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Velocity dependent invariants for hard particles in one dimension

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Abstract. The relative motion of N impenetrable mass points in one dimension is shown to be equivalent to a billiard in a simplex of $N-1$ dimension, the orientation of the confining hyperplanes being fixed by the mass ratios. The discrete group generated by reflections in these planes and its closure in $SO(N-1)$ are used to show that the only invariant functions of the particle velocities are total momentum and total energy, if $N > 3$ and at least one mass is different from the others.

1. Introduction

For a long time systems of hard particles which move on a line or ring and interact through elastic collisions have been studied to get more insight into the foundations of statistical mechanics. Results for finite systems ($N < \infty$) of identical particles ('rods') can be found in Kasperkovitz and Reisenberger (1985a) and the references cited therein. These systems are known to be integrable, i.e. the motion of the N particles is equivalent to the free motion on a torus. There are two ways to establish this equivalence. The first approach is to consider the hard-core potential as the limit of the repulsive potential $V_g(x) = g/\sin x$ for $g \downarrow 0$. Linear chains of N particles with nearest-neighbour interaction V_g , $g > 0$, meet the criterion of integrability because they possess N linearly independent analytical integrals of motion which are in involution (Olshanetsky and Perelomov 1981). These invariants are closely related to a Lie algebra which can be characterised by a finite group generated by reflections (Weyl group). A complete set of invariants allows us, at least in principle, to construct action and angle variables for the system, thereby establishing the connection with the free motion on the torus (Arnold 1980), but to our knowledge this has not yet been done for this chain. The second approach to proving integrability is straightforward. Since equal masses exchange their velocities in a collision, the symmetric polynomials $S_n(\mathbf{V}) = \sum_{i=1}^N v_i^n$, $n = 1, \dots, N$, are invariant under the evolution. However, these invariants are unsuited to determining the evolution completely because the velocities of colliding particles are undefined at the instant of the collision. An efficient method, not related to the invariants S_n , to describe the evolution of phase space functions has been introduced by Jepsen (1965) and used in subsequent work on hard rod systems. Although initially considered only as a trick it anticipated the definition of action and angle variables. The systematic construction of these variables, described in Kasperkovitz and Reisenberger (1985b), exploits the fact that the relative motion of the N particles may be transformed into a billiard in $N-1$ dimensions. The volume of the billiard is a simplex from which a tiling of \mathbf{R}^{N-1} is obtained by iterative reflections in the bounding

hyperplanes. The unit cell of the resulting periodic structure corresponds to the torus and the evolution appears as free motion in \mathbf{R}^{N-1} . The relation to the integrable chain is seen in the set of reflections that leave a corner of the simplex, in which the billiard takes place, invariant; this group is isomorphic to the Weyl group mentioned above.

Much less is known for systems with different masses ('inhomogeneous systems'). Computer simulations have been performed for mixtures of two different masses (Masoliver and Marro 1983, Marro and Masoliver 1985a, b) and a mass $m(\neq 1)$ in a bath of particles of unit mass (Omerti *et al* 1986, Foidl 1987). For these systems time averages of various phase space functions (one-particle velocity distribution, collision frequency, etc) have been found to agree, for most of the runs, with the averages over all states having the same total momentum and total energy as the initial state (Foidl *et al* 1987, Foidl 1987). This suggests non-existence of additional invariants besides total momentum and energy, at least for large systems ($N \sim 10^3$), and favours the ergodic hypothesis. However, numerical simulation of three-particle systems (Casati and Ford 1976, Rabouw and Ruijgrok 1981) revealed unexpected discrepancies of time and ensemble averages. On the theoretical side Hobson (1975) showed that the relative motion of three hard points on a ring is equivalent to a billiard in a triangle, no matter how the masses are chosen, and that a third invariant exists for a countable set of mass ratios. Apart from three integrable systems all these exceptional cases belong to the class of pseudo-integrable or almost integrable systems which take an intermediate position between integrable and ergodic systems (Zemlyakov and Katok 1976, Richens and Berry 1981, Eckhardt *et al* 1984, Gutkin 1986).

In this paper the results of Hobson (1975) are extended to systems with more than three particles. In § 2 the dynamics of N hard particles enclosed by a massless freely movable box is formulated as a billiard in a tube of dimension N ; for a fixed container this equivalence has been shown by Cornfeld *et al* (1982, p 152). In § 3 the reflections in the confining hyperplanes are used to characterise and classify those invariants which depend on the velocities only. The result of this discussion is summarised in § 4.

2. Equivalence with a billiard problem

The model considered in the following consists of N particles labelled by $i = 1, \dots, N$. The velocities of the particles, $v_i \in \mathbf{R}$, may be combined into a column vector $\mathbf{V} \in \mathbf{R}^N$ the transpose of which is $\mathbf{V}^T = (v_1, \dots, v_N)$. We also assume $x_i \in \mathbf{R}$, meaning that the particles move on a straight line, and denote \mathbf{X} or $\mathbf{X}^T = (x_1, \dots, x_N)$ as the configuration of the system. The particles are assumed to be enclosed by a box (or frame) which is rigid, massless and freely movable along the line. This device makes the first and the last particle interact like nearest neighbours and serves to define the volume of the system (cf figure 1 of Kasperkovitz and Reisenberger (1985a)). The mass of particle i is denoted by m_i and the sequence m_1, \dots, m_N is called the mass distribution of the system. The particles are assumed to move freely until two of them, say i and $i+1$, collide. In such an event the velocity vector \mathbf{V} is changed into $A_i \mathbf{V}$ where A_i is the following block diagonal matrix:

$$A_i = E(i-1) \oplus a_i \oplus E(N-1-i) \quad (1)$$

$$a_i = \frac{1}{m_i + m_{i+1}} \begin{pmatrix} m_i - m_{i+1} & 2m_{i+1} \\ 2m_i & m_{i+1} - m_i \end{pmatrix} \quad (2)$$

$$E(s) = \text{unit matrix of dimension } s. \quad (3)$$

It should be noted that the dynamics remains well defined if some of the masses tend to infinity. For instance, if $m_{i+1} \uparrow \infty$ then v_i changes into $-v_i + 2v_{i+1}$ in a collision while v_{i+1} remains unchanged. Since we consider only systems where E/N , the average energy per particle, is finite the limit $m_j \uparrow \infty$ will always include the limit $v_j \downarrow 0$, i.e. infinite masses are always assumed to be at rest. It is intuitively clear and may easily be derived from the form of the matrices A_i , (1)-(3), that the infinite masses divide the system into subsystems consisting of finite masses which move as if they were trapped by fixed walls. Since these subsystems evolve in time independently of each other it is sufficient to consider two prototypes only: (i) $m_i < \infty$ for $i = 1, \dots, N$ and (ii) $m_i < \infty$ for $i = 1, \dots, N - 1$ and $m_N = \infty$; in this case the fixed walls are formed by the mass m_N and the massless box linked to it.

In principle each of the particles could have its own diameter so that the hard core of particle i would extend from $x_i - (d_i/2)$ to $x_i + (d_i/2)$. This kind of inhomogeneity, however, does not affect the dynamics in an essential way since one may always pass from extended particles to point particles by a linear transformation in the positional variables ($x_1 \rightarrow x_1, x_2 \rightarrow x_2 - (d_1 + d_2)/2, x_3 \rightarrow x_3 - (d_1 + 2d_2 + d_3)/2, \dots$; $L \rightarrow L - (d_1 + \dots + d_N)$). Finite diameters only show up in spatial expectation values such as pair distribution functions or static structure factors. This topic has been discussed in detail elsewhere (Foidl 1986); we therefore restrict the following discussion to point particles.

In the following we always consider first a system consisting of finite masses only, discussing the limit $m_N \uparrow \infty$ afterwards whenever this is formally possible. Let the matrix M and the vector \mathbf{M} be defined by

$$M = \text{diag}(m_1, \dots, m_N) \quad \mathbf{M}^T = (m_1, \dots, m_N). \tag{4}$$

It then follows from (1)-(3) that

$$A_i^T M A_i = M \quad A_i^T \mathbf{M} = \mathbf{M}. \tag{5}$$

These equations show that the total energy and the total momentum

$$E = \frac{1}{2} \mathbf{V}^T M \mathbf{V} \quad \mathbf{P} = \mathbf{M}^T \mathbf{V} \tag{6}$$

are conserved in a collision. In (5) and (6) we used the notation A^T for the transpose of the matrix A and $\mathbf{U}^T \mathbf{W}$ for the scalar product of two column vectors. To show the equivalence with a billiard problem we need the matrix

$$L = M^{1/2} = \text{diag}(\sqrt{m_1}, \dots, \sqrt{m_N}) = L^T. \tag{7}$$

This matrix transforms A_i into

$$B_i = L A_i L^{-1} = E(i-1) \oplus b_i \oplus E(N-1-i) = B_i^T \tag{8}$$

with

$$b_i = \begin{pmatrix} \Delta_i & \Gamma_i \\ \Gamma_i & -\Delta_i \end{pmatrix} = b_i^T \tag{9}$$

$$\Delta_i = \frac{m_i - m_{i+1}}{m_i + m_{i+1}} \quad \Gamma_i = \frac{2(m_i m_{i+1})^{1/2}}{m_i + m_{i+1}} > 0. \tag{10}$$

$$\Delta_i^2 + \Gamma_i^2 = 1 \tag{11}$$

$$B_i^2 = E(N). \tag{12}$$

Equations (12) imply conservation of total energy E . Conservation of total momentum P is contained in the relation

$$B_i \mathbf{K} = \mathbf{K} \quad (13)$$

where

$$\mathbf{K}^T = (L^{-1} \mathbf{M})^T = (\sqrt{m_1}, \dots, \sqrt{m_N}). \quad (14)$$

The positions and the velocities of the particles are transformed according to $\mathbf{X} \rightarrow \mathbf{Y}$, $\mathbf{V} \rightarrow \mathbf{W}$, where

$$\begin{aligned} \mathbf{Y}^T &= (L\mathbf{X})^T = (\sqrt{m_1}x_1, \dots, \sqrt{m_N}x_N) \\ \mathbf{W}^T &= (L\mathbf{V})^T = (\sqrt{m_1}v_1, \dots, \sqrt{m_N}v_N). \end{aligned} \quad (15)$$

In these new coordinates the change of velocities caused by a collision of particles i and $i+1$ appears now as $\mathbf{W} \rightarrow B_i \mathbf{W}$. Introducing unit vectors \mathbf{E}_j , $j = 1, \dots, N$, with components

$$(\mathbf{E}_j)_i = \delta_{i,j} \left(\frac{m_{j+1}}{m_j + m_{j+1}} \right)^{1/2} - \delta_{i,j+1} \left(\frac{m_j}{m_j + m_{j+1}} \right)^{1/2} \quad (16)$$

we may write the spectral decomposition of B_i as

$$B_i = E(N) - 2\mathbf{E}_i \mathbf{E}_i^T. \quad (17)$$

This equation allows us to interpret the transition $\mathbf{W} \rightarrow B_i \mathbf{W} = \mathbf{W} - 2\mathbf{E}_i (\mathbf{E}_i^T \mathbf{W})$ as reflection of the vector \mathbf{W} in the hyperplane $\mathbf{E}_i^T \mathbf{W} = 0$. This transition occurs when the two particles approach each other before they get into contact, i.e. for $\mathbf{E}_i^T \mathbf{W} > 0$ ($\Leftrightarrow v_i > v_{i+1}$) and

$$\mathbf{E}_i^T \mathbf{Y} = 0 \quad (\Leftrightarrow x_i = x_{i+1}). \quad (18)$$

Up to now we have tacitly assumed that i ranges from 1 to $N-1$. For the furthest particles, N and 1, the non-vanishing elements of the collision matrix B_N are $(B_N)_{2,2} = \dots = (B_N)_{N-1,N-1} = 1$ and $(B_N)_{N,N} = -(B_N)_{1,1} = \Delta_N$, $(B_N)_{N,1} = (B_N)_{1,N} = \Gamma_N$, where Δ_N and Γ_N are given by (10) with $i=N$ and $i+1=1$. This collision occurs for $\mathbf{E}_N^T \mathbf{W} > 0$ ($\Leftrightarrow v_N > v_1$) and

$$\mathbf{E}_N^T \mathbf{Y} = L \left(\frac{m_N m_1}{m_N + m_1} \right)^{1/2} \quad (\Leftrightarrow x_N = x_1 + L) \quad (19)$$

where

$$(\mathbf{E}_N)_i = \delta_{i,N} \left(\frac{m_1}{m_N + m_1} \right)^{1/2} - \delta_{i,1} \left(\frac{m_N}{m_N + m_1} \right)^{1/2}. \quad (20)$$

Note that all unit vectors \mathbf{E}_j are orthogonal to the vector \mathbf{K} .

The region confined by the N hyperplanes (18) and (19) is a cartesian product $\mathbf{R} \times \Sigma^{N-1}$ where Σ^{N-1} is a simplex of dimension $N-1$ (a triangle for $N=3$, a tetrahedron for $N=4$, etc). This domain has the form of a straight pipe with cross section Σ^{N-1} , extending to infinity in the direction of the vector (14). Moving in this direction corresponds to a rigid translation of the whole system. Since $\mathbf{K}^T \mathbf{Y}$ is the position of the centre of mass, moving normal to \mathbf{K} corresponds to a relative motion of the particles which leaves the centre of mass unchanged. This kind of motion is limited by the fact that the particles are assumed to be impenetrable and to be enclosed

by a movable box of length L . To require that $\mathbf{Y} \in \mathbf{R} \times \Sigma^{N-1}$, i.e. $\mathbf{E}_1^T \mathbf{Y} < 0, \mathbf{E}_2^T \mathbf{Y} < 0, \dots, \mathbf{E}_{N-1}^T \mathbf{Y} < 0$, and $\mathbf{E}_N^T \mathbf{Y} < L[m_N m_1 / (m_N + m_1)]^{1/2}$, is nothing but the requirement $x_1 < x_2 < \dots < x_1 + L$. As long as \mathbf{Y} is in the interior of $\mathbf{R} \times \Sigma^{N-1}$ the evolution is given by $\mathbf{Y}_{t+t'} = \mathbf{Y}_t + \mathbf{W}_t t'$ since the velocities contained in \mathbf{W} do not change. If \mathbf{Y} hits one of the confining planes \mathbf{W} is changed as in a specular reflection. Along the axis of the tube the representative point \mathbf{Y} moves freely

$$\mathbf{K}^T \mathbf{Y}_t = \mathbf{K}^T (\mathbf{Y}_0 + \mathbf{W}_0 t) \tag{21}$$

in accordance with the conservation of the total momentum P . Note that the motions parallel and normal to \mathbf{K} do not interfere with each other.

3. Velocity dependent invariants and groups generated by reflections

Formally, the evolution of the system is described by functions $\mathbf{W}_t[\mathbf{W}, \mathbf{Y}]$ and $\mathbf{Y}_t[\mathbf{W}, \mathbf{Y}]$, $t \in \mathbf{R}$, whose values $(\mathbf{W}_t, \mathbf{Y}_t)$ characterise the state of the system at time t if its state at $t = 0$ has been (\mathbf{W}, \mathbf{Y}) . A function that does not change its value along the orbits in phase space

$$g(\mathbf{W}, \mathbf{Y}) = g(\mathbf{W}_t[\mathbf{W}, \mathbf{Y}], \mathbf{Y}_t[\mathbf{W}, \mathbf{Y}]) \quad \text{for all } t \in \mathbf{R} \tag{22}$$

is called an invariant. To make a complete list of all the invariants of a hard rod system with arbitrary masses is still an open problem. However, it is possible to classify those invariants that do not depend on the position variables. These functions satisfy, by definition, the following equation:

$$\tilde{g}(\mathbf{W}) = \tilde{g}(\mathbf{W}_t[\mathbf{W}, \mathbf{Y}]) \quad \text{for all } t \in \mathbf{R} \text{ and all } \mathbf{Y} \in \mathbf{R} \times \Sigma^{N-1}. \tag{23}$$

Examples of such invariants are the total momentum, $P = \mathbf{K}^T \mathbf{W}$, and the total energy, $E = \frac{1}{2} \mathbf{W}^T \mathbf{W}$. Equation (23) is obviously satisfied if

$$\tilde{g}(\mathbf{W}) = \tilde{g}(B_i \mathbf{W}) \quad \text{for } i = 1, \dots, N. \tag{24}$$

That this condition is also necessary for (23) to hold, if \tilde{g} is continuous, can be seen as follows. Since \tilde{g} is continuous we may assume without loss of generality that $w_i \neq w_{i+1}$ in the argument. Moreover we may choose \mathbf{Y} in such a way that the particles i and $i+1$ are arbitrarily close to each other. Therefore these particles will either collide next ($w_i > w_{i+1}, t > 0$) or else they took part in the last collision ($w_i < w_{i+1}, t < 0$); in both cases $\mathbf{W}_t = B_i \mathbf{W}$ and (23) yields (24) for this transformation B_i .

The same reasoning applies for time averages

$$\bar{g}(\mathbf{W}, \mathbf{Y}) = \lim_{T', T'' \rightarrow \infty} \frac{1}{T' + T''} \int_{-T'}^{T''} dt g(\mathbf{W}_t[\mathbf{W}, \mathbf{Y}], \mathbf{Y}_t[\mathbf{W}, \mathbf{Y}]) \tag{25}$$

which obviously satisfy (22). If such an average turns out to be independent of the initial configuration \mathbf{Y} , then the function $\bar{g}(\mathbf{W}, \mathbf{Y}) = \bar{g}(\mathbf{W})$ has to satisfy (24).

The equivalence of (23) and (24) may also be described in terms of ensembles. The smallest stationary ensemble containing the subset $\mathbf{R} \times \Sigma^{N-1} \times \{\mathbf{W}\}$ is $\mathbf{R} \times \Sigma^{N-1} \times \{G\mathbf{W} | G \in \mathcal{G}\}$ where

$$\mathcal{G} = \text{matrix group generated by } B_1, \dots, B_N. \tag{26}$$

In this proposition \mathbf{R} may be replaced by a singleton set $\{x_{CM}\}$ if $P = \mathbf{K}^T \mathbf{W} = 0$.

To classify these stationary ensembles and the invariants (24) as functions of the masses m_1, \dots, m_N we have to determine the structure of \mathcal{G} as a function of these parameters. It follows from the very definition of \mathcal{G} that it is a countable group

generated by a finite number of elements of order two (see (12)). Groups of this kind have been studied for a long time (Coxeter and Moser 1965, Hiller 1982) and it has been shown that the cardinality of these groups is uniquely determined by the orders of those group elements that are formed by a pair of generators. In the present case, $B_i B_j$ is of order two if $i \neq j \pm 1$ (modulo N). If no special relations between the masses m_i, m_{i+1}, m_{i+2} are assumed to exist the element $B_i B_{i+1}$ will be of infinite order and hence \mathcal{G} will be a countable group. As will be shown later, \mathcal{G} is an infinite group even if all elements $B_i B_{i+1}$ (indices modulo N) are of finite order, the only exceptions being the free homogeneous system ($m_1 = \dots = m_{N-1} = m_N < \infty$) and the homogeneous system with fixed walls ($m_1 = \dots = m_{N-1} < m_N = \infty$).

However, these results do not give much insight into the problem at hand. For if \mathcal{G} is infinite it is obvious that the set $\{GW_0 | G \in \mathcal{G}\}$ must have accumulation points on the reduced energy surface $\{E = E_0\} \cap \{P = P_0\}$; but proving the infinity of \mathcal{G} along the lines of Coxeter and Moser (1965) and Hiller (1982) does not tell us how many of these points exist nor where they might be located. Moreover, it is impossible to infer from this proof whether the set $\{GW_0 | G \in \mathcal{G}\}$ is contained in a proper closed subset of the sphere

$$S_0^{N-2} = \{W | W^T W = W_0^T W_0, K^T W = K^T W_0\} \tag{27}$$

which would indicate the existence of constants of motion in addition to total energy and total momentum. In the present context it is therefore more useful to investigate the status of \mathcal{G} as a subgroup of $\mathcal{O}(N)$, the symmetry group of the energy surfaces $E = W^T W = \text{constant}$. Because of (13) \mathcal{G} is actually a subgroup of that subgroup of $\mathcal{O}(N)$ which leaves K invariant. To make this fact more transparent we pass from the variables W, Y to new variables U, Z which are essentially the well known Jacobi coordinates (Blochinzew 1953, p 532).

$$U = R^T W \quad Z = R^T Y \quad R^T R = R R^T = E(N) \tag{28}$$

$$j = 1, \dots, N-1 \quad R_{i,j} = \begin{cases} 0 & \text{for } i < j \\ (M_{j+1}/M_j)^{1/2} & \text{for } i = j \\ -(m_i m_j / M_j M_{j+1})^{1/2} & \text{for } i > j \end{cases} \tag{29}$$

$$j = N \quad R_{i,N} = (m_i / M_1)^{1/2} \tag{30}$$

$$M_k = \sum_{i=k}^N m_i. \tag{31}$$

Under this transformation the matrices B_i are transformed into the matrices

$$C_i = R^T B_i R = C_i^T \tag{32}$$

$$i = 1, \dots, N-1 \quad C_i = E(i-1) \oplus c_i \oplus E(N-1-i) \tag{33}$$

$$c_i = \begin{pmatrix} \delta_i & \gamma_i \\ \gamma_i & -\delta_i \end{pmatrix} = c_i^T \tag{34}$$

$$\delta_i^2 + \gamma_i^2 = 1 \tag{35}$$

$$i = 1, \dots, N-2 \quad \delta_i = \frac{m_i M_{i+2} - m_{i+1} M_i}{(m_i + m_{i+1}) M_{i+1}} \tag{36}$$

$$\gamma_i = \frac{2(m_i m_{i+1} M_i M_{i+2})^{1/2}}{(m_i + m_{i+1}) M_{i+1}} > 0$$

$$i = N-1 \quad \delta_{N-1} = -1 \quad \gamma_{N-1} = 0. \tag{37}$$

Because

$$\sqrt{M_1}u_N = P \tag{38}$$

the last component of U is not changed by any of the transformations C_i . The group \mathcal{H}' ,

$$\mathcal{H}' = \text{matrix group generated by } C_1, \dots, C_N \tag{39}$$

is therefore considered as a subgroup of $\mathcal{O}(N-1)$

$$\mathcal{O}(N-1) = \text{group of orthogonal matrices leaving } z_N \text{ invariant} \tag{40}$$

which is the symmetry group of the $(N-1)$ -dimensional sphere (27). For technical reasons we first study the group

$$\mathcal{H} = \text{matrix group generated by } C_1, \dots, C_{N-1} \tag{41}$$

and discuss its extension $\mathcal{H}' (\simeq \mathcal{G})$ afterwards.

The group $\mathcal{O}(N-1)$ is one of the classical Lie groups. The groups \mathcal{H} and \mathcal{H}' are subgroups in the algebraic sense, but in general not topological subgroups of $\mathcal{O}(N-1)$. The smallest analytical subgroup containing \mathcal{H} is the group

$$\bar{\mathcal{H}} = \text{closure of } \mathcal{H} \tag{42}$$

which is considered as the topological subspace of the topological space $\mathcal{O}(N-1)$ (Cohn 1961, pp 39, 53, 123, 127). This group contains a normal subgroup

$$\bar{\mathcal{H}}_0 = \text{identity component of } \bar{\mathcal{H}} \tag{43}$$

which is both open and closed. Therefore the factor group

$$\bar{\mathcal{H}}/\bar{\mathcal{H}}_0 = \mathcal{F} \tag{44}$$

is discrete and, since $\mathcal{O}(N-1)$ is compact, even finite. Keeping in mind that the sphere S^{N-2} may be identified with the homogeneous space $\mathcal{SO}(N-1)/\mathcal{SO}(N-2)$ we therefore arrive at the following picture. The set $\{HW_0 | H \in \mathcal{H}\}$ is a dense subset of the set $\{\bar{H}W_0 | \bar{H} \in \bar{\mathcal{H}}\}$ which consists of a finite number of disjoint subsets of S_0^{N-2} .

The result obtained up to now holds for any subgroup of $\mathcal{O}(N-1)$. However the definition of \mathcal{H} by means of generators, (41), and the special form of these matrices, (33)-(37), admit only two possibilities: either $\bar{\mathcal{H}} = \mathcal{O}(N-1)$ and $\{HW_0 | H \in \mathcal{H}\}$ is dense in S_0^{N-2} ; or $\bar{\mathcal{H}} = \mathcal{H}$ is a finite group and $\{HW_0 | H \in \mathcal{H}\}$ consists of a finite number of points on S_0^{N-2} .

To prove this proposition let us consider the Lie algebra of $\bar{\mathcal{H}}$, i.e.

$$\mathfrak{h} = \text{Lie algebra of } \bar{\mathcal{H}} \subseteq \mathfrak{so}(N-1). \tag{45}$$

The elements of \mathfrak{h} are closely related to infinite cyclic subgroups of \mathcal{H} . For if H is the product of an even number of generators C_i then $\det H = 1$ and H corresponds to a set of finite rotations, simultaneously performed in two-dimensional subspaces orthogonal to each other. If H is of infinite order then each neighbourhood of the unit matrix $E(N)$ contains infinitely many powers of H . The cyclic group generated by such a transformation H is embedded in a one-parameter subgroup of $\bar{\mathcal{H}}_0 = \{\exp L | L \in \mathfrak{h}\}$ if we pass from \mathcal{H} to $\bar{\mathcal{H}}$. Thus $\mathfrak{h} \neq 0$ if \mathcal{H} contains at least one element of infinite order. On the other hand, if $\mathfrak{h} = 0$ then $\bar{\mathcal{H}}_0 = \{E(N)\}$ and \mathcal{H} is finite because $\mathcal{F} \simeq \mathcal{H}$ in this case and \mathcal{F} is a finite group.

The form of the algebra \mathfrak{h} , which determines the group \mathcal{H}_0 , emerges from the fact that the mappings $L \rightarrow C_n L C_n, L \in \mathfrak{h}, n \in \{1, \dots, N-1\}$, are automorphisms of \mathfrak{h} because $C_n \in \mathcal{H}$ and \mathcal{H}_0 is a normal subgroup of \mathcal{H} . To discuss these automorphisms let us consider first the transformations $L \rightarrow C_n L C_n$ for the elements $L \in \mathfrak{so}(N-1)$. This algebra consists of all real skew-symmetric matrices of the form

$$M = \bar{M} \oplus E(1). \tag{46}$$

In the following discussion we shall consider only the submatrices \bar{M} of the matrices $M = L, C_n, \dots$, but retain the symbols L, C_n, \dots , to avoid a clumsy notation. With these conventions it is obvious that the matrices $L_{i,j}, i \in \{1, \dots, N-2\}, i < j < N$, with elements

$$(L_{i,j})_{k,l} = \delta_{i,k} \delta_{j,l} - \delta_{i,l} \delta_{j,k} \tag{47}$$

form a basis of $\mathfrak{so}(N-1)$. Under the mapping $L \rightarrow C_n L C_n$ these matrices are either invariant or transform according to the following rules ($j > i+1$):

$$\begin{aligned} C_{i-1} L_{i,j} C_{i-1} &= \gamma_{i-1} L_{i-1,j} - \delta_{i-1} L_{i,j} \\ C_j L_{i,j} C_j &= \gamma_j L_{i,j+1} + \delta_j L_{i,j} \end{aligned} \tag{48}$$

$$\begin{aligned} C_i L_{i,j} C_i &= \gamma_i L_{i+1,j} + \delta_i L_{i,j} \\ C_{j-1} L_{i,j} C_{j-1} &= \gamma_{j-1} L_{i,j-1} - \delta_{j-1} L_{i,j}. \end{aligned} \tag{49}$$

Moreover

$$C_i L_{i,i+1} C_i = -L_{i,i+1}. \tag{50}$$

As the coefficients γ_n are positive (cf (36)) it is possible to obtain from one element $L_{i,j}$ all the others by applying the transformations $L \rightarrow C_n L C_n$ and forming suitable linear combinations. In the generic case, where no special relations exist between the masses m_i , the matrix

$$D_{N-2,N-1} = C_{N-2} C_{N-1} = E(N-3) \oplus d_{N-2,N-1} \tag{51}$$

$$d_{N-2,N-1} = \begin{pmatrix} \cos \psi & -\sin \psi \\ \sin \psi & \cos \psi \end{pmatrix} \quad \cos \psi = \delta_{N-1} \quad \sin \psi = \gamma_{N-1} \tag{52}$$

is a finite rotation of infinite order ($\psi \neq$ rational multiple of 2π). The closure of this cyclic group is $\{\exp \lambda L_{N-2,N-1} \mid \lambda \in \mathbf{R}\}$ so that $L_{N-2,N-1} \in \mathfrak{h}$; because of (49), (50) and $C_n \mathfrak{h} C_n = \mathfrak{h}$, this entails $\mathfrak{h} = \mathfrak{so}(N-1)$ and hence $\mathcal{H} = \mathcal{O}(N-1)$.

It remains to discuss what happens if $D_{N-2,N-1}$ is of finite order but $\mathfrak{h} \neq 0$. We now show that also in this case the whole algebra $\mathfrak{so}(N-1)$ may be generated from one element $L \in \mathfrak{h}, L \neq 0$. If $\mathfrak{h} \neq 0$ then there exists an element $L_{(1)} = \sum \lambda_{i,j} L_{i,j}$ with $\lambda_{i,j} = \lambda_{(1)} \neq 0$ for some pair i, j . Applying a series of transformations $L \rightarrow C_n L C_n, n = a, b, \dots, z$, to $L_{(1)}$ we obtain an element $L_{(2)} = \lambda_{(2)} L_{1,2} + \dots$ with $\lambda_{(2)} = \gamma_z, \dots, \gamma_b \gamma_a \lambda_{(1)} \neq 0$. From $L_{(2)}$ we pass to the matrix $L_{(3)} = L_{(2)} - C_1 L_{(2)} C_1$ whose definition implies $C_1 L_{(3)} C_1 = -L_{(3)}$. The matrix $L_{(3)}$ has the form

$$L_{(3)} = \begin{pmatrix} 0 & \lambda_{(3)} & -\gamma_1 \xi^T \\ -\lambda_{(3)} & 0 & (1 + \delta_1) \xi^T \\ \gamma_1 \xi & -(1 + \delta_1) \xi & O(N-3) \end{pmatrix} \tag{53}$$

where $\lambda_{(3)} = 2\lambda_{(2)} \neq 0$ (cf (50)), $O(N-3)$ is the null matrix of dimension $N-3$ and $\xi^T = (\xi_3, \dots, \xi_{N-1})$ is a vector depending on $L_{(1)}$ and the way $L_{(2)}$ has been obtained from $L_{(1)}$.

To show how to get rid of ξ , if $\xi \neq 0$, we introduce matrices $C_i^{(r)}$, $r \in \{0, 1, \dots, N-2\}$, and groups $\mathcal{H}^{(r)}$ by the following definitions:

$$i > r \quad C_i = E(r) \oplus C_i^{(r)} \tag{54}$$

$$\mathcal{H}^{(r)} = \text{matrix group generated by } C_{r+1}^{(r)}, C_{r+2}^{(r)}, \dots, C_{N-1}^{(r)}. \tag{55}$$

These equations show that the group $\mathcal{H}^{(r)}$ is generated by block diagonal matrices of dimension $N-1-r$ which contain the two-dimensional matrices c_{r+1}, \dots, c_{N-1} in the appropriate places. It will be shown below that these matrix groups are irreducible, i.e. there exists no orthogonal matrix that transforms all matrices $H^{(r)} \in \mathcal{H}^{(r)}$ into block form. For $r=2$ this result implies that, given a vector $\xi \neq 0$, we can always find matrices $H_1^{(2)}, H_2^{(2)}, \dots, H_{N-3}^{(2)}$ such that

$$\xi = \sum_{s=1}^{N-3} \kappa_s H_s^{(2)} \xi \quad \sum_{s=1}^{N-3} \kappa_s = \kappa \neq 1 \tag{56}$$

for, if $\mathcal{H}^{(2)}$ is irreducible and $\xi \neq 0$, there exist matrices $H_1^{(2)}, \dots, H_{N-3}^{(2)}$ such that the vectors

$$\eta_s = H_s^{(2)} \xi \quad s = 1, \dots, N-3 \tag{57}$$

span the carrier space of $\mathcal{H}^{(2)}$. With respect to this basis ξ has the representation

$$\xi = \sum_{s=1}^{N-3} \kappa_s \eta_s. \tag{58}$$

If the vectors ζ_t are reciprocal to the vectors η_s ,

$$\zeta_t^T \eta_s = \delta_{t,s} \tag{59}$$

and

$$\zeta = \sum_{s=1}^{N-3} \zeta_s \tag{60}$$

then

$$\xi^T \zeta = \sum_{s=1}^{N-3} \kappa_s. \tag{61}$$

If this sum is different from 1 then relation (56) is satisfied; if it happens to be equal to 1 then we have to look for a new basis. If we transform the basis (57) with a matrix $H^{(2)} \in \mathcal{H}^{(2)}$ we obtain instead of (58) and (61) the following equations:

$$\xi = \sum_{s=1}^{N-3} \kappa_s [H^{(2)}] H^{(2)} \eta_s \tag{62}$$

$$\xi^T H^{(2)} \zeta = \sum_{s=1}^{N-3} \kappa_s [H^{(2)}]. \tag{63}$$

Next we choose a vector $\chi \in \mathbf{R}^{N-3}$ such that

$$\xi^T \chi = 1. \tag{64}$$

Now let us assume that

$$\xi^T (H^{(2)} \zeta - \chi) = \sum_{s=1}^{N-3} \kappa_s [H^{(2)}] - 1 = 0 \quad \text{for all } H^{(2)} \in \mathcal{H}^{(2)}. \tag{65}$$

Since the carrier space of $\mathcal{H}^{(2)} (= \mathbf{R}^{N-3})$ is irreducible it is spanned by the vectors $H^{(2)}\xi$, $H^{(2)} \in \mathcal{H}^{(2)}$, or equivalently by the vectors $H^{(2)}\xi - \chi$, $H^{(2)} \in \mathcal{H}^{(2)}$, χ fixed. The irreducibility of $\mathcal{H}^{(2)}$ and (65) imply $\xi = 0$, contrary to what has been assumed in the beginning. It is therefore always possible, at least after a suitable transformation of the basis chosen initially, to find matrices $H_1^{(2)}, \dots, H_{N-3}^{(2)} \in \mathcal{H}^{(2)}$ such that (56) is satisfied. Assuming such a set to be given we can form the matrix

$$L_{(4)} = L_{(3)} - \sum_{s=1}^{N-3} \kappa_s H_s L_{(3)} H_s = \lambda_{(4)} L_{1,2} \tag{66}$$

where $\lambda_{(4)} = (1 - \kappa)\lambda_{(3)} \neq 0$. Having now obtained the matrix $L_{1,2} \in \mathfrak{so}(N-1)$ we may generate the remaining basis elements by means of (49).

It remains for us to prove that the matrix groups $\mathcal{H}^{(r)}$ are irreducible. We do this by induction. Assume that $\mathcal{H}^{(r)}$ is irreducible; then a real symmetric matrix commuting with $C_{r+1}^{(r)}, \dots, C_{N-1}^{(r)}$ and hence with all matrices $H^{(r)} \in \mathcal{H}^{(r)}$ has to be of the form $aE(N-1-r)$, $a \in \mathbf{R}$. Considering now the direct sum of the identical representation, $H^{(r)} \rightarrow E(1)$, and the defining representation, $H^{(r)} \rightarrow H^{(r)}$, we see that a matrix commuting with all matrices $E(1) \oplus H^{(r)}$, $H^{(r)} \in \mathcal{H}^{(r)}$, has to be of the form $bE(1) \oplus aE(N-1-r)$. This matrix commutes with $C_r^{(r-1)}$ if and only if $a = b$ (cf (34) and (36)). Therefore the matrix group $\mathcal{H}^{(r-1)}$ is irreducible if the matrix group $\mathcal{H}^{(r)}$ has this property. Now $\mathcal{H}^{(N-1)}$ is one dimensional and thus trivially irreducible so that all matrix groups $\mathcal{H}^{(N-1)}, \dots, \mathcal{H}^{(0)}$ are irreducible. This concludes the proof that $\mathfrak{h} \neq 0$ implies $\mathfrak{h} = \mathfrak{so}(N-1)$.

Therefore, if $\bar{\mathcal{H}}_0 \neq \{E(N)\}$ then $\bar{\mathcal{H}}_0 = \mathcal{SO}(N-1)$ and $\bar{\mathcal{H}} = \mathcal{O}(N-1)$ since $\det C_n = -1$. Inclusion of C_N into the set of generators does not change this result since $C_N \in \mathcal{O}(N-1)$. The same holds in the limit $m_N \uparrow \infty$ where

$$\begin{aligned} R &\rightarrow E(N) & C_i &\rightarrow B_i (\delta_i \rightarrow \Delta_i, \gamma_i \rightarrow \Gamma_i) \\ C_{N-1} &= B_{N-1} = \text{diag}(1, \dots, 1, -1, 1) \\ C_N &= B_N = \text{diag}(-1, 1, \dots, 1) \end{aligned} \tag{67}$$

and all the arguments used before apply as well.

We now have to discuss the structure of \mathcal{H} if $\mathfrak{h} = 0$. In this case $\bar{\mathcal{H}}_0 = \{E(N)\}$ and $\bar{\mathcal{H}} = \mathcal{F}$ is a finite group which coincides with \mathcal{H} since \mathcal{H} is dense in $\bar{\mathcal{H}}$. The group \mathcal{H} is then a finite group generated by reflections. These groups have been classified a long time ago (Coxeter and Moser 1965), where it has been shown that their structure is uniquely determined by the order of the finite rotations formed by pairs of generators

$$(C_i C_j)^{p_{i,j}} = (B_i B_j)^{p_{i,j}} = E(N). \tag{68}$$

The transformation $B_i B_j$ is a rotation in the plane spanned by the vectors E_i and E_j , (16), the angle of rotation being twice the acute angle between the reflecting hyperplanes:

$$-E_i^T E_j = \cos(\pi/p_{i,j}). \tag{69}$$

It follows both from (8) and (16) that

$$p_{i,j} = 2 \quad \text{for } i+1 < j. \tag{70}$$

If this condition holds for the $N-1$ generators and if $N > 3$ the group has to be isomorphic to one of the following groups: the symmetric group \mathcal{S}_N (order $N!$) or the hyperoctahedral group Ω_{N-1} (order $2^{N-1}(N-1)!$). In both cases

$$p_{i,i+1} = 3 \quad \text{for } i = 1, \dots, N-3 \tag{71}$$

and therefore

$$(-\mathbf{E}_i^T \mathbf{E}_{i+1})^{-2} = [\cos(\pi/3)]^{-2} = (1 + m_{i+1}/m_i)(1 + m_{i+1}/m_{i+2}) = 4$$

$$\text{for } i = 1, \dots, N-3. \tag{72}$$

Using these equations we can express the mass ratios $m_1/m_2, \dots, m_{N-2}/m_{N-1}$ as functions of one single ratio m_i/m_{i+1} . Note that (72) admit only configurations where the masses, if they are different, are arranged in a monotonic sequence, i.e. $m_1 < m_2 \dots < m_{N-1}$ or $m_1 > m_2 \dots > m_{N-1}$. If $\mathcal{H} = \mathcal{S}_N$ (71) and (72) have to be supplemented by the equations

$$p_{N-2, N-1} = 3 \tag{73}$$

$$(1 + m_{N-1}/m_{N-2})(1 + m_{N+1}/m_N) = 4. \tag{74}$$

Because of (74) m_N has to follow the monotonicity of the preceding masses ($m_1 < \dots < m_N$ or $m_1 > \dots > m_N$ or $m_1 = \dots = m_N$). If $\mathcal{H} = \Omega_{N-1}$ one has, instead of (73) and (74), the following relations (cf (69)):

$$p_{N-2, N-1} = 4 \tag{75}$$

$$(1 + m_{N-1}/m_{N-2})(1 + m_{N-1}/m_N) = 2. \tag{76}$$

If we resolve (76) for m_{N-1}/m_{N-2} we see that in this case there are only two possibilities for the mass configuration, namely either $m_1 > \dots > m_{N-1}$ and $m_{N-1} < m_N < \infty$ or $m_1 = \dots = m_{N-1}$ and $m_n = \infty$. In any case we are left with a one-parameter family of matrix groups whose members are uniquely fixed by the value of the mass ratio

$$\mu = m_{N-1}/m_N. \tag{77}$$

The generators $C_i(\mu)$ and $C_i(\mu')$ of two members of the one-parameter family are related by an orthogonal transformation and the same holds for the corresponding matrices B_i :

$$B_i(\mu) = U(\mu, \mu') B_i(\mu') U(\mu, \mu')^T \quad \text{for } i = 1, \dots, N-1 \tag{78}$$

$$U(\mu, \mu') U(\mu, \mu')^T = U(\mu, \mu')^T U(\mu, \mu') = E(N). \tag{79}$$

This result follows from the following facts. (i) As can be seen from their spectral decomposition (17) the matrices B_i are uniquely determined by the vectors \mathbf{E}_i . (ii) The unit vectors $\mathbf{E}_1, \dots, \mathbf{E}_{N-1}$ and $\mathbf{K}/|\mathbf{K}|$ form a basis of \mathbf{R}^N . (iii) The angles between these vectors depend only on the structure of the abstract group to which $\mathcal{H}(\mu)$ is isomorphic and not on the value of the parameter μ (cf (69)). The transition from μ to μ' is therefore performed by means of an orthogonal transformation U which is a continuous function of both μ and μ' because the basis vectors $\mathbf{E}_1, \dots, \mathbf{K}/|\mathbf{K}|$ depend continuously on the mass ratios.

If we extend the finite group \mathcal{H} by including the matrix C_N into the set of generators we obtain, in general, an infinite group \mathcal{H}' which is dense in $\mathcal{O}(N-1)$. For if the parameter μ does not fix the mass ratios in a very special way the rotations $C_N C_1$ and $C_{N-1} C_N$ will be of infinite order and \mathfrak{h}' , the Lie algebra of \mathcal{H}' , will therefore be non-empty. But even if these rotations are of finite order we see from the arguments used before for \mathcal{H} that here too there are only two alternatives: either $\mathfrak{h}' \neq \mathbf{0}$ and $\mathcal{H}' = \mathcal{O}(N-1)$ or $\mathfrak{h}' = \mathbf{0}$ and $\mathcal{H}' = \mathcal{H}$ is finite. In the latter case there are again only two possibilities: either $C_N \notin \mathcal{H}$ and \mathcal{H}' is a proper extension of \mathcal{H} or $C_N \in \mathcal{H}$ and $\mathcal{H}' = \mathcal{H}$. As will be shown immediately only the second case can be realised for the matrix groups considered here.

It follows from the definition of the generators B_i that

$$B_i B_N = B_N B_i \quad \text{for } i \neq 1, N-1 \tag{80}$$

or, in the notation of (68), that

$$p_{i,N} = 2 \quad \text{for } i \neq 1, N-1. \tag{81}$$

The only extensions of \mathcal{S}_N compatible with condition (81) are \mathcal{S}_{N+1} and Ω_N . If $\mathcal{H} \approx \mathcal{S}_N$ and $\mathcal{H}' \approx \mathcal{S}_{N+1}$ then either

$$p_{1,N} = 3 \quad (1 + m_1/m_N)(1 + m_1/m_2) = 4 \tag{82}$$

$$p_{N-1,N} = 2 \quad [(1 + m_N/m_{N-1})(1 + m_N/m_1)]^{-1} = 0 \tag{83}$$

or

$$p_{N-1,N} = 3 \quad (1 + m_N/m_{N-1})(1 + m_N/m_1) = 4 \tag{84}$$

$$p_{1,N} = 2 \quad [(1 + m_1/m_N)(1 + m_1/m_2)]^{-1} = 0. \tag{85}$$

For the mass distributions considered here $0 < m_i < \infty$ for $i < N$. These conditions show that (85) can never be satisfied. Likewise the only solution of (83) is $m_N = \infty$; but this implies $m_1 < \dots < m_{N-1} < m_N = \infty$ which contradicts (82). Analogous reasoning eliminates the possibility $\mathcal{H} \approx \mathcal{S}_N, \mathcal{H}' \approx \Omega_N$ in which case (82) has to be substituted by

$$p_{1,N} = 4 \quad (1 + m_1/m_N)(1 + m_1/m_2) = 2 \tag{86}$$

and (84) by

$$p_{N-1,N} = 4 \quad (1 + m_N/m_{N-1})(1 + m_N/m_1) = 2. \tag{87}$$

If $\mathcal{H} \approx \Omega_{N-1}$ then condition (80) admits only the extension $\mathcal{H}' \approx \Omega_N$. In that case the necessary conditions for the new generator are again (82) and (83). Here too the solution of the second of these equations is $m_N = \infty$, but this now entails $m_{N-1} = \dots = m_2 = m_1$ (cf (72) and (76)) and again violates (82).

If $C_N \in \mathcal{H}$ then it must be possible to represent C_N as a product of the generators C_1, \dots, C_{N-1} . For $\mathcal{H} \approx \mathcal{S}_N$ this relation is

$$C_N = C_1 C_2 \dots C_{N-2} C_{N-1} C_{N-2} \dots C_2 C_1. \tag{88}$$

The corresponding relation for B_N is easily verified for $\mu = 1$ ($m_1 = \dots = m_N < \infty$) by direct calculation. Because of (78) the same relation between the group element $B_N(\mu)$ and the generators $B_1(\mu), \dots, B_{N-1}(\mu)$ has to hold for all values of μ for which $B_N(\mu) \in \mathcal{H}(\mu)$. If the matrix on the RHS of (88) is multiplied by C_1 from the right the resulting matrix is of order three as can be seen again from the matrix group \mathcal{G} for $\mu = 1$:

$$p_{N,1} = 3 \quad (1 + m_1/m_N)(1 + m_1/m_2) = 4. \tag{89}$$

This equation excludes inhomogeneous mass distributions with $m_1 < \dots < m_N$ or $m_1 > \dots > m_N$, so that $\mathcal{G} \approx \mathcal{H}' \approx \mathcal{H} \approx \mathcal{S}_N$ if and only if the system is homogeneous and $m_n < \infty$. Equation (88) is also valid if $C_N \in \mathcal{H}$ and $\mathcal{H} \approx \Omega_{N-1}$ for the corresponding relation holds for the B in the case $\mu = 0$ ($m_1 = \dots = m_{N-1} < m_N = \infty$). If relation (88) holds true for $\mu = 0$ it has to be valid whenever $B_N(\mu) \in \mathcal{G}(\mu)$. It then follows from (88) that $(B_N B_1)^4 = E(N)$, i.e.

$$p_{N,1} = 4 \quad (1 + m_1/m_N)(1 + m_1/m_2) = 2 \tag{90}$$

which shows that in this case the mass distribution has to be $m_1 = \dots = m_{N-1} < m_N = \infty$.

All these considerations apply also to the three-particle system except that \mathcal{H} can be finite without being isomorphic to \mathcal{S}_3 ($\approx \mathcal{D}_3$) or Ω_2 ($\approx \mathcal{D}_4$). For this system the simplex Σ^2 is a triangle with acute angles, one of which becomes a right angle in the limit $m_3 \uparrow \infty$. Whenever these angles are rational multiples of π the group \mathcal{G} is isomorphic to a dihedral group of finite order and the system is pseudo-integrable.

4. Conclusions

The results of this paper may be summarised as follows. In § 2 we showed that the relative motion of N hard rods is equivalent to a billiard problem in a properly chosen simplex of dimension $N - 1$. If the N hyperplanes confining the simplex are translated into the origin then the group \mathcal{G} generated by reflections on these new hyperplanes characterises the set of velocities that can occur in the system in the course of time. The corresponding vectors $\mathbf{W}^T = (\sqrt{m_1}v_1, \dots, \sqrt{m_N}v_N) \in \mathbf{R}^N$ lie on a sphere S_0^{N-2} which is uniquely determined by the total energy E_0 and the total momentum P_0 of the system. The symmetry group of this sphere is the orthogonal group $\mathcal{O}(N - 1)$ and the group \mathcal{G} is a countable subgroup of it. The main result of § 3 is that \mathcal{G} is dense in $\mathcal{O}(N - 1)$ or finite. For $N > 3$ the second case occurs if, and only if, all masses are equal, with the possible exception of one infinite mass which then acts like a pair of fixed walls enclosing the other particles. In these exceptional cases the system is known to be integrable and there exist N analytic invariants which are polynomial functions of the velocities only. Moreover iterated reflections of the simplex Σ^{N-1} in its confining hyperplanes results in a tiling of \mathbf{R}^{N-1} which can be used to construct action and angle variables for the relative motion. This construction breaks down in the generic case where no special relations between the masses exist. In this case our result shows that the only continuous invariant functions of the velocities are total energy and total momentum. This holds true whenever the system contains at least two different masses, no matter how small this difference may be and which special relations exist between the N masses. These results—as well as computer simulations of inhomogeneous systems—lead us to the conjecture that inhomogeneous hard rod systems (with more than three particles) are ergodic.

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