the orbit, which we will denote Z. The equation determining Z is that $d(Z,Y)+d(A',Z)$ should be minimized. Similarly, the equation determining A' is that $d(A',Z)+d(B',A')$ be minimized. But $d(B',A')=d(B,A)\exp(-\epsilon\Delta z)$, where Δz is the change in z over the whole orbit. Thus the values of all the angles can be found simultaneously by minimizing

$$\left\{ \frac{\partial}{\partial \vartheta_B}[d(B,A)+d(C,B)] \right\}^2 + \left\{ \frac{\partial}{\partial \varphi_B}[d(B,A)+d(C,B)] \right\}^2 + \cdots + \left\{ \frac{\partial}{\partial \varphi_A}[d(A',Z)+d(B,A)\exp(-\epsilon\Delta z)] \right\}^2 . \quad (24)$$

The above expression is certainly very complicated, but it can be expressed analytically, which may be an advantage over current numerical techniques, which use root finding algorithms to locate a collision. Note that it is also a minimum even if the path length should turn out to be a maximum.

The one-particle problem also has direct relevance to some other systems, for which the thermostated dynamics is exact. For example, the above form of the metric is equivalent to Fermat's principle for light passing through glass with a refractive index $n=e^{-\epsilon z}$. In addition, the $\beta=-1$ form of the Hamiltonian is that of an electron moving in a potential $V=e^{-2\epsilon z}/2$ with a total energy of zero. This could be relevant to recent work on ballistic motion of electrons in semiconductors, where refraction effects can be observed [21]. Quantum-mechanical effects are also important here and are discussed below.

IV. DISCUSSION

In this final section, we will put the above results in the perspective of nonequilibrium statistical mechanics and seek a deeper understanding of the nature of thermostated systems. The first thing to note is that there is a distinct difference between a thermostat that preserves kinetic energy and a thermostat that preserves internal energy. They yield the same linear response, but differ in the microscopic features. Both the NHIK thermostat described above and the GIK thermostat admit a Hamiltonian description, but simple modifications of these Hamiltonians that we have tried do not generate isoenergetic thermostats, that is, it is easy to write down a Hamiltonian tht preserves internal energy. An example would be

$$H_{\mathrm{IE}}=\frac{1}{2}e^{2\Phi_{\mathrm{ext}}}\sum_{i=1}^{N} \boldsymbol{\pi}_i^2+\Phi_{\mathrm{int}}, \quad (25)$$

but this does not generate the GIE equations, as α can no longer be written $\Sigma_{i=1}^{N}\mathbf{F}_{\mathrm{ext}\,i}\cdot\mathbf{p}_i$; the denominator in Eq. (9) is no longer constant. Similarly, there is no known Hamiltonian formulation of the NHIE thermostat.

Another way of looking at the difference between isokinetic and isoenergetic constraints is to note the different manner in which the thermodynamical relations are satisfied. The rate of increase of the entropy of the thermal reservoir is $\dot{S}=\mathbf{J}\cdot\mathbf{F}/T$. The rate of decrease of the entropy of the system is equal to k_B multiplied by the phase-space contraction rate, which is $-(3N-1)\alpha$ for either type of thermostat. In the isokinetic case, these two have exactly the same magnitude at all times, whereas in the isoenergetic case, the equality is only evident after a long time average. In terms of a Hamiltonian, the total amount of phase-space contraction is obvious from the transformation used to relate the canonical variables to the measured ones. In the isokinetic case, this is a known function of Φ, while in the isoenergetic case, the average value of $-(3N-1)\alpha$ is path dependent.

Also, we note that recently the conjugate pairing rule has been proved for the GIK thermostat [22]. This is the statement that pairs of Lyapunov exponents sum to a constant C, so that, if λ is one exponent, then so is $C-\lambda$, with the exception of one or two of the exponents. The proof relies heavily on the isokinetic property and shows that the linear time evolution matrix always has a symplectic structure when represented using the correct basis. Our own computations show that simulations using a GIE thermostat obey the conjugate pairing rule, but there is no analytic treatment yet. Perhaps the pairing only occurs as the result of long time averaging.

Another important point relates to boundary conditions. For an equilibrium system, periodic boundary conditions may be used without affecting the Hamiltonian structure of the equations. All that happens is that $\mathbf{q}$ becomes a compact manifold. In our case, enforcing periodic boundary conditions results in abrupt changes in Φ, so that the Hamiltonian is not conserved. It is clear that the imposition of periodic boundary conditions breaks the global Hamiltonian structure, as multifractal attractors appear [8]. Nonetheless, it is still valid to view a periodic system as a Hamiltonian system with a potential that is in some sense periodic.

Finally, we consider the possibility of quantizing the thermostated dynamics. Quantum dissipative systems are an active area of research at present, using both canonical [23] and path-integral [24] quantization. In this paper we have an approach where the heat bath is not modeled explicitly; it appears classically as a deterministic modification of the equations of motion. Quantum mechanically, this means that the system can be expressed in terms of pure states rather than density matrices. In addition, the semiclassical techniques of Gutzwiller [25] and Cvitanovic *et al.* [26] become available. There are potential problems and ambiguities whichever value of β is used: if $\beta\neq-1$ there are ambiguities with regard to operator ordering, which occur also if the curved space representation is used; see Ref. [27], where an attempt is made to resolve such questions. If $\beta\neq 0$ the question arises as to whether the different times used in the formulation have any effect on the quantization, and if $\beta\neq 1$ the constraint $H=0$ must be implemented without trivializing the time evolution. Here also the issue of boundary conditions becomes of paramount importance. Nonetheless, it is clear that the physical systems referred to at the end of Sec. III can be consistently and uniquely quantized. Once these questions are resolved, we believe that a quantum treatment of the GIK thermostat would make an important contribution to the study of dissipative dynamics.

Note added in proof. A Hamilton containing an exponential was given for the Lorentz gas in Ref. [27].

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[1] D. Ruelle (unpublished).
[2] P. Gaspard and G. Nicolis, Phys. Rev. Lett. **65**, 1693 (1990).
[3] P. Gaspard and J. R. Dorfman, Phys. Rev. E **52**, 3525 (1995).
[4] D. J. Evans and G. P. Morriss, *Statistical Mechanics of Nonequilibrium Liquids* (Academic, London, 1990).
[5] D. J. Evans and S. Sarman, Phys. Rev. A **48**, 65 (1993).
[6] L. A. Pars, *A Treatise on Analytical Dynamics* (Heinemann, London, 1968).
[7] G. P. Morriss, Phys. Rev. A **39**, 4811 (1989).
[8] W. G. Hoover and B. Moran, Phys. Rev. A **40**, 5319 (1989).
[9] H. Goldstein, *Classical Mechanics* (Addison-Wesley, Reading, MA, 1980), p. 346.
[10] B. Moran and W. G. Hoover, J. Stat. Phys. **48**, 709 (1987).
[11] W. N. Vance, Phys. Rev. Lett. **69**, 1356 (1992).
[12] J. Lloyd, M. Niemeyer, L. Rondoni, and G. P. Morriss, CHAOS **5**, 536 (1995).
[13] S. Nosé, J. Chem. Phys. **81**, 511 (1984).
[14] S. Nosé, Mol. Phys. **52**, 255 (1984).
[15] W. G. Hoover, Phys. Rev. A **31**, 1695 (1985).
[16] S. Nosé, Prog. Theor. Phys. Suppl. **103**, 1 (1991).
[17] C. W. Misner, K. S. Thorne, and J. A. Wheeler, *Gravitation* (Freeman, San Francisco, 1973), p. 654.
[18] M. Szydłowski and M. Biesiada, Phys. Rev. D **44**, 2369 (1991).
[19] W. G. Hoover, B. Moran, C. G. Hoover, and W. J. Evans, Phys. Lett. A **133**, 114 (1988).
[20] H. van Beijeren and J. R. Dorfman, Phys. Rev. Lett. **74**, 4412 (1995).
[21] J. Spector, J. S. Weiner, H. L. Stormer, K. W. Baldwin, L. N. Pfeiffer, and K. W. West, Surf. Sci. **263**, 240 (1992).
[22] C. P. Dettmann and G. P. Morriss, Phys. Rev. E **53**, R5545 (1996).
[23] V. E. Tarasov, Theor. Math. Phys. **100**, 1100 (1994).
[24] N. Makri, J. Math. Phys. **36**, 2430 (1995).
[25] M. C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer, New York, 1990).
[26] P. Cvitanovic *et al.* (unpublished).
[27] A. Foerster, H. O. Girotti, and P. S. Kuhn, Phys. Lett. A **195**, 301 (1994).