Breaking conjugate pairing in thermostated billiards by a magnetic field

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We demonstrate that in the thermostated three-dimensional Lorentz gas, the symmetry of the Lyapunov spectrum can be broken by adding to the system an external magnetic field not perpendicular to the electric field. For perpendicular field vectors, there is a Hamiltonian reformulation of the dynamics and the conjugate pairing rule still holds. This indicates that symmetric Lyapunov spectra have nothing to do with time-reversal symmetry or reversibility; instead, it seems to be related to the existence of a Hamiltonian connection.

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I. INTRODUCTION

Thermostated dynamical systems have raised considerable interest recently as a testing ground for ideas in nonequilibrium statistical mechanics [1]. In particular, questions concerning the role played by chaotic dynamics in the appearance of nonequilibrium stationary states in dissipative systems have been in the focus of research activities [2]. One of the most remarkable features of these models is that they are dissipative *and* time reversal symmetric at the same time. Some, but not all, thermostated systems have another interesting common property known as the *conjugate pairing rule* (CPR): the Lyapunov exponents of the system form pairs summing up to the same (negative) value [3]. With the CPR, one pair of Lyapunov exponents is enough to determine the sum of *all* the exponents, which is known to be connected to the transport properties of the system [4]. The CPR is trivially present in conservative Hamiltonian systems (the sum being zero due to symplecticity); however, there is no obvious reason to expect anything similar in dissipative systems. In fact, the CPR in thermostated systems was first discovered by numerical studies [3].

The simplest system in which the CPR can be checked is the three-dimensional (periodic) Lorentz gas (3DLG): due to its three degrees of freedom, it has four nontrivial Lyapunov exponents. Dettmann *et al.* have shown numerically [5] that the 3DLG with an external electric field and a Gaussian isokinetic (GIK) thermostat exhibits conjugate pairing; later, this was proven analytically for conservative forces and hard-wall scatterers [6]. It has also been demonstrated [7] that this system can be connected to a Hamiltonian dynamics.

In this paper, we check the effect of an external magnetic field on the validity of the CPR in the GIK thermostated cubic lattice 3DLG. In particular, we will focus on two features possibly related to the CPR: reversibility (an extension of time-reversal symmetry) and the existence of a Hamiltonian formulation. Both can be controlled by the direction of the magnetic field with respect to that of the electric field and the lattice. Our numerical results show that the CPR is not affected by breaking reversibility, and it also holds for cases with perpendicular electric- and magnetic-field vectors for which there is a connection to Hamiltonian dynamics. However, the CPR breaks down for nonperpendicular fields, i.e., in the case when no Hamiltonian connection has been found.

In Sec. II, the equations of motion for billiards with a GIK thermostat in magnetic field are presented, together with a discussion of reversibility and the Hamiltonian connection for perpendicular fields. The numerical results for the 3DLG and our conclusions are presented in Secs. III and IV, respectively.

II. THERMOSTATED BILLIARDS IN MAGNETIC FIELD

A. The dynamics

The kinetic energy of a particle moving under the influence of external fields can be kept constant by adding a special frictionlike force to the system. Since this force can be deduced from Gauss's principle of least constraint, and it is kinetic energy that is kept constant, the technique is called the Gaussian isokinetic (GIK) thermostat [1]. In billiards, this is equivalent of particle momentum $\mathbf{p}$ changing only in direction, but not in magnitude p, during the ''free'' flights between collisions with the hard-wall boundaries. Choosing the unit of mass to be the mass of the particle, the corresponding equations of motion are

$$\dot{\mathbf{q}}=\mathbf{p}, \quad \dot{\mathbf{p}}=\mathbf{F}_e-\alpha\mathbf{p}, \tag{1}$$

where $\mathbf{q}=(x,y,z)$ is the position of the particle, $\mathbf{F}_e$ stands for the external forces, while the GIK thermostat corresponds to the choice

$$\alpha=\frac{\mathbf{F}_e\mathbf{p}}{p^2}. \tag{2}$$

For simplicity, we will choose length and time units in our studies so that $p=1$, but care must be taken when substituting 1 for p^2 in terms like α above, especially in the derivation of tangent space equations for the calculation of Lyapunov exponents.

In our model, the external force $\mathbf{F}_e$ contains the (constant) electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$:

$$\mathbf{F}_e=\mathbf{E}+\mathbf{p}\times\mathbf{B} \tag{3}$$

(we have defined the unit of electric charge to be that of the particle). The full dynamics also includes the secular collisions with the hard-wall boundaries, changing the momentum $\mathbf{p}_i$ to $\mathbf{p}_f$ instantaneously:

$$\mathbf{p}_f = (I - 2\mathbf{n} \circ \mathbf{n})\mathbf{p}_i, \tag{4}$$

where I is the (3×3) identity matrix, $\mathbf{n}$ is the normal vector of the boundary at the collision point, and ''$\circ$'' denotes the diadic product. In our 3DLG, the scatterers are hard spheres of radius R, arranged into a regular cubic lattice with distance d between the centers of nearest-neighbor scatterers. For simplicity, we choose the length scale so that $R=1$.

B. Reversibility

Without magnetic field, Eqs. (1) and (2) ensure time-reversal symmetry for the dynamics, which means that for each solution $\Gamma_+(t) = (\mathbf{q}(t),\mathbf{p}(t))^T$ there exists another one tracing the same path backward in time:

$$\Gamma_-(t) = (\mathbf{q}(-t), -\mathbf{p}(-t))^T. \tag{5}$$

The pairing of solutions by time-reversal symmetry is important in these models: it is used, e.g., in showing that the average current flows in the direction of the external electric field [8]. This symmetry cannot hold if $\mathbf{B}\neq 0$, but the more general property of *reversibility* [9] may still be true, depending on the particular choice of $\mathbf{E}$ and $\mathbf{B}$. Reversibility means the existence of a transformation G in phase space, which is an involution (i.e., G^2 is the identity) mapping each solution $\Gamma_+(t)$ to another one $\Gamma_-(t)$ in the following manner:

$$\Gamma_-(t) = G\Gamma_+(-t). \tag{6}$$

In terms of the phase-space flow ϕ^t defined by $\Gamma(t) = \phi^t\Gamma(0)$, this requirement can be written as

$$G\phi^t G = \phi^{-t}, \tag{7}$$

i.e., bracketing the flow by G ''reverses the direction of time.''

Ordinary time-reversal symmetry is equivalent to $G = G_0$ just flippping the direction of the momentum: $G_0(\mathbf{q},\mathbf{p}) = (\mathbf{q},-\mathbf{p})^T$. For $\mathbf{B}\neq 0$, the flow can be reversed by the transformation $G_B = MG_0$, where M is a mirroring of $\mathbf{q}$ and $\mathbf{p}$ with respect to the plane containing $\mathbf{E}$ and $\mathbf{B}$ (the proof of this statement is left to the Appendix). In the Lorentz gas, reversibility of the full dynamics also requires that the invariant plane of M be a symmetry plane of the lattice, too. This gives us an easy way to control reversibility in the Lorentz gas: choosing directions for $\mathbf{E}$ and $\mathbf{B}$ in a symmetry plane of the lattice leads to reversible dynamics, otherwise we have no reversibility.

C. Hamiltonian formalism

A nontrivial result for GIK thermostated systems without magnetic field is that a Hamiltonian formulation of the dynamics exists provided the force $\mathbf{F}_e$ is the gradient of a scalar field $-\Phi(\mathbf{q})$ [7]. Then there is a Hamiltonian $H(\mathbf{Q},\mathbf{P})$ so that the GIK equations of motion for the physical variables $\mathbf{q}$ and $\mathbf{p}$ can be obtained from the canonical equations of motion for $\mathbf{Q}$ and $\mathbf{P}$ through a suitable coordinate transformation. It is straightforward to check that the Hamiltonian $H(\mathbf{Q},\mathbf{P}) = \frac{1}{2}[e^{\Phi}\mathbf{P}^2 - e^{-\Phi}]$ has canonical equations leading to Eq. (1) if one assumes the transformations $\mathbf{q}=\mathbf{Q}$ and $\mathbf{p} = e^{\Phi}\mathbf{P}$. However, it is important to stress that this connection holds only if we make explicit use of the constraint $p=1$ and its equivalent $H=0$ in the GIK and canonical equations, respectively.

The extension of the Hamiltonian formulation to cases with $\mathbf{B}\neq 0$ is not as obvious as for conservative systems because of the factor e^{Φ} in front of $\mathbf{P}^2$ in the ''kinetic-energy'' term of the Hamiltonian. Nevertheless, we may still follow a similar route by defining $\Phi(\mathbf{q})$ through $\mathbf{E} = -\boldsymbol{\nabla}\Phi$ as usual and replacing $\mathbf{P}$ by $\mathbf{P}-\mathbf{a}(\mathbf{q})$ in H, where the vector $\mathbf{a}(\mathbf{q})$ is connected to the magnetic field. This leads to the Hamiltonian

$$H_B(\mathbf{Q},\mathbf{P}) = \tfrac{1}{2}[e^{\Phi}(\mathbf{P}-\mathbf{a})^2 - e^{-\Phi}]. \tag{8}$$

A lengthy but straightforward calculation shows [10] that the canonical equations for $H_B=0$ can be connected to the GIK equations of motion for $p=1$ by the transformation

$$\mathbf{q}=\mathbf{Q}, \quad \mathbf{p} = e^{\Phi}(\mathbf{P}-\mathbf{a}) \tag{9}$$

if we assume the following relationship between $\mathbf{B}$ and $\mathbf{a}$:

$$\mathbf{B} = e^{\Phi}\,\mathrm{rot}\,\mathbf{a}. \tag{10}$$

Note that this is an extension of the usual relationship $\mathbf{B} = \mathrm{rot}\,\mathbf{a}$ for the GIK thermostat. However, due to the presence of e^{Φ} in Eq. (10), we do not necessarily have a solution $\mathbf{a}$ for arbitrary $\mathbf{E}$ and $\mathbf{B}$. Indeed, since $\mathbf{B}$ must satisfy Maxwell's equation $\mathrm{div}\,\mathbf{B}=0$, this condition leads to the restriction $\mathbf{EB}=0$. Therefore, we can use the Hamiltonian formulation given above only in the case when $\mathbf{B}$ is perpendicular to $\mathbf{E}$.

III. NUMERICAL RESULTS

We have calculated numerically the Lyapunov spectrum of the GIK thermostated 3DLG with constant electric and magnetic fields. The Lyapunov exponents $\lambda_1 > \lambda_2 > \cdots > \lambda_6$ can be measured by following the evolution of a full set of linearly independent tangent space vectors along a very long trajectory and applying repeated reorthogonalization and rescaling to them; see Ref. [11] for a detailed description of this method. Collisions were taken into account by the formula presented in Ref. [12], with suitable modifications to include the effect of the magnetic field. In all cases studied, we have obtained finite time exponents converging to their infinite time limits, as in the example plotted in Fig. 1. The fluctuations in the measured values typically tend to zero as $1/\sqrt{N}$, where N is the number of collisions, so for reliable results we needed very long runs with $N=10^7$ collisions or more. The data also show that the largest Lyapunov exponent is positive, i.e., the motion is chaotic, and that two of the exponents are zero as expected.

We have chosen the coordinate axes x, y, and z aligned with the lattice axes. Through the directions of the field vectors, we can have reversible or nonreversible dynamics in our model, with or without a Hamiltonian representation, independently. In the simulations, we fixed $\mathbf{E}$ along the x axis, so that it lies in the symmetry planes $y=0$ and $z=0$, and controlled the above properties by chosing the direction of $\mathbf{B}$ accordingly. In particular, the dynamics is reversible, e.g., for $B_y=0$; meanwhile, there exists a Hamiltonian formulation as given in Sec. II C for $B_x=0$.

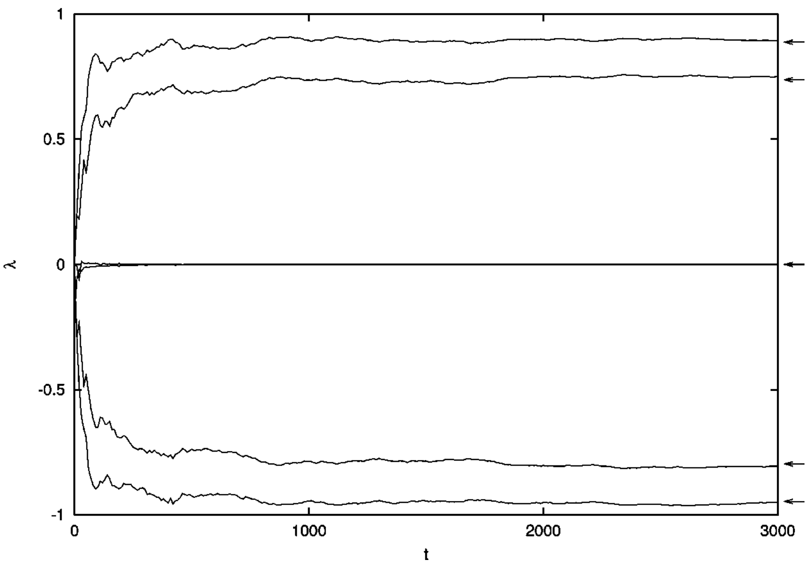

FIG. 1. Time evolution of the measured Lyapunov exponents $\lambda_1 > \lambda_2 > \cdots > \lambda_6$ in the 3DLG, in dimensionless variables defined in Sec. II A. The scatterers are balls with radius $R=1$ arranged in a cubic lattice with lattice constant $d=2.3$. The external fields are $\mathbf{E}=(0.3,0,0)$ and $\mathbf{B}=(0,0.5\cos\phi,0.5\sin\phi)$ with $\phi=\pi/20$. The arrows show the long-time values of the exponents ($t=10^8$); λ_3 and λ_4 converge to 0 as expected.

Figure 1 shows the results of a simulation for $\mathbf{B}=(0,B\cos\phi,B\sin\phi)$ with $\phi=\pi/20$, i.e., for perpendicular fields and *without* reversibility. In Fig. 2, we plotted the Lyapunov pair sum $s_1=\lambda_1+\lambda_6$ and its deviation from the other sum $s_2=\lambda_2+\lambda_5$ as functions of time. The sums converge to the same value, thus the CPR seems to hold in this case. It is also worth noticing that the difference $\Delta(t)=s_1(t)-s_2(t)$ disappears much faster (approximately as $1/t$) than the fluctuations in the individual sums. We have obtained similar results for other values of the angle ϕ, including reversible flows (e.g., $\phi=0$). These results demonstrate that reversibility is not needed for the CPR to hold.

In the second type of simulations, we have chosen $\mathbf{B}=(B\sin\phi,0,B\cos\phi)$, so that for $\phi\neq 0$ the two field vectors are not perpendicular and the Hamiltonian formulation of Sec. II C does not apply. The numerical Lyapunov spectrum looks qualitatively the same as in Fig. 1, but the sums s_1 and s_2 seem to converge to different values as shown in Fig. 3 for the angle $\phi=7\pi/20$. In other words, the CPR is broken in this case; other values of $\phi\neq 0$ have led to similar results. The difference between Figs. 2 and 3 is very clear: the quantity Δ converges to zero quite fast if the CPR holds, while it stays definitely away from zero in the case without the CPR.

IV. CONCLUSIONS

We have demonstrated that in the GIK thermostated 3DLG, the CPR can be broken by an external magnetic field that is not perpendicular to the electric field. For perpendicular fields, however, the CPR holds, and the convergence of the pair sums to each other seems to be much faster than that of the sums to their long-time value, indicating that the CPR is valid for all times in these cases just as in the 3DLG without magnetic field [5]. This phenomenon is called the *strong* CPR. The perpendicular cases are also characterized by the existence of a Hamiltonian formulation. There exist other nontrivial examples for systems with the strong CPR and a Hamiltonian formulation, too: e.g., the Gaussian isoenergetic thermostat with a special interparticle potential [13] or the ideal Sllod gas [14,10]. These examples suggest that there may be a direct connection between the strong CPR and the existence of a Hamiltonian formulation. We will examine this question in a separate paper [10]. Although we are not aware of any counterexamples, the question concerning

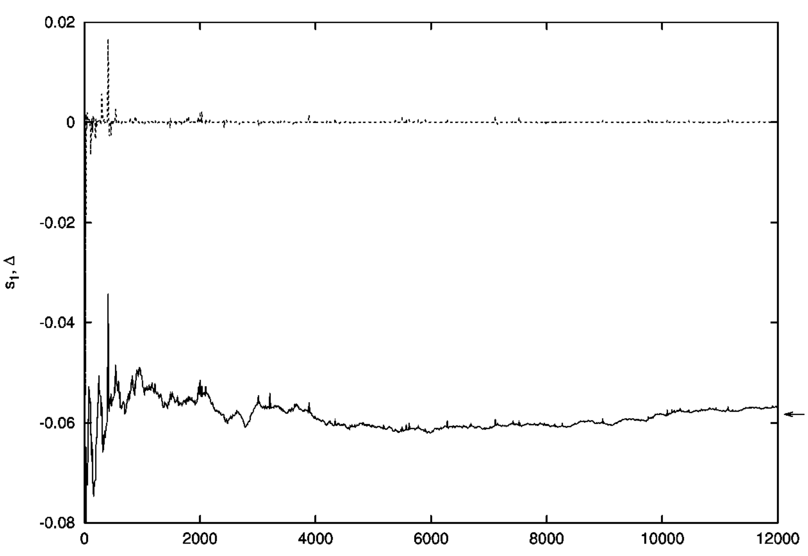

FIG. 2. Time evolution of the sum $s_1=\lambda_1+\lambda_6$ (solid line) and its deviation Δ from $s_2=\lambda_2+\lambda_5$ (dotted line) obtained for the same parameters as in Fig. 1. The arrow shows the long-time value of the sums ($t=10^8$).

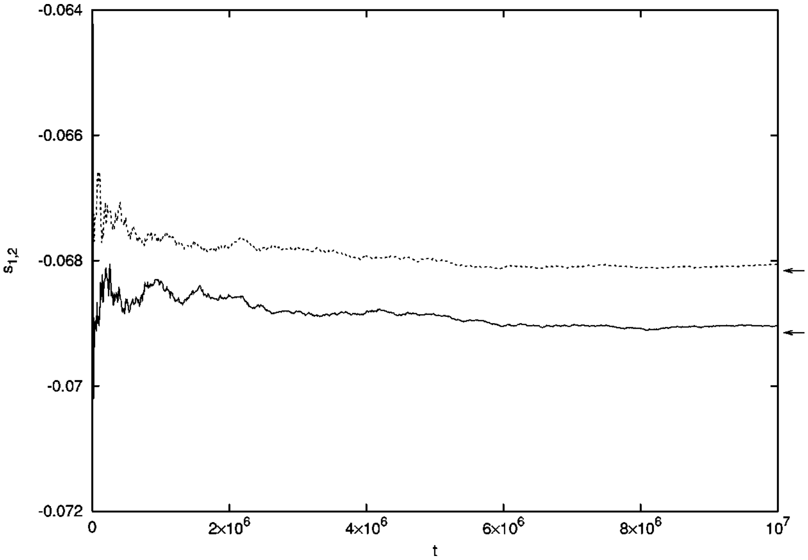

FIG. 3. Time evolution of the sums s_1 (solid line) and s_2 (dotted line) for nonperpendicular fields; $\mathbf{B}=(0.5\sin\phi,0,0.5\cos\phi)$ with $\phi=7\pi/20$. The arrows show the long-time values of the sums ($t=10^8$). Notice the change of scales with respect to Fig. 2.

the existence of systems with the strong CPR but without a Hamiltonian formulation is still open.

Our results also show that time-reversal symmetry, or reversibility in general, is not needed for the CPR to hold. Indeed, one of the first examples for the CPR in dissipative systems has been a Hamiltonian system with a constant viscous damping [15] that has no time-reversal symmetry.

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APPENDIX

We show that the flow defined by Eqs. (1)–(3) is reversible with respect to the transformation $G_B=MG_0$ as given in Sec. II B. Equation (7) can be rewritten for the time derivative F of the flow as $GFG=-F$. From Eq. (1), one can see that $F(\mathbf{q},\mathbf{p})=(\mathbf{p},\mathbf{f})^T$, with $\mathbf{f}(\mathbf{q},\mathbf{p})$ given by the expression for $\dot{\mathbf{p}}$. Now we can write that $G_BFG_B(\mathbf{q},\mathbf{p})=G_BF(M\mathbf{q},-M\mathbf{p})=G_B(-M\mathbf{p},\mathbf{f}(M\mathbf{q},-M\mathbf{p}))=(-\mathbf{p},-M\mathbf{f}(M\mathbf{q},-M\mathbf{p}))^T$. Comparison with $(-\mathbf{p},-\mathbf{f})^T$ gives us the condition

$$\mathbf{f}(\mathbf{q},\mathbf{p})=M\mathbf{f}(M\mathbf{q},-M\mathbf{p}) \tag{A1}$$

for the force acting on the particle.

Since $\mathbf{f}$ consists of the two parts of the Lorentz force and the thermostat, we can check these terms separately. For the electric field, this means that $\mathbf{E}=M\mathbf{E}$, i.e., $\mathbf{E}$ must be in the invariant plane of M. For the term $\mathbf{p}\times\mathbf{B}$, the right-hand side of Eq. (A1) reads as $M(-M\mathbf{p}\times\mathbf{B})=-M(\mathbf{p}_\parallel\times\mathbf{B}-\mathbf{p}_\perp\times\mathbf{B})=-M(\mathbf{p}_\parallel\times\mathbf{B})+M(\mathbf{p}_\perp\times\mathbf{B})$, where $\mathbf{p}_\parallel$ and $\mathbf{p}_\perp$ denote the components of $\mathbf{p}$ parallel and perpendicular to the invariant plane of M, respectively. If $\mathbf{B}$ is in this plane, then $-M(\mathbf{p}_\parallel\times\mathbf{B})=\mathbf{p}_\parallel\times\mathbf{B}$ and $M(\mathbf{p}_\perp\times\mathbf{B})=\mathbf{p}_\perp\times\mathbf{B}$, so the magnetic part of the Lorentz force also satisfies Eq. (A1). As for the thermostating force, $M((\mathbf{E}\cdot M\mathbf{p})M\mathbf{p})=(\mathbf{E}\cdot M\mathbf{p})M^2\mathbf{p}=(\mathbf{E}\cdot\mathbf{p})\mathbf{p}$ also holds if $\mathbf{E}=M\mathbf{E}$. Thus the flow is reversed by $G_B=MG_0$ if the field vectors $\mathbf{E}$ and $\mathbf{B}$ are invariant under M.

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