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An Elementary Proof of Lyapunov Exponent Pairing for Hard-Sphere Systems at Constant Kinetic Energy

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The conjugate pairing of Lyapunov exponents for a field-driven system with smooth inter-particle interaction at constant total kinetic energy was first proved by Dettmann and Morriss [*Phys. Rev. E* **53**:R5545 (1996)] using simple methods of geometry. Their proof was extended to systems interacting via hard-core inter-particle potentials by Wojtkowski and Liverani [*Comm. Math. Phys.* **194**:47 (1998)], using more sophisticated methods. Another, and somewhat more direct version of the proof for hard-sphere systems has been provided by Ruelle [*J. Stat. Phys.* **95**:393 (1999)]. However, these approaches for hard-sphere systems are somewhat difficult to follow. In this paper, a proof of the pairing of Lyapunov exponents for hard-sphere systems at constant kinetic energy is presented, based on a very simple explicit geometric construction, similar to that of Ruelle. Generalizations of this construction to higher dimensions and arbitrary shapes of scatterers or particles are trivial. This construction also works for hard-sphere systems in an external field with a Nosé–Hoover thermostat. However, there are situations of physical interest, where these proofs of conjugate pairing rule for systems interacting via hard-core inter-particle potentials break down.

KEY WORDS: Lorentz gas; hard-sphere systems; lyapunov exponents; conjugate pairing rule.

1. INTRODUCTION

Thermostatted, field-driven systems have been popular models for non-equilibrium molecular dynamics (NEMD) simulation studies of transport processes in fluids. NEMD studies consider systems with a large number of particles interacting with each other, driven by an external field.[1, 2] In these studies, the thermostat continuously removes the energy generated

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inside the system due to the work done on it by the external field, by means of a dynamical friction term in the equations of motion. One finds that for these systems, a non-equilibrium steady state (NESS), homogeneous in space, is reached after a sufficiently long time.[3–8] Here we consider a particular kind of thermostat, where the friction is linearly coupled to the laboratory momenta and keeps the total laboratory kinetic energy of the particles constant (i.e., isokinetic Gaussian thermostat coupled to the laboratory momenta). The dynamical description of these systems, would be Hamiltonian in the absence of this thermostat, and the corresponding Hamiltonian system, obtained by dropping the dynamical friction term from the equations of motion, will be referred to as the *background Hamiltonian system*. Due to the presence of the dynamical friction terms in the equations of motion, such a system is no longer Hamiltonian with a conservation of phase space volumes, but instead is phase-space contracting.[1,9] The sum of all the Lyapunov exponents, which measures the rate of long-time exponential growth of phase-space volume, for such a system is thus negative.[9] Of course, the background Hamiltonian system, if chaotic, is such that the Lyapunov exponents sum up to zero. Furthermore, due to its symplectic form, the Lyapunov exponents of the background system come in pairs such that the sum of each such pair is also zero.[10,11] The phenomenon of such pairing of Lyapunov exponents, where the sum of each pair of non-zero exponents takes a constant value independent of the particular pair, is known as the *conjugate pairing rule* (CPR). Dettmann and Morriss[12] have studied the isokinetic Gaussian thermostatted field-driven systems that are under consideration here, assuming that the particles of the system interact with smooth pair potential energies, and that the forces on the particles due to the external field depends *only on their positions*. They have proved that under these conditions, in a restricted subspace of the phase space of all the particles, characterized by all the non-zero Lyapunov exponents, such a system is μ-symplectic.[2] As a consequence, the CPR is exactly satisfied in that subspace, and it is independent of the number of particles in the system (corresponding simulation results can be found in refs. 13 and 14)—the sum of each pair comes out to be the same negative constant. One important consequence of this result is that the macroscopic transport coefficients of these systems, in the linear order, can be obtained from this constant value of the sum (see, for example ref. 15). The restricted subspace, characterized by all the non-zero Lyapunov exponents, is identified by observing that with an isokinetic Gaussian thermostat, trajectories of the system always lie on a constant total kinetic energy

[2] For a definition of μ-symplecticity condition, see Eqs. (8) and (9) of this paper. The usual symplectic condition is a particular case of Eq. (8) with $\mu = 1$.

hypersurface in the phase space of all the particles. This constraint generates a zero Lyapunov exponent. Also, two points in the phase space do not separate exponentially in time if one point is chosen in the direction of flow of the other. This generates another zero Lyapunov exponent.

As hard-core inter-particle interaction can be dealt as a limiting case of a very short range smooth potential, one would expect that in this restricted subspace, the system is still μ-symplectic, and as a result, the CPR will continue to hold for a field-driven isokinetic Gaussian thermostatted system with hard-core inter-particle interactions. The corresponding pairing of Lyapunov exponents for hard-sphere systems has been proved by direct means using the differential geometric structure of the phase space, by Wojtkowski and Liverani.[16] Another version of the proof for hard-sphere systems has been obtained by Ruelle.[17] The above two approaches for hard-sphere systems are somewhat difficult to follow. The purpose of this paper therefore, is to present a proof of the pairing of Lyapunov exponents (also by direct means) for hard-sphere systems at constant kinetic energy, based on a very simple explicit geometric construction, similar to that used by Ruelle. Two kinds of field-driven isokinetic Gaussian thermostatted systems with hard-core interaction are considered here: in Section 2, the proof of the CPR is carried out for the three-dimensional Lorentz gas, where mutually non-interacting point particles suffer specular collisions with fixed spherical scatterers. In Section 3, the proof is then carried out for a gas of hard spheres. The explicit method of this paper allows one to identify the dependence of these approaches (described in refs. 16 and 17 and here) on the geometrical shapes of the scatterers (or the particles, as the case may be) and on the nature of the externally applied field. Based on it, generalizations to higher dimensions, to arbitrary geometry of the scatterers or the particles, and to the case where the masses of the particles are arbitrary, become trivial. Finally, in Section 4, we argue that this construction can be used to prove the CPR for hard-sphere systems in an external field with a Nosé–Hoover thermostat. We also identify situations of physical interest, where these approaches break down.

2. PROOF OF THE CPR FOR THREE-DIMENSIONAL LORENTZ GAS

The Lorentz gas model consists of a set of scatterers fixed in space together with mutually non-interacting moving particles that suffer elastic, specular collisions with the scatterers. Here we consider the version of the model in three dimensions where the scatterers are hard spheres, and are placed in space without overlapping. Each of the moving particles is a point particle with unit mass ($m = 1$), and is subjected to an external force that depends *only on its position*, as well as a Gaussian thermostat which is designed to keep its kinetic energy at a constant value. During a flight, the equation of motion of a particle is

$$\dot{\mathbf{\Gamma}} = [\dot{\vec{r}}, \dot{\vec{p}}] = [\vec{p}, \vec{F} - \alpha\vec{p}], \tag{1}$$

where $\vec{F} = -\vec{\nabla}\phi$ is the force on the particle due to the external field and α is the coefficient of dynamical friction representing the isokinetic Gaussian thermostat. The value of α is obtained from the fact that the kinetic energy of the particle $\frac{p^2}{2}$ is constant during a flight, i.e.,

$$\alpha = \frac{\vec{F} \cdot \vec{p}}{p^2} \tag{2}$$

and without any loss of generality, the time hereafter is rescaled such that $p^2 = 1$. At a collision with a scatterer, the post-collisional position and momentum of a particle, $\mathbf{\Gamma}_+ = [\vec{r}_+, \vec{p}_+]$, are related to its pre-collisional position and momentum $\mathbf{\Gamma}_- = [\vec{r}_-, \vec{p}_-]$, by

$$\mathbf{\Gamma}_+ = \mathbf{Q}\mathbf{\Gamma}_- = [\vec{r}_-, \vec{p}_- - 2\,(\vec{p}_- \cdot \hat{n})\,\hat{n}], \tag{3}$$

where $\hat{n}$ is the unit vector from the center of the scatterer to the point of collision (see Fig. 1).

It is sufficient to consider the motion of only one of the moving particles in its six-dimensional phase space to investigate the chaotic properties of this system, since they do not interact with each other. To obtain the Lyapunov exponents, we consider a particle at the phase space location $\mathbf{\Gamma}_0 \equiv [\vec{r}_0, \vec{p}_0]$ at time $t = 0$. In time t, it suffers s sequential collisions at time instants $t_1, t_2, \ldots, t_s$ with the scatterers. In between collisions, the particle undergoes flights, acted upon by the external field. We refer to the phase

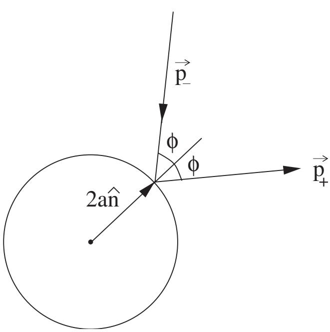

Fig. 1. Dynamics of the point particle at a collision in two-dimensional projection.

space trajectory of it as the "reference trajectory." We also consider another particle at $\mathbf{\Gamma}_0 + \delta\mathbf{\Gamma}_0 \equiv [\vec{r}_0 + \vec{\delta r}_0, \vec{p}_0 + \vec{\delta p}_0]$ at time $t = 0$, such that $\mathbf{\Gamma}_0$ and $\mathbf{\Gamma}_0 + \delta\mathbf{\Gamma}_0$ are infinitesimally apart from each other. This particle suffers the same sequence of collisions and likewise its movement in the phase space generates the "adjacent trajectory." The two trajectories remain infinitesimally apart from each other at all times. Let $\mathbf{H}(t_j - t_{j-1})$ denote the time evolution operator for $\delta\mathbf{\Gamma}(t)$ due to a flight between time instants t_{j-1} and t_j and let $\mathbf{M}_i$ denote the evolution operator for $\delta\mathbf{\Gamma}(t)$ at the ith collision. For $0 < t_1 < t_2 < \cdots < t_s < t$, we therefore have

$$\delta\mathbf{\Gamma}(t) = \mathbf{H}(t - t_s)\, \mathbf{M}_s \mathbf{H}(t_s - t_{s-1}) \cdots \mathbf{M}_1 \mathbf{H}(t_1)\, \delta\mathbf{\Gamma}_0 = \mathbf{L}(t)\, \delta\mathbf{\Gamma}_0 . \tag{4}$$

Let us now also define another six-dimensional matrix $\mathbf{T}(t)$, such that during a flight

$$\delta\dot{\mathbf{\Gamma}}(t) = \mathbf{T}(t)\, \delta\mathbf{\Gamma}(t) . \tag{5}$$

The matrix $\mathbf{L}(t)$ can then be obtained from the solution of the differential equation

$$\dot{\mathbf{H}}(t) = \mathbf{T}(t)\, \mathbf{H}(t), \tag{6}$$

and Eq. (4), with the boundary condition that $\mathbf{H}(0) = \mathbf{L}(0) = \mathbf{I}$. The Lyapunov exponents, measuring the rate of exponential separation between the reference point and adjacent point in this six-dimensional phase space for long times, are then defined as the logarithms of the eigenvalues of the matrix $\mathbf{\Lambda}$, where

$$\mathbf{\Lambda} = \lim_{t \to \infty} \{[\mathbf{L}(t)]^{\mathrm{T}}\, \mathbf{L}(t)\}^{1/2t} . \tag{7}$$

Clearly, there can be at most six Lyapunov exponents of this system, two of which are zero due to the reasons explained in the introduction. For our purpose, we need to select out a four-dimensional subspace of this six-dimensional phase space where all the Lyapunov exponents may be non-zero. In this four-dimensional subspace, the proof of the CPR would follow from the μ-symplecticity property of $\mathbf{L}(t)$.[12, 16, 17] Thus, all we need to prove to establish the CPR in this four-dimensional subspace is that there exists a $\mu(t)$, such that with the four-dimensional subspace representation of $\mathbf{L}(t)$,

$$\mu(t)\, [\mathbf{L}(t)]^{\mathrm{T}}\, \mathbf{J}[\mathbf{L}(t)] = \mathbf{J}, \tag{8}$$

which is the μ-symplecticity condition. Here, $\mathbf{J}$ is a 4×4 matrix with each entry being a 2×2 matrix :

$$\mathbf{J} = \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{I} & \mathbf{0} \end{bmatrix}. \tag{9}$$

Our goal is to prove Eq. (8) by means of the geometric construction, developed in ref. 12.

The identification of this four-dimensional subspace is facilitated by decomposing the six-dimensional position and momentum space of the particle at every point on the reference trajectory, into two separate three-dimensional subspaces, one for the position-space and the other for the momentum-space. Next, in each of these two three-dimensional subspaces, a unit vector $\hat{e}_0 = \vec{p}$ is chosen and two other unit vectors $\hat{e}_1$ and $\hat{e}_2$ are also chosen to form a complete set of orthonormal basis. One zero Lyapunov exponent, which occurs due to the fact that $\vec{\delta p}$ must be chosen orthogonal to $\hat{e}_0$ in order to respect the constraint that $p^2 = 1$, is avoided by measuring $\vec{\delta p}$ by its components along the local directions of $\hat{e}_1$ and $\hat{e}_2$, i.e.,

$$\vec{\delta p} = \sum_{i=1}^{2} \delta p_i \, \hat{e}_i \, . \tag{10}$$

The other zero Lyapunov exponent, which occurs due to the fact that the adjacent point does not exponentially separate from the reference point if $\vec{\delta r}_0$ is chosen along $\hat{e}_0(t = 0)$, is avoided by measuring $\vec{\delta r}$ also by its components along the local directions of $\hat{e}_1$ and $\hat{e}_2$, i.e.,

$$\vec{\delta r} = \sum_{i=1}^{2} \delta r_i \, \hat{e}_i \, . \tag{11}$$

Albeit $\hat{e}_0$, being the momentum of the particle, is uniquely defined at each point on the reference trajectory, $\hat{e}_1$ and $\hat{e}_2$ can be chosen arbitrarily at every point of the reference trajectory, maintaining the orthonormality condition. This ambiguity in the local orientations of $\hat{e}_1$ and $\hat{e}_2$ can be removed by an initial choice of $\hat{e}_1(t = 0)$ and $\hat{e}_2(t = 0)$ at $(\vec{r}_0, \vec{p}_0)$ and subsequently connecting the orthonormal set of basis vectors at different points on the reference trajectory by means of a "parallel transport." The construction and parallel transport of these basis vectors are the key components of the proof of the μ-symplecticity in this procedure.

To this end, we first concentrate on the evolution of $\delta\boldsymbol{\Gamma}(t)$ during the process of a flight of the particle, which is a special case of the systems that

Dettmann and Morriss[12] have considered, where ϕ is the potential due to *only* the external field. Following their construction, we therefore use

$$\dot{\hat{e}}_i = -(\vec{F}\cdot\hat{e}_i)\,\hat{e}_0, \qquad i=1,2 \tag{12}$$

while the parallel transport of $\hat{e}_0$ is obtained from the equations of motion, Eq. (1), i.e.,

$$\dot{\hat{e}}_0 = \sum_{i=1}^{2} (\vec{F}\cdot\hat{e}_i)\,\hat{e}_i\ . \tag{13}$$

From Eq. (1), having obtained

$$\dot{\mathbf{\Gamma}} = \left[\hat{e}_0,\ \sum_{i=1}^{2} (\vec{F}\cdot\hat{e}_i)\,\hat{e}_i\right], \tag{14}$$

it is then easy to show that during a flight

$$\dot{\delta r}_i = \delta p_i \qquad \text{and} \qquad \dot{\delta p}_i = \sum_{j=1}^{2}\left[-\nabla_i\nabla_j\phi - (\vec{F}\cdot\hat{e}_i)(\vec{F}\cdot\hat{e}_j)\right]\delta r_j - \alpha\,\delta p_i\ . \tag{15}$$

Consequently, the matrix $\mathbf{T}$ can be expressed as

$$\mathbf{T} = \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{R}_f & -\alpha\mathbf{I} \end{bmatrix}, \tag{16}$$

where each of the elements in $\mathbf{T}$ above is a 2×2 matrix and $\mathbf{R}_f$ is a symmetric matrix. The matrix $\mathbf{T}$ in Eq. (16) has the property that

$$\mathbf{T}^{\mathrm{T}}\mathbf{J} + \mathbf{J}\mathbf{T} = -\alpha\mathbf{J}, \tag{17}$$

from which it can be easily shown that for a flight between t_{j-1} and t_j

$$\mu(t_j - t_{j-1})\,[\mathbf{H}(t_j - t_{j-1})]^{\mathrm{T}}\,\mathbf{J}\,[\mathbf{H}(t_j - t_{j-1})] = \mathbf{J}, \tag{18}$$

where $\mu(t_j - t_{j-1}) = \exp\left[\int_{t_{j-1}}^{t_j} \alpha(t')\,dt'\right]$ along the reference trajectory.

Next, we study the evolution of the infinitesimal volume element $\delta\mathbf{\Gamma}$ due to a collision with a scatterer to obtain a similar four-dimensional representation of the matrix $\mathbf{M}$, defined in Eq. (4). We notice that even though Eqs. (12) and (13) uniquely determine the orientations of the basis vectors over a flight given their orientation at the initiation of the flight, the equations of parallel transport connecting the pre-collisional and post-collisional basis vectors are still lacking. As the post-collisional momentum of the particle $\hat{e}_{0+}$ can be related to its pre-collisional momentum $\hat{e}_{0-}$ by

$$\hat{e}_{0+} = \hat{e}_{0-} - 2\,(\hat{e}_{0-}\cdot\hat{n})\,\hat{n}, \tag{19}$$

over a collision [see Eq. (3)], a parallel transport of the orthonormal basis vectors that serves our purpose, can be completed also by using

$$\hat{e}_{i+} = \hat{e}_{i-} - 2\,(\hat{e}_{i-} \cdot \hat{n})\,\hat{n} \qquad i = 1, 2. \tag{20}$$

With the use of Eqs. (10), (11), (19), and (20), we now show that as the infinitesimal pre-collisional phase space separation can be written as

$$\boldsymbol{\delta\Gamma}_- = [\vec{\delta r}_-, \vec{\delta p}_-] = \left[\sum_{i=1}^{2} \delta r_{i-}\,\hat{e}_{i-}, \sum_{i=1}^{2} \delta p_{i-}\,\hat{e}_{i-}\right], \tag{21}$$

the corresponding infinitesimal post-collisional separation, $\delta\boldsymbol{\Gamma}_+$, can then be expressed as

$$\boldsymbol{\delta\Gamma}_+ = [\vec{\delta r}_+, \vec{\delta p}_+] = \left[\sum_{i=1}^{2} \delta r_{i+}\,\hat{e}_{i+}, \sum_{i=1}^{2} \delta p_{i+}\,\hat{e}_{i+}\right], \tag{22}$$

which would also reduce the collision dynamics of $\delta\boldsymbol{\Gamma}(t)$ to four dimensions. We want to obtain the symplectic property of the 4×4 matrix $\mathbf{M}$, defined by

$$\boldsymbol{\delta\Gamma}_+ = \mathbf{M}\,\boldsymbol{\delta\Gamma}_-. \tag{23}$$

We begin by studying Fig. 2, which is the two-dimensional projection of an exaggerated picture of a collision that is taking place in three-dimensions. The plane Δ_-, perpendicular to the reference trajectory at its point of collision A intersects the adjacent trajectory at B. While $\vec{\delta r}_- = \vec{AB}$, $\vec{\delta p}_-$ too lies on the plane Δ_-. Similarly, Δ_+ is the plane that is perpendicular to the reference trajectory at D passing through C, the point of collision of the adjacent trajectory. The post-collisional position-space separation between the two trajectories, $\vec{\delta r}_+ = \vec{DC}$ and $\vec{\delta p}_+$ also lies on the plane Δ_+. Clearly, there is a time gap $\delta\tau$ between the two collisions at A and C (i.e., the time required for the adjacent point to travel from B to C), given by

$$\delta\tau = -\frac{\vec{\delta r}_- \cdot \hat{n}}{\hat{e}_{0-} \cdot \hat{n}}. \tag{24}$$

Following the procedure outlined in ref. 18, we find that the infinitesimal phase space separation of the two trajectories just before the two collisions at A and C is

$$\delta\boldsymbol{\Gamma}^* = \boldsymbol{\delta\Gamma}_- + \dot{\boldsymbol{\Gamma}}_-\,\delta\tau \tag{25}$$

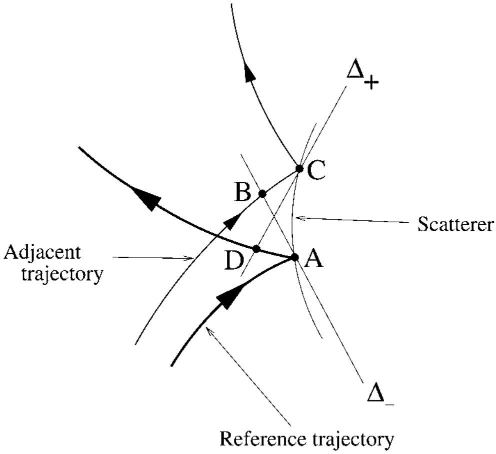

Fig. 2. A two-dimensional projection of the three-dimensional collision dynamics of the reference and adjacent trajectories.

and consequently,

$$\delta \Gamma_+ = \frac{\partial \mathbf{Q}}{\partial \mathbf{\Gamma}_-} \cdot \delta \mathbf{\Gamma}^* - \dot{\mathbf{\Gamma}}_+ \, \delta\tau \tag{26}$$

where $\dot{\mathbf{\Gamma}}_-$ ($\dot{\mathbf{\Gamma}}_+$) is obtained from the equations of motion of the particle for the flight immediately before and after the collision at A [see Eq. (14)], i.e.,

$$\dot{\mathbf{\Gamma}}_\pm = \left[\hat{e}_{0\pm}, \sum_{i=1}^{2} (\vec{F}^* \cdot \hat{e}_{i\pm}) \, \hat{e}_{i\pm} \right] \tag{27}$$

($\vec{F}^*$ is the force on the reference point due to the external field at the point of collision at A) and

$$\frac{\partial \mathbf{Q}}{\partial \mathbf{\Gamma}_-} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ -2\,\hat{e}_{0-} \cdot \left[\dfrac{\partial \hat{n}}{\partial \vec{r}_-} \hat{n} + \hat{n} \dfrac{\partial \hat{n}}{\partial \vec{r}_-} \right] & \mathbf{I} - 2\hat{n}\hat{n} \end{bmatrix} \tag{28}$$

[obtained from Eq. (3)]. Starting with the expression of $\vec{\delta r}_+$, we obtain, from Eqs. (19) and (24)–(28) that

$$\vec{\delta r}_+ = \vec{\delta r}_- - 2(\vec{\delta r}_- \cdot \hat{n})\, \hat{n}, \tag{29}$$

which, together with Eqs. (20)–(22) yields

$$\hat{e}_{0+} \cdot \vec{\delta r}_{+} = 0 \qquad \text{and} \qquad \delta r_{i+} = \delta r_{i-} \qquad i = 1, 2 \tag{30}$$

In a similar manner, the expression of $\vec{\delta p}_{+}$ can also be easily obtained from Eqs. (26)–(28), i.e.,

$$\begin{aligned} \vec{\delta p}_{+} &= \mathbf{A} \cdot \vec{\delta r}^{\,*}_{-} + (\mathbf{I} - 2\hat{n}\hat{n})\, \vec{\delta p}_{-} + (\mathbf{I} - 2\hat{n}\hat{n}) \\ &\quad \times \sum_{i=1}^{2} (\vec{F}^{*} \cdot \hat{e}_{i-})\, \hat{e}_{i-}\, \delta\tau - \sum_{i=1}^{2} (\vec{F}^{*} \cdot \hat{e}_{i+})\, \hat{e}_{i+}\, \delta\tau, \end{aligned} \tag{31}$$

where $\mathbf{A} = -2\hat{e}_{0-} \cdot [\frac{\partial \hat{n}}{\partial \vec{r}_{-}}\, \hat{n} + \hat{n}\, \frac{\partial \hat{n}}{\partial \vec{r}_{-}}]$ and $\vec{\delta r}^{\,*}_{-} = (\vec{\delta r}_{-} + \hat{e}_{0-}\, \delta\tau)$ is the infinitesimal vector $\vec{AC}$ lying on the surface of the scatterer (see Fig. 2).

The simplification of the expression on the r.h.s. of Eq. (31) is carried out in Appendix A. After collecting all the terms together from Eqs. (A1), (A2), and (A5), we obtain

$$\begin{aligned} \delta p_{i+} = \sum_{j=1}^{2} \Bigg[\delta_{ij}\, \delta p_{j-} - 2 \Bigg\{ \frac{(\vec{F}^{*} \cdot \hat{n})(\hat{e}_{i-} \cdot \hat{n})(\hat{e}_{j-} \cdot \hat{n})}{(\hat{e}_{0-} \cdot \hat{n})} \\ + \frac{1}{a}\, \frac{(\hat{e}_{i-} \cdot \hat{n})(\hat{e}_{j-} \cdot \hat{n}) + \delta_{ij}\, (\hat{e}_{0-} \cdot \hat{n})^{2}}{(\hat{e}_{0-} \cdot \hat{n})} \Bigg\} \delta r_{j-} \Bigg]. \end{aligned} \tag{32}$$

One can now see from Eqs. (23), (29) and (32) that the 4×4 matrix $\mathbf{M}$ has the following structure

$$\mathbf{M} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{R}_c & \mathbf{I} \end{bmatrix}, \tag{33}$$

where the 2×2 matrix $\mathbf{R}_c$ is symmetric. This allows us to conclude that in the four-dimensional subspace representation, the transformation of $\delta\boldsymbol{\Gamma}$ over a collision is symplectic, i.e.,

$$\mathbf{M}^{\mathrm{T}} \mathbf{J} \mathbf{M} = \mathbf{J}. \tag{34}$$

Finally, using Eqs. (4), (18), and (34) and $\mu(t) = \exp\,[\int_0^t \alpha(t')\, dt']$, the four-dimensional subspace representation, $\mathbf{L}(t)$ is seen to be μ-symplectic. The four non-zero Lyapunov exponents of this system can therefore be arranged in pairs such that the sum of each pair is exactly equal to $-\langle \alpha \rangle_t$, the negative of the long time average of α along the reference trajectory, i.e., the CPR is exactly satisfied for this system in the restricted four-dimensional subspace.

2.1. Further Generalizations of this Geometric Construction

We end this section with the following generalizations:

(i) The proof can be extended to any arbitrary dimensions, simply by including appropriate number of unit vectors $\hat{e}_i$'s.

(ii) Equation (32) demonstrates the role of geometry of the scatterers and the effect of the external field on the symmetry property of $\mathbf{R}_c$, as *having a symmetric* $\mathbf{R}_c$ *is essential for the symplecticity of* $\mathbf{M}$ [and consequently, the μ-symplecticity of $\mathbf{L}(t)$]. The effect of the geometry of the scatterers is coded in the $\mathbf{A}\cdot\vec{\delta r}^*_-$ term of Eq. (31). For nonspherical scatterers, this geometric construction works, so long as the surfaces of the scatterers are smooth. One has to notice that at the collision point A (see Fig. 1) on an $(n-1)$-dimensional surface embedded in an n-dimensional Euclidean manifold, $\vec{\delta r}^*_-$ is the infinitesimal vector $\vec{AC}$ along the surface of the scatterer, and since $\vec{\delta n}$ appearing in Eq. (A4) is the infinitesimal difference between the two unit normal vectors to the surface of the scatterer at A and C, for a smooth surface, one can define an $n\times n$ *symmetric* matrix $\mathbf{B}$, such that $\vec{\delta n}=\mathbf{B}\cdot\vec{\delta r}^*_-$. In general, the form of the matrix $\mathbf{B}$ depends on the shape of the surface of the scatterer at collision point A. As a special case, if the scatterer is spherical, then $\mathbf{B}$ can be explicitly constructed to be the identity matrix times the inverse radius of curvature of the sphere. In terms of $\mathbf{B}$, one then simply needs to obtain the form of $\mathbf{A}\cdot\vec{\delta r}^*_-$, analogous to Eq. (A5), given below as

$$\mathbf{A}\cdot\vec{\delta r}^*_- = 2\sum_{i,j=1}^{n-1}\Bigg[(\hat{e}_{i-}\cdot\hat{n})(\hat{e}_{j-}\cdot\mathbf{B}\cdot\hat{e}_{0-})+(\hat{e}_{j-}\cdot\hat{n})(\hat{e}_{i-}\cdot\mathbf{B}\cdot\hat{e}_{0-}) - (\hat{e}_{0-}\cdot\hat{n})(\hat{e}_{i-}\cdot\mathbf{B}\cdot\hat{e}_{j-}) - \frac{\hat{e}_{0-}\cdot\mathbf{B}\cdot\hat{e}_{0-}}{\hat{e}_{0-}\cdot\hat{n}}(\hat{e}_{i-}\cdot\hat{n})(\hat{e}_{j-}\cdot\hat{n})\Bigg]\delta r_{j-}\,\hat{e}_{i+}\,. \tag{35}$$

The term in square bracket in Eq. (35) is symmetric in i and j, which contributes the symmetry of the matrix $\mathbf{R}_c$ in Eq. (33). However, the role of external field on the symmetry of $\mathbf{R}_c$ is a bit more subtle—the $\vec{F}^*$-dependent term in Eq. (32) arises due to the fact that *the reference and the adjacent trajectories do not collide the same scatterer at the same instant, despite the fact that collisions between the particles and the scatterers are instantaneous*. As Eq. (27) shows, we have used the fact that both the dynamics of $\mathbf{\Gamma}_-$ and $\mathbf{\Gamma}_+$ involve the *same* force $\vec{F}^*$, which is possible *only* if the pre- and the post-collisional values of $\vec{F}^*$ (i.e., appropriate $\vec{F}^*_-$ and $\vec{F}^*_+$) are the same. One can therefore conclude that this construction can be generalized to prove CPR for arbitrary (smooth) shapes of the scatterers in any dimensions, when the forces on the particles due to the external field depends only the particles' positions.

(iii) The proof does not depend on the specific locations of the scatterers, and hence the CPR holds for any arrangement of the scatterers in space.

3. PROOF OF THE CPR FOR HARD SPHERE GAS IN THREE DIMENSIONS

In this section, we consider a gas of N identical moving spheres in three-dimensions. Each of the spheres has a unit mass and is subjected to an external force that depends *only on its position*, as well as a Gaussian thermostat which keeps the total kinetic energy of the system at a constant value. The spheres interact with each other by means of binary elastic collisions. During a flight, where no collision takes place between any two of the spheres, the equations of motion of the system are

$$\dot{\vec{r}}_{i'} = \vec{p}_{i'}, \dot{\vec{p}}_{i'} = \vec{F}_{i'} - \alpha\vec{p}_{i'}, \qquad i' = 1 \cdots N \tag{36}$$

where $\vec{F}_{i'}$ is the external force on the i'th sphere and α is the coefficient of dynamical friction representing the isokinetic Gaussian thermostat (hereafter primed indices will always indicate sphere numbers). The value of α is set in a way that it keeps the total kinetic energy of the system, $\sum_{i'=1}^{N} \frac{p_{i'}^2}{2}$ constant, i.e.,

$$\alpha = \left[\sum_{i'=1}^{N} \vec{F}_{i'} \cdot \vec{p}_{i'}\right] \Big/ \left[\sum_{i'=1}^{N} p_{i'}^2\right]. \tag{37}$$

As before, we rescale the time such that $\sum_{i'=1}^{N} p_{i'}^2 = 1$. At a collision between the i'th and the j'th spheres, the post-collisional positions and momenta are related to the pre-collisional values by

$$\vec{r}_{i'+} = \vec{r}_{i'-}, \quad \vec{r}_{j'+} = \vec{r}_{j'-}, \quad \vec{p}_{i'+} = \vec{p}_{i'-} - \{(\vec{p}_{i'-} - \vec{p}_{j'-}) \cdot \hat{n}_{i'j'}\}\, \hat{n}_{i'j'} \qquad \text{and}$$
$$\vec{p}_{j'+} = \vec{p}_{j'-} + \{(\vec{p}_{i'-} - \vec{p}_{j'-}) \cdot \hat{n}_{i'j'}\}\, \hat{n}_{i'j'}, \tag{38}$$

where $\hat{n}_{i'j'}$ is the unit vector along the line joining the center of the i'th sphere to the j'th sphere at the time of the collision. Since such a collision is instantaneous, during any such binary collision process, the positions and momenta of the spheres not participating in the collision do not change.

We define the $3N$-dimensional vectors $\vec{R}$ and $\vec{P}$, assembled respectively from the three-dimensional position and momentum vectors of the N spheres, such that

$$\vec{R}=[\vec{r}_1, \vec{r}_2,..., \vec{r}_N] \qquad \text{and} \qquad \vec{P}=[\vec{p}_1, \vec{p}_2,..., \vec{p}_N], \tag{39}$$

with $P^2=1$. We also form two more $3N$-dimensional vectors $\vec{F}$ and $\hat{N}_{i'j'}$: $\vec{F}$ describes the external force on the spheres, and $\hat{N}_{i'j'}$ is assembled from the unit vector $\hat{n}_{i'j'}$; i.e.,

$$\vec{F}=[\vec{F}_1, \vec{F}_2,..., \vec{F}_N] \qquad \text{and} \qquad \hat{N}_{i'j'}=\frac{1}{\sqrt{2}}[\vec{0}, \vec{0},..., \hat{n}_{i'j'},..., , -\hat{n}_{i'j'},..., \vec{0}], \tag{40}$$

such that the i'th and the j'th entries of $\hat{N}_{i'j'}$ (they are the only non-zero entries) are $\hat{n}_{i'j'}/\sqrt{2}$ and $-\hat{n}_{i'j'}/\sqrt{2}$ respectively [satisfying the normalization condition $\hat{N}_{i'j'}\cdot\hat{N}_{i'j'}=1$]. Equations (36) and (37) can now be rewritten [in the same form as Eqs. (1) and (2)] as

$$\dot{\mathbf{\Gamma}}=[\dot{\vec{R}}, \dot{\vec{P}}]=[\vec{P}, \vec{F}-\alpha\vec{P}], \qquad \text{with} \quad \alpha=\vec{F}\cdot\vec{P}, \tag{41}$$

while the collision dynamics can be rewritten as

$$\mathbf{\Gamma}_+=\mathbf{Q}\mathbf{\Gamma}_-=[\vec{R}_-, \vec{P}_- -2(\vec{P}_-\cdot\hat{N}_{i'j'})\,\hat{N}_{i'j'}], \tag{42}$$

analogous to Eq. (3). As discussed in the introduction, the geometric construction associated with Eqs. (39)–(42) can be obtained as an extension of the corresponding constructions for the three-dimensional Lorentz gas. We will see that the construction of the unit normal vector $\hat{N}_{i'j'}$ is the key component of the proof of μ-symplecticity and the CPR for hard-sphere gases.

The proof of the CPR proceeds exactly in the same way as it has been described in Section 2. The time evolution of the infinitesimal $6N$-dimensional phase space separation $\mathbf{\Gamma}(t)$ between the reference and the adjacent trajectories can be decomposed by means of $6N$-dimensional $\mathbf{H}$ and $\mathbf{M}$ matrices as in Eq. (4). The $(6N-2)$-dimensional reduction of $\mathbf{H}$ matrices can be subsequently obtained by constructing N $3N$-dimensional basis vectors $\hat{e}_0(t=0)$, $\hat{e}_1(t=0)$, ., ., ., ., $\hat{e}_{(3N-1)}(t=0)$ at $\mathbf{\Gamma}_0$, and then parallelly transporting them using equations analogous to Eqs. (12) and (13) and choosing to measure both $\delta\vec{R}$ and $\delta\vec{P}$ in directions orthogonal to $\hat{e}_0$ in the same manner as in Eqs. (10) and (11). As a special case of what Dettmann and Morriss considered,[12] in terms of the $(6N-2)$-dimensional representation, the matrix $\mathbf{H}(t_j-t_{j-1})$ is easily seen to be μ-symplectic with

$\mu(t_j - t_{j-1}) = \exp\left[\int_{t_{j-1}}^{t_j} \alpha(t')\, dt'\right]$ along the reference trajectory, for a flight between t_{j-1} and t_j. What remains to be shown, therefore, is that the matrix **M** describing the transformation of $\delta\boldsymbol{\Gamma}(t)$ due to a binary collision is also symplectic. To this end, following Section 2 of this paper, we use a simple extension, comprising of the same form of parallel transport (as in Eqs. (19) and (20)) of the N basis vectors $\hat{e}_0, \hat{e}_1,..., \hat{e}_{(3N-1)}$ over the binary collision between the i'th and the j'th sphere, i.e.,

$$\begin{aligned} \hat{e}_{0+} &= \hat{e}_{0-} - 2(\hat{e}_{0-} \cdot \hat{N}_{i'j'})\, \hat{N}_{i'j'} \qquad \text{and} \\ \hat{e}_{i+} &= \hat{e}_{i-} - 2(\hat{e}_{i-} \cdot \hat{N}_{i'j'})\, \hat{N}_{i'j'} \qquad 1 \leqslant i \leqslant (3N-1) \end{aligned} \tag{43}$$

Evaluation of the expression of **M** in this $(6N-2)$-dimensional representation is a bit more involved than that presented in Section 2. Nevertheless, one can still use Fig. 2 to illustrate the collisions at A and C and the construction of the planes Δ_- and Δ_+ in a schematic way, keeping in mind that this time the diagram describes quantities in $3N$-dimensions (for another version of Fig. 2 in the context of hard-sphere gases, the reader may also find Fig. 6 in ref. 19 helpful). We will follow the logical steps described in Eqs. (24)–(28) to obtain the expressions of $\delta\vec{X}_+$ and $\delta\vec{P}_+$. Let us first define below the $6N$ dimensional vector $\delta\boldsymbol{\Gamma}_\pm$ describing the infinitesimal post(pre)-collisional phase-space separations of the two trajectories

$$\begin{aligned} \boldsymbol{\delta\Gamma}_\pm &= [\delta\vec{R}_\pm, \delta\vec{P}_\pm] = [\delta\vec{r}_{1\pm},..., \delta\vec{r}_{N\pm}, \delta\vec{p}_{1\pm},..., \delta\vec{p}_{N\pm}] \\ &= \left[\sum_{i=1}^{3N-1} \delta R_{i\pm}\, \hat{e}_{i\pm}, \sum_{i=1}^{3N-1} \delta P_{i\pm}\, \hat{e}_{i\pm}\right]. \end{aligned} \tag{44}$$

We observe that the time lag between the binary collisions, involving the i'th and the j'th sphere on the reference and the adjacent trajectories (schematically at A and C respectively in Fig. 2) is

$$\delta\tau = -\frac{(\delta\vec{r}_{j'-} - \delta\vec{r}_{i'-}) \cdot \hat{n}_{i'j'}}{(\vec{p}_{j'-} - \vec{p}_{i'-}) \cdot \hat{n}_{i'j'}} = -\frac{\delta\vec{R}_- \cdot \hat{N}_{i'j'}}{\hat{e}_{0-} \cdot \hat{N}_{i'j'}}. \tag{45}$$

Following the procedure outlined in ref. 18, we find that the infinitesimal phase space separation of the two trajectories at A and C is, as before,

$$\delta\boldsymbol{\Gamma}^* = \boldsymbol{\delta\Gamma}_- + \dot{\boldsymbol{\Gamma}}_-\, \delta\tau \qquad \text{and} \qquad \boldsymbol{\delta\Gamma}_+ = \frac{\partial \mathbf{Q}}{\partial \boldsymbol{\Gamma}_-} \cdot \delta\boldsymbol{\Gamma}^* - \dot{\boldsymbol{\Gamma}}_+\, \delta\tau, \tag{46}$$

where $\dot{\boldsymbol{\Gamma}}_-$ ($\dot{\boldsymbol{\Gamma}}_+$) is obtained from the equations of motion of the system for the flight immediately before and after the collision at A [from Eq. (41)], i.e.,

$$\dot{\boldsymbol{\Gamma}}_\pm = \left[\hat{e}_{0\pm}, \sum_{i=1}^{2} (\vec{F}^* \cdot \hat{e}_{i\pm})\, \hat{e}_{i\pm} \right]. \tag{47}$$

Here $\vec{F}^*$ is the force on the reference point, described in Eq. (40), due to the external field at the point of collision at A. Using Eq. (42),

$$\frac{\partial \mathbf{Q}}{\partial \boldsymbol{\Gamma}_-} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ -2\, \hat{e}_{0-} \cdot \left[\frac{\partial \hat{N}_{i'j'}}{\partial \vec{R}_-} \hat{N}_{i'j'} + \hat{N}_{i'j'} \frac{\partial \hat{N}_{i'j'}}{\partial \vec{R}_-} \right] & \mathbf{I} - 2\hat{N}_{i'j'} \hat{N}_{i'j'} \end{bmatrix}, \tag{48}$$

where each entry of the matrix on the r.h.s. of Eq. (48) is a $3N \times 3N$ matrix.

Starting with the expression of $\delta\vec{R}_+$, once again we obtain, from Eqs. (43) and (45)–(48) that

$$\delta\vec{R}_+ = \delta\vec{R}_- - 2\, (\delta\vec{R}_- \cdot \hat{N}_{i'j'})\, \hat{N}_{i'j'}, \tag{49}$$

which, together with Eq. (43) yields

$$\hat{e}_{0+} \cdot \delta\vec{R}_+ = 0 \qquad \text{and} \qquad \delta R_{i+} = \delta R_{i-} \qquad 1 \leqslant i \leqslant (3N-1) \tag{50}$$

In a similar manner, the expression of $\delta\vec{P}_+$ can also be easily obtained from Eqs. (46)–(48), i.e.,

$$\begin{aligned} \delta\vec{P}_+ &= \mathbf{A} \cdot \delta\vec{R}^*_- + (\mathbf{I} - 2\hat{N}_{i'j'}\hat{N}_{i'j'})\, \delta\vec{P}_- \\ &\quad + (\mathbf{I} - 2\hat{N}_{i'j'}\hat{N}_{i'j'}) \sum_{i=1}^{3N-1} (\vec{F}^* \cdot \hat{e}_{i-})\, \hat{e}_{i-}\, \delta\tau - \sum_{i=1}^{3N-1} (\vec{F}^* \cdot \hat{e}_{i+})\, \hat{e}_{i+}\, \delta\tau, \end{aligned} \tag{51}$$

where $\mathbf{A} = -2\hat{e}_{0-} \cdot [\frac{\partial \hat{N}_{i'j'}}{\partial \vec{R}_-} \hat{N}_{i'j'} + \hat{N}_{i'j'} \frac{\partial \hat{N}_{i'j'}}{\partial \vec{R}_-}]$ and $\delta\vec{R}^*_- = (\delta\vec{R}_- + \hat{e}_{0-}\, \delta\tau)$. The simplification of the expression of $\delta\vec{P}_+$ is carried out in Appendix B. Finally, using Eqs. (B1) and (B2) and (B6) and (B7), we obtain that in terms of the $(6N-2)$-dimensional representation, the matrix $\mathbf{M}$ can be written in the form

$$\delta P_{i+} = \sum_{j=1}^{3N-1} \left[\delta_{ij}\, \delta P_{i-} + \left\{ W_{ij} - 2 \sum_{i,j=1}^{3N-1} \frac{(\vec{F}^* \cdot \hat{N}_{i'j'})(\hat{e}_{i-} \cdot \hat{N}_{i'j'})(\hat{e}_{j-} \cdot \hat{N}_{i'j'})}{(\hat{e}_{0-} \cdot \hat{n})} \right\} \delta R_{j-} \right] \tag{52}$$

where $W_{ij} = W_{ji}$ has been evaluated in Eq. (B18) in Appendix B. Equation (52), together with Eqs. (50)–(51) implies that $\mathbf{M}$ has the same form as in

Eq. (33), where the $(3N-1)\times(3N-1)$ matrix $\mathbf{R}_c$ is symmetric. This again allows us to conclude that in the $(6N-2)$-dimensional subspace representation, $\mathbf{M}$ is symplectic, and $\mathbf{L}(t)$ is μ-symplectic with $\mu(t)=\exp[\int_0^t \alpha(t')\,dt']$, i.e., the CPR is exactly satisfied in the restricted $(6N-2)$-dimensional subspace for this system.

3.1. Further Generalizations of this Geometric Construction

We end this section with the following observations:

(i) the condition that each sphere is of unit mass is not essential—if the i'th particle has a mass $m_{i'}$, one can define the new quantities $\vec{r}\,'_{i'}=m_{i'}^{\frac{1}{2}}\vec{r}_{i'}$, $\vec{p}\,'_{i'}=m_{i'}^{-\frac{1}{2}}\vec{p}_{i'}$ and $\vec{F}'_{i'}=m_{i'}^{-\frac{1}{2}}\vec{F}_{i'}$ and then begin with the Eqs. (36)–(38) replacing $\vec{r}_{i'}$'s, $\vec{p}_{i'}$'s and $\vec{F}_{i'}$'s by the corresponding primed variables. One also needs to use

$$\hat{N}'_{i'j'}=\left[\vec{0},\vec{0},\ldots,\sqrt{\frac{m_{j'}}{m_{i'}+m_{j'}}}\,\hat{n}_{i'j'},\ldots,,-\sqrt{\frac{m_{i'}}{m_{i'}+m_{j'}}}\,\hat{n}_{i'j'},\ldots,\vec{0}\right], \tag{53}$$

such that the i'th and the j'th entries of $\hat{N}'_{i'j'}$ (they are the only non-zero entries) are $\sqrt{\frac{m_{j'}}{m_{i'}+m_{j'}}}\,\hat{n}_{i'j'}$ and $-\sqrt{\frac{m_{i'}}{m_{i'}+m_{j'}}}\,\hat{n}_{i'j'}$ respectively (satisfying the normalization condition $\hat{N}'_{i'j'}\cdot\hat{N}'_{i'j'}=1$) and define a corresponding $6N\times 6N$ matrix $\mathbf{U}'$ (see Eqs. (B12) in Appendix B and its preceding paragraph) such that

$$\mathbf{U}'_{i'i'}=\frac{m_{j'}}{m_{i'}}\mathbf{U}'_{j'j'}=-\sqrt{\frac{m_{j'}}{m_{i'}}}\,\mathbf{I},\qquad \mathbf{U}'_{i'j'}=\mathbf{U}'_{j'i'}=\mathbf{I}; \tag{54}$$

(ii) the proof can be trivially extended to any arbitrary dimensions by including appropriate number of unit vectors $\hat{e}_i$'s and

(iii) Following point (ii) of Section 2.1, it is easy to generalize this construction, and hence the proof, to arbitrary (smooth) shapes of the particles. One simply needs to use an analogous *symmetric* matrix $\mathbf{B}$ such that $\delta\vec{N}_{i'j'}=\mathbf{B}\cdot\delta\vec{R}^*_-$. Just from Eq. (B3), one then obtains the same equation as Eq. (35):

$$\begin{aligned}\mathbf{A}\cdot\delta\vec{R}^*_-&\\ =2\sum_{i,j=1}^{n-1}\Bigg[&(\hat{e}_{i-}\cdot\hat{N}_{i'j'})(\hat{e}_{j-}\cdot\mathbf{B}\cdot\hat{e}_{0-})+(\hat{e}_{j-}\cdot\hat{N}_{i'j'})(\hat{e}_{i-}\cdot\mathbf{B}\cdot\hat{e}_{0-})\\ &-(\hat{e}_{0-}\cdot\hat{N}_{i'j'})(\hat{e}_{i-}\cdot\mathbf{B}\cdot\hat{e}_{j-})-\frac{\hat{e}_{0-}\cdot\mathbf{B}\cdot\hat{e}_{0-}}{\hat{e}_{0-}\cdot\hat{N}_{i'j'}}(\hat{e}_{i-}\cdot\hat{N}_{i'j'})(\hat{e}_{j-}\cdot\hat{N}_{i'j'})\Bigg]\delta R_{j-}\,\hat{e}_{i+}\,.\end{aligned} \tag{55}$$

Notice already the striking similarity of the term inside the square brackets in Eqs. (35) and (55) to the form of W_{ij} in Eq. (B18). When the $nN \times nN$ matrix $\mathbf{B}$ is decomposed into $N \times N$ blocks of $n \times n$ matrices, the only non-zero entries are $\mathbf{B}_{i'i'}$, $\mathbf{B}_{i'j'}$, $\mathbf{B}_{j'i'}$ and $\mathbf{B}_{j'j'}$, corresponding to the two colliding particles i' and j'. As a special case, if these particles are spheres, then the matrix $\mathbf{B}$ can be explicitly constructed to be $\mathbf{U}/[\sqrt{2}\,(a_{i'} + a_{j'})]$, where $a_{i'}$ and $a_{j'}$ are the radii of the colliding particles[21] (in Appendix B, we have used $a_{i'} = a_{j'} = a$). The factor of $\sqrt{2}$ follows from Eqs. (40) and (B4). Once again, the form of Eqs. (55) contributes the symmetry of $\mathbf{R}_c$. In a similar manner as explained in point (iii) of Section 2.1, the symplecticity property of $\mathbf{M}$ (and hence the μ-symplecticity of $\mathbf{L}(t)$ crucially hinges upon the symmetry of $\mathbf{R}_c$, for which it is necessary to have the expression of $\vec{F}^*$ to be invariant under a collision.

4. DISCUSSION

While much of the content of this paper is technical, the underlying principle behind our discussion of the CPR is similar to those in the existing literature.[16, 17] First, the dimension of the phase space is identified where all the Lyapunov exponents are non-zero. The dimension of this reduced phase space, characterized by all the non-zero Lyapunov exponents, depends on the number of macroscopic conserved quantities in the problem (such as total momentum, total angular momentum, total energy etc.) that are consistent with the dynamics. By means of confining the dynamics to a hypersurface of dimension 1 less than that of the full phase space, each such conserved quantity reduces the dimension of the phase space characterized by all the non-zero Lyapunov exponents by 1. In addition, the fact that two points in the phase space do not separate exponentially in time if one point is chosen in the direction of flow of the other, reduces the dimension of the phase space characterized by the non-zero Lyapunov exponents also by 1. The dynamics for systems with hard-core inter-particle interactions are then decomposed into flights and collisions. The dynamics of a flight segment in the reduced phase space is shown to be μ-symplectic as a special case of the explicit geometric construction in ref. 12. By means of another simple explicit geometric construction, it is also possible to incorporate the collisions in this formalism, which subsequently leads one to evaluate the matrix $\mathbf{M}$ and demonstrate that it is symplectic. Finally, the matrix $\mathbf{L}(t)$, assembled from the sequential products of the $\mathbf{H}$ and $\mathbf{M}$ matrices, is easily seen to be μ-symplectic using the fact that the product of a symplectic and a μ-symplectic transformation is μ-symplectic. We must note here that the proof of CPR by this construction is *sufficient and not necessary*; and as a result, if a system does not satisfy this proof, it is *not* guaranteed that CPR would not be satisfied for it. Moreover, this explicit geometric construction, used in this paper for the parallel transport of basis vectors, is by no means unique. One could conceivably use a different set of equations for the parallel transport mechanisms for both flight and collision parts of the dynamics to prove the CPR for a dynamical system.

Questions naturally arise about the applicability of this construction for other hard-particle systems. It turns out that using the same explicit geometric construction that is presented here, CPR can also be proved for a gas of hard particles (of finite sizes) in an external field (such that the forces on the particles due to this field depend only on their positions of the particles) under a Nosé–Hoover thermostat. One simply has to separate the time evolution of $\delta\mathbf{\Gamma}$ in terms of the $\mathbf{H}$ and the $\mathbf{M}$ matrices in an appropriately reduced phase space. The μ-symplecticity of the $\mathbf{H}$ matrices can be trivially obtained as a special case of ref. 20, where the CPR has been proved for a system of particles that interact with each other by means of smooth interparticle potentials. The symplecticity property of the $\mathbf{M}$ matrices can also be easily seen to be valid, if one combines the observation of point (ii) of Section 3.1 with Eq. (15) of ref. 20. We have seen in point (ii) of Section 3.1 that for $\mathbf{M}$ to be symplectic, it is necessary that $\vec{F}^*$ be invariant under a collision, and it is definitely the case with Eq. (15) of ref. 20.

Clearly, this explicit geometric construction allows one to see the role of the external field in between collisions (that it is necessary for the force on the particles due to the external field be dependent only on their positions), the role of $\vec{F}^*$ and the geometry of the colliding particles (or scatterers, as the case may be) for it to prove the CPR. However, these conditions, under which this construction works to prove the CPR, are rather restrictive in the context of NEMD studies of the transport quantities of the systems of physical interest, as they exclude a class of very interesting systems where the external force may depend on the momenta of the particles—for example, when the system is subjected to an additional external magnetic field. Nevertheless, it has allowed us to prove an important theoretical result regarding the CPR, for a gas of hard spheres under shear ref. 21. It is also possible that this choice of parallel transport can be used for numerical computations to achieve higher accuracy for the Lyapunov exponents.

We end this paper with the observation that while this construction uses explicit dependence on the co-ordinate system on a Euclidean manifold, there exists a (co-ordinate independent) differential geometric method (for example, in ref. 16) that allows one to work easily on non-Euclidean manifolds[22] as well. How this present construction can be generalized to such non-Euclidean manifolds is presently unclear, but it remains a challenging task for the future.

APPENDIX A

To simplify the expression of $\vec{\delta p}_+$, we break the r.h.s. of Eq. (31) into several parts. First we notice that

$$(\mathbf{I}-2\hat{n}\hat{n})\,\vec{\delta p}_- = \sum_{i=1}^{2} \delta p_{i-}\,\hat{e}_{i+} \qquad \text{and} \tag{A1}$$

$$\begin{aligned}(\mathbf{I}-2\hat{n}\hat{n}) &\sum_{i=1}^{2} (\vec{F}^*\cdot\hat{e}_{i-})\,\hat{e}_{i-}\,\delta\tau - \sum_{i=1}^{2} (\vec{F}^*\cdot\hat{e}_{i+})\,\hat{e}_{i+}\,\delta\tau \\ &= -2\sum_{i,j=1}^{2} \frac{(\vec{F}^*\cdot\hat{n})(\hat{e}_{i-}\cdot\hat{n})(\hat{e}_{j-}\cdot\hat{n})}{(\hat{e}_{0-}\cdot\hat{n})}\,\delta r_{j-}\,\hat{e}_{i+}\,.\end{aligned} \tag{A2}$$

Next, we observe that the rest of the r.h.s. of Eq. (31), i.e., $\mathbf{A}\cdot\vec{\delta r}^*_-$ describes the effect of the orientation of $\hat{n}$ on $\vec{\delta p}_+$. Having denoted the unit vector normal to the surface of the scatterer at C by $\hat{n}'$, which can be related to $\hat{n}$ by

$$\hat{n}' = \hat{n} + \vec{\delta n}\,, \tag{A3}$$

($\hat{n}\cdot\vec{\delta n} = 0$), it is easily seen from Eqs. (25), (26), and (28) that

$$\mathbf{A}\cdot\vec{\delta r}^*_- = -2\,[(\hat{e}_{0-}\cdot\vec{\delta n})\,\hat{n} + (\hat{e}_{0-}\cdot\hat{n})\,\vec{\delta n}\,]. \tag{A4}$$

Furthermore, using $\vec{\delta n} = \vec{\delta r}^*_-/a$, where a is the radius of the scatterer, The expression of $\mathbf{A}\cdot\vec{\delta r}^*_-$ can be readily simplified as

$$\mathbf{A}\cdot\vec{\delta r}^*_- = -\frac{2}{a}\sum_{i,j=1}^{2} \frac{(\hat{e}_{i-}\cdot\hat{n})(\hat{e}_{j-}\cdot\hat{n}) + \delta_{ij}\,(\hat{e}_{0-}\cdot\hat{n})^2}{(\hat{e}_{0-}\cdot\hat{n})}\,\delta r_{j-}\,\hat{e}_{i+}\,. \tag{A5}$$

APPENDIX B

Two terms on the r.h.s. of Eq. (51) simplify as before, i.e.,

$$(\mathbf{I}-2\hat{N}_{i'j'}\hat{N}_{i'j'})\,\vec{\delta P}_- = \sum_{i=1}^{3N-1} \delta P_{i-}\,\hat{e}_{i+} \qquad \text{and} \tag{B1}$$

$$\begin{aligned}(\mathbf{I}-2\hat{N}_{i'j'}\hat{N}_{i'j'}) &\sum_{i=1}^{3N-1} (\vec{F}^*\cdot\hat{e}_{i-})\,\hat{e}_{i-}\,\delta\tau - \sum_{i=1}^{3N-1} (\vec{F}^*\cdot\hat{e}_{i+})\,\hat{e}_{i+}\,\delta\tau \\ &= -2\sum_{i,j=1}^{3N-1} \frac{(\vec{F}^*\cdot\hat{N}_{i'j'})(\hat{e}_{i-}\cdot\hat{N}_{i'j'})(\hat{e}_{j-}\cdot\hat{N}_{i'j'})}{(\hat{e}_{0-}\cdot\hat{n})}\,\delta R_{j-}\,\hat{e}_{i+}\,.\end{aligned} \tag{B2}$$

Following Section 2, the term $\mathbf{A}\cdot\delta\vec{R}^*_-$ can be expressed as

$$\mathbf{A}\cdot\delta\vec{R}^*_- = -2\,[(\hat{e}_{0-}\cdot\delta\vec{N}_{i'j'})\,\hat{N}_{i'j'} + (\hat{e}_{0-}\cdot\hat{N}_{i'j'})\,\delta\vec{N}_{i'j'}], \tag{B3}$$

where

$$\delta\vec{N}_{i'j'} = \frac{1}{\sqrt{2}}\,[\vec{0}, \vec{0},\ldots, \delta\vec{n}_{i'j'},\ldots, , -\delta\vec{n}_{i'j'},\ldots, \vec{0}], \tag{B4}$$

satisfying $\hat{n}_{i'j'}\cdot\delta\vec{n}_{i'j'} = 0$. This orthogonality condition between $\hat{n}_{i'j'}$ and $\delta\vec{n}_{i'j'}$ also implies that $\hat{N}_{i'j'}\cdot\delta\vec{N}_{i'j'} = 0$; from which it can be readily shown that

$$\hat{e}_{0+}\cdot[\,\mathbf{A}\cdot\delta\vec{R}^*_-] = 0, \tag{B5}$$

In other words, we have

$$\mathbf{A}\cdot\delta\vec{R}^*_- = \sum_{i=1}^{3N-1}\,\{[\mathbf{A}\cdot\delta\vec{R}^*_-]\cdot\hat{e}_{i+}\}\,\hat{e}_{i+}\ . \tag{B6}$$

The full simplification of the expression $[\,\mathbf{A}\cdot\delta\vec{R}^*_-]\cdot\hat{e}_{i+}$ is carried out below, where it is shown that

$$[\mathbf{A}\cdot\delta\vec{R}^*_-]\cdot\hat{e}_{i+} = \sum_{j=1}^{3N-1} W_{ij}\,\delta\vec{R}_j, \tag{B7}$$

with the property that $W_{ij} = W_{ji}$ (see Eq. (B18)). The expression $\mathbf{A}\cdot\delta\vec{R}^*_-$, using Eq. (B3), can be written in the following form

$$\mathbf{A}\cdot\delta\vec{R}^*_- = [\vec{0}, \vec{0},\ldots, \vec{A}_{i'},\ldots, , -\vec{A}_{j'},\ldots, \vec{0}]; \tag{B8}$$

such that all but the i'th and the j'th entries on the r.h.s. of Eq. (B8) are zero, while the j'th entry $\vec{A}_{j'}$ is related to the i'th entry $\vec{A}_{i'}$ by [using Eq. (B4)]

$$\vec{A}_{j'} = -\vec{A}_{i'} = [\{(\vec{p}_{i'-} - \vec{p}_{j'-})\cdot\delta\vec{n}n_{i'j'}\}\,\hat{n}_{i'j'} + \{(\vec{p}_{i'-} - \vec{p}_{j'-})\cdot\delta\vec{n}_{i'j'}\}\,\delta\vec{n}_{i'j'}]. \tag{B9}$$

To obtain an expression for $\delta\vec{n}_{i'j'}$ analogous to $\delta\vec{n} = \delta\vec{r}^*_-/a$ as used in Appendix A, we need to take a look at Figs. 3 and 4. Figure 3 describes, in the laboratory frame, the binary collision process between the i'th and the j'th sphere on the reference and adjacent trajectories; the thick-lined spheres are on the reference trajectory whereas the thin-lined spheres are on the adjacent trajectory. Figure 4 describes the same binary collision process in the reference frame of the i'th sphere (with center C). In Fig. 3, the thick-lined j'th sphere (with center D) on the left depicts the collision situation

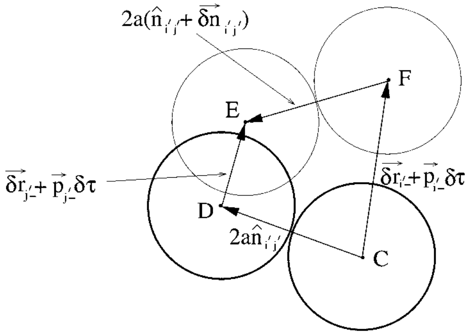

Fig. 3. Collision between the i'th and the j'th sphere on the reference and adjacent trajectories in the laboratory frame. Thick-lined spheres are on the reference trajectory whereas the thin-lined spheres are on the adjacent trajectory.

on the reference trajectory and the thin-lined j'th sphere (with center E) on the left depicts the collision situation on the adjacent trajectory. Clearly, in Fig. 4, the infinitesimal vector $\vec{DE}$ is given by

$$\vec{\delta r}^{\,*}_{i'j'} = \vec{\delta r}_{j'_-} - \vec{\delta r}_{i'_-} + (\vec{p}_{j'_-} - \vec{p}_{i'_-})\,\delta\tau \tag{B10}$$

and since the lengths of both the lines CD and CE are $2a$ (a is the radius of each sphere), we have

$$\vec{\delta n}_{i'j'} = \frac{1}{2a}\,\vec{\delta r}^{\,*}_{i'j'}\,. \tag{B11}$$

Starting with the expression in Eq. (B6), we proceed to calculate the quantity $[\mathbf{A}\cdot\vec{\delta R}^*_-]\cdot\hat{e}_{i+}$. Let us first define a $3N\times 3N$ matrix $\mathbf{U}$ composed of

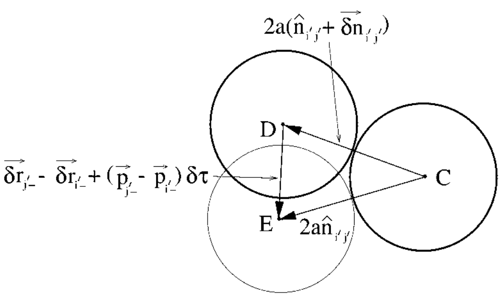

Fig. 4. Same collisions as in Fig. 3, in the reference frame of the i'th sphere.

$N \times N$ blocks of 3×3 matrices, such that, in terms of the block indices the only non-zero entries of $\mathbf{U}$ are

$$\mathbf{U}_{i'i'} = -\mathbf{U}_{i'j'} = -\mathbf{U}_{j'i'} = \mathbf{U}_{j'j'} = -\mathbf{I}, \tag{B12}$$

where $\mathbf{I}$ is the 3×3 unit matrix. The matrix $\mathbf{U}$ has the property that

$$\mathbf{U}^{\mathrm{T}} = \mathbf{U} \qquad \text{and} \qquad \mathbf{U} \cdot \hat{N}_{i'j'} = -2\hat{N}_{i'j'} \ . \tag{B13}$$

Using Eqs. (B8)–(B11,) and (B13), one can then simplify $[\mathbf{A} \cdot \delta\vec{R}^*_-] \cdot \hat{e}_{i+}$ as

$$\begin{aligned}
&[\mathbf{A} \cdot \delta\vec{R}^*_-] \cdot \hat{e}_{i+} \\
&= \frac{\sqrt{2}}{2a} (\hat{e}_{i-} \cdot \hat{N}_{i'j'}) \sum_{j=1}^{3N-1} \left[(\hat{e}_{j-} \cdot \mathbf{U} \cdot \hat{e}_{0-}) - (\hat{e}_{0-} \cdot \mathbf{U} \cdot \hat{e}_{0-}) \frac{(\hat{e}_{j-} \cdot \hat{N}_{i'j'})}{(\hat{e}_{0-} \cdot \hat{N}_{i'j'})} \right] \delta R_{j-} \\
&\quad - \frac{\sqrt{2}}{2a} (\hat{e}_{0-} \cdot \hat{N}_{i'j'}) \sum_{j=1}^{3N-1} \left[(\hat{e}_{i+} \cdot \mathbf{U} \cdot \hat{e}_{j-}) - (\hat{e}_{i+} \cdot \mathbf{U} \cdot \hat{e}_{0-}) \frac{(\hat{e}_{j-} \cdot \hat{N}_{i'j'})}{(\hat{e}_{0-} \cdot \hat{N}_{i'j'})} \right] \delta R_{j-} \ .
\end{aligned} \tag{B14}$$

Equation (B14) can be further simplified by using

$$(\hat{e}_{i+} \cdot \mathbf{U} \cdot \hat{e}_{0-}) (\hat{e}_{j-} \cdot \hat{N}_{i'j'}) = \{(\hat{e}_{i-} \cdot \mathbf{U} \cdot \hat{e}_{0-}) + 4 (\hat{e}_{i-} \cdot \hat{N}_{i'j'}) (\hat{e}_{0-} \cdot \hat{N}_{i'j'})\} (\hat{e}_{j-} \cdot \hat{N}_{i'j'}), \tag{B15}$$

$$(\hat{e}_{i+} \cdot \mathbf{U} \cdot \hat{e}_{j-}) (\hat{e}_{0-} \cdot \hat{N}_{i'j'}) = \{(\hat{e}_{i-} \cdot \mathbf{U} \cdot \hat{e}_{j-}) + 4 (\hat{e}_{i-} \cdot \hat{N}_{i'j'}) (\hat{e}_{j-} \cdot \hat{N}_{i'j'})\} (\hat{e}_{0-} \cdot \hat{N}_{i'j'}) \tag{B16}$$

and Eq. (B13), to obtain

$$[\mathbf{A} \cdot \delta\vec{R}^*_-] \cdot \hat{e}_{i+} = \sum_{j=1}^{3N-1} W_{ij} \, \delta R_{j-}, \tag{B17}$$

where

$$\begin{aligned}
W_{ij} = W_{ji} = \frac{1}{\sqrt{2}\, a} \Bigg[& (\hat{e}_{i-} \cdot \hat{N}_{i'j'}) (\hat{e}_{j-} \cdot \mathbf{U} \cdot \hat{e}_{0-}) + (\hat{e}_{j-} \cdot \hat{N}_{i'j'})(\hat{e}_{i-} \cdot \mathbf{U} \cdot \hat{e}_{0-}) \\
& - (\hat{e}_{i-} \cdot \mathbf{U} \cdot \hat{e}_{j-}) (\hat{e}_{0-} \cdot \hat{N}_{i'j'}) - (\hat{e}_{j-} \cdot \hat{N}_{i'j'}) (\hat{e}_{i-} \cdot \hat{N}_{i'j'}) \frac{(\hat{e}_{0-} \cdot \mathbf{U} \cdot \hat{e}_{0-})}{(\hat{e}_{0-} \cdot \hat{N}_{i'j'})} \Bigg].
\end{aligned} \tag{B18}$$

Equation (B18) is then used in Eq. (B7).

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