Dynamics of two interacting particles in classical billiards

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The problem of two interacting particles moving in a d-dimensional billiard is considered here. A suitable coordinate transformation leads to the problem of a particle in an unconventional hyperbilliard. A dynamical map can be readily constructed for this general system, which greatly simplifies calculations. As a particular example, we consider two identical particles interacting through a screened Coulomb potential in a one-dimensional billiard. We find that the screening plays an important role in the dynamical behavior of the system and only in the limit of vanishing screening length can the particles be considered as bouncing balls. For more general screening and energy values, the system presents strong non-integrability with resonant islands of stability.

A system of two interacting bodies moving in an otherwise free space, is one of the few integrable problems known. The reduction to the one-body central force problem allows a solution by quadratures \( \mathbb{I} \). However, once the translational symmetries are broken, as when the system is placed inside a billiard, the center-of-mass (CM) and angular momenta are in general no longer constants of motion. In this case, the classical dynamics of the system may be chaotic even when the geometry yields an otherwise fully integrable one-particle case, as we shall see below.

On the other hand, recent experimental realizations of billiards, such as suitably shaped resonators and quantum dots \( \mathbb{E} \), have allowed the study of the quantum manifestations of well-known classical non-integrability in some billiards \( \mathbb{I} \). In the case of quantum dots, disagreement between theory and experiment has been attributed to geometrical factors \( \mathbb{I} \). A considerable amount of theoretical work exists on the effect that geometry has on the integrability of billiards \( \mathbb{I} \), as well as on their quantum analogs \( \mathbb{E} \). However, the possibility of more than one particle in the quantum dot leaves the usual one-particle approach incomplete. In fact, some experiments have pointed out the importance of electron-electron interaction on various features observed in such mesoscopic systems \( \mathbb{E} \). In this article, we explore the role of the electrostatic interaction introduced when two particles are in the billiard. A formalism for billiards in any dimensions is developed, and as an example, we apply it to the one-dimensional case. Since we are interested in the role of the electrostatic interaction in mesoscopic systems, we consider particles interacting through a screened Coulomb potential.

The hyperbilliard. The problem of two point masses moving along a finite line and suffering elastic impacts with the end walls and between themselves, can be transformed to the motion of one ‘particle’ moving in a triangular billiard. The coordinates of the particle in this billiard are the coordinates of the original masses. The ratio of the masses determines the integrability of the system \( \mathbb{I} \), being regularizable for a particle mass ratio of 1 and 3 (or \( \frac{1}{2} \) \( \mathbb{I} \)).

We now introduce an interaction between the particles and consider the d-dimensional case. Let \( \mathbf{q}_i, \mathbf{p}_i \) (\( i = 1,2 \)) be the position and linear momentum of the \( i \)-th particle. The motion takes place in a d-dimensional billiard, a compact simply-connected region of \( \mathbb{R}^d \) whose boundary is denoted by \( \Gamma \). We assume that \( \Gamma \) is piecewise smooth and defined by \( \nu \) surfaces, \( \Gamma_j = \{ \mathbf{q} : f_j(\mathbf{q}, \alpha_j) = 0 \} \), \( j = 1,\ldots,\nu \), where \( f_j \) and \( \alpha_j \) denote the function and the set of constants which characterize the \( j \)-th surface. These functions define subspaces of dimension \( d-1 \) in \( \mathbb{R}^d \). To fix ideas, we restrict ourselves to flat surfaces, i.e., for \( d = 2 \) (3) the billiards are simple polygons (polyhedrons).

The formalism developed here can be applied to any central-force interaction between the particles. We have selected the screened Coulomb potential, i.e., the Yukawa potential given by \( V(\mathbf{q}_1, \mathbf{q}_2) = e^{-\lambda|\mathbf{q}_2-\mathbf{q}_1|}/|\mathbf{q}_2-\mathbf{q}_1| \), where \( \lambda \) is the screening length. Notice that this potential goes to a \( \delta \)-function when \( \lambda \to \infty \). In this limit, the particles behave as bouncing hard-core balls, i.e., non-interacting impenetrable point particles, for which the dynamics can be integrable, as described above. Hence, for a given energy, \( \lambda \) plays the role of the perturbation parameter. Due to the interaction, a finite value of \( \lambda \) determines the finite effective radius of the particles for a given total energy, as described below.

Considering for simplicity identical-mass particles \( m_1 = m_2 = 1 \), the Hamiltonian for the system is written as

\[
H = \frac{p_1^2}{2} + \frac{p_2^2}{2} + V(\mathbf{q}_1, \mathbf{q}_2) + \sum_{i=1}^{2} \sum_{j=1}^{\nu} U[f_j(\mathbf{q}_i, \alpha_j)],
\]

where the function \( U[f_j(\mathbf{q}_i, \alpha_j)] \) represents the infinite repulsion potential exerted by the \( j \)-th hard wall on the \( i \)-th particle. Analytically, this function could be written in terms of Heaviside functions with a large prefactor. In practice, the normal component of the velocity of the incident particle will be reversed at the moment of bouncing on the billiard walls.
The Hamilton equations can be written as \( \dot{q}_i = p_i \), and \( \dot{p}_i = -\nabla_q V(q_1, q_2) + \sum_{j=1}^{\nu} A_j(p_j) \delta[f_j(q_1, \alpha_j)] \), where \( i = 1, 2 \) and the vector function \( A_j \) represents the change of momentum due to the bounce on the \( j \)-th wall. Given \( d \), the number of degrees of freedom is \( 2d \). Hence, the phase space of the system is \( 4d \)-dimensional.

We now introduce a transformation to center-of-mass and relative coordinates \( \mathbf{R} = (\mathbf{q}_1 + \mathbf{q}_2)/M \), and \( \mathbf{r} = \mathbf{q}_2 - \mathbf{q}_1 \), respectively, where the total mass \( M = 2 \), and the reduced mass \( \mu = \frac{1}{2} \). These equations define a new space of coordinates \( \rho = (\mathbf{r}, \mathbf{R}) \), which is \( 2d \)-dimensional. In this space, we have a new set of equations for the boundary of the billiard, say \( F_j(\rho, \alpha_j) \), \( j = 1, \ldots, \nu \). Every function \( F_j \) now defines a subspace of \( 2d - 1 \) dimensions in \( \rho \)-space.

The Hamilton equations are transformed then to \( \dot{\mathbf{r}} = \frac{\mathbf{p}}{\mu}, \dot{\mathbf{R}} = \frac{\mathbf{P}}{M} \), and

\[
\dot{\mathbf{p}} = -\nabla_V(r) + \sum_{j=1}^{\nu} A_j(p, P) \delta[F_j(r, \mathbf{R}, \alpha_j)],
\]

\[
\dot{\mathbf{P}} = \sum_{j=1}^{\nu} B_j(p, P) \delta[F_j(r, \mathbf{R}, \alpha_j)].
\]

As before, \( A_j \) and \( B_j \) represent the change of the momenta \( \mathbf{p} \) and \( \mathbf{P} \), respectively, due to the bounce on the \( j \)-th wall.

Notice that these equations describe the motion of one particle in the \( \rho \) hyperspace, i.e., we have constructed the hyperbilliard. The description of a system composed by a few masses in terms of one particle in a hyperspace has been used for several cases, including billiards 1, 2, 3. Usually, the hyperspace is constructed without introducing transformations of the coordinates. Here, however, the change to the CM coordinates allows one to get a map in a simple way.

Notice that bounces of the particle in the hyperbilliard correspond to bounces of the masses in the real billiard. The walls of the billiard cause the breaking of the translational symmetry of the system, and as a consequence, the CM momentum is no longer a constant of motion. In the case of non-interacting and equal-mass particles, the changes in the CM momentum are determined only by the geometry of the billiard. In our case, however, the interaction couples the CM and relative momenta after a bounce, which in turn depend on the momenta of each of the original masses. The rotational symmetry is also broken in general and the generator of rotations is no longer a constant of motion either.

The map. Hamilton equations in \( \rho \)-space indicate that between bounces the particle moves freely along the CM coordinate whereas the central force \( V(r) \) acts only along \( \mathbf{r} \). The motions are independent, and only become correlated at each bounce, as the corresponding momenta are changed while keeping the total energy constant. We take advantage of this fact: Consider that the particle at the \( n \)-th bounce has the coordinate \( \rho_n = (r_n, \mathbf{R}_n) \). The condition that the time spent by the particle until the next bounce on the \( j \)-th wall be the same along the \( \mathbf{r} \) and \( \mathbf{R} \) coordinates,

\[
\tau_r(\rho_n, \rho_{n+1}) = \tau_{R_k}(\rho_n, \rho_{n+1}), \quad k = 1, \ldots, d,
\]

represents an interesting opportunity. Here, \( \tau_r(\tau_{R_k}) \) refers to the time along the relative (\( k \)-component of CM) coordinate. The times \( \tau_{R_k} \) for the free motion between collisions can be calculated easily. The l.h.s. in (3) can be obtained by noting that the motion along \( \mathbf{r} \) becomes separable and the time \( \tau_r \) can then be calculated by quadratures, as illustrated below. Equations (3) and the equation corresponding to \( F_j \) result in a set of nonlinear algebraic equations for \( \rho_{n+1} \). We call this set the map of the billiard since it indeed expresses \( \rho_{n+1} \) in terms of \( \rho_n \). This procedure can be easily carried out at least formally in the general case. Notice that this map has not been obtained by means of the usual linearization procedure 1, but rather as an extension of Benettin’s procedure 13. The 1D case, explained in detail now, provides a clear example of this procedure.

The 1D billiard. This system is defined by walls at the end points \( q = \pm \frac{1}{2} \). Because of the interparticle repulsion, the particle 1 (2) never reaches the boundary 2 (1). This implies that \( A_j \), here associated with bounces on the \( j \)-th wall, will describe bounces of the \( j \)-th particle only. The Hamilton equations for the \( r - R \) coordinates are then \( p = \mu \dot{r}, P = MR \dot{R} \), and

\[
\dot{r} = -\frac{dV(r)}{dr} + A_1 \delta(R + \frac{1}{2} - \frac{r}{2}) + A_2 \delta(R - \frac{1}{2} - \frac{r}{2}),
\]

\[
\dot{R} = B_1 \delta(R + \frac{1}{2} - \frac{r}{2}) + B_2 \delta(R - \frac{1}{2} - \frac{r}{2}).
\]

According to the arguments of the \( \delta \)-functions, the point boundaries are transformed into lines in \( \rho \)-space, which define a billiard with an isosceles-triangle shape, similar to the case of non-interacting hard core particles 1, although here is in the \( r - R \) space. The base of this triangle in our case acts as a repulsive wall of potential \( V(r) \). The closest approach to the repulsive wall by the particle (the turning point), depends on the energy associated with the relative motion, \( \epsilon = E - P^2/2M \).

The functions giving the change of momentum are simple. For example, for bounces of the \( i \)-th particle (on \( i-th \) wall) we have \( A_i = -p \pm 2\mu P/M \), where \( P \) and \( p \) are the momenta before the collision, and the + (−) sign refers to \( i = 1 \) (2).

For a pure Coulomb potential \( \lambda = 0 \), \( \tau_r \) can be calculated analytically, so Eq. (3) can be written in the form

\[
\tau\{T_e(\rho_n), T_e(\rho_{n+1})\} = \left| \frac{R_{n+1} - R_n}{P/M} \right|,
\]

where \( \tau \) is the time elapsed going from \( \rho_n \) to \( \rho_{n+1} \), expressed in terms of the time \( T \) spent by the particle from the turning point to \( \rho \),

\[
T_e(\rho) = \frac{r P}{2\epsilon} + \left( \frac{\mu}{2\epsilon} \right)^{\frac{1}{2}} \cosh^{-1}(r\epsilon)^{\frac{1}{2}}.
\]
For $\lambda \leq 1$ we can expand $V(r)$ to first order and obtain the same expression, except that $E$ is shifted to $E - \lambda$. For all different initial conditions there are only a few possible trajectories which can be determined by analyzing the momenta. A simple algorithm can then be obtained to determine the Poincaré surfaces of section. (The details of the motion in $\rho$-space will be presented elsewhere.) This nontrivial algebraic map provides a full description of the dynamics. Its use simplifies calculations a great deal, and allows one to better characterize the system, as we describe below.

To characterize the dynamics, we determine the Poincaré section (PS) at a phase such that one of the masses is fixed, say, as it just bounces on the wall. Then we plot the position and momentum of the other mass due to the inter-particle interaction $[11]$ and correspond in the secondary islands become unstable for the "short-range" case because for some instants the particles are nearly free, the memory of the previous motion is lost, and the correlation is destroyed. Hence, as $\lambda$ decreases (Fig. 2b), the number of stability islands increases. In this case $q_2 = \frac{1}{2}$, so that the PS shows the position and momentum of particle 1 when particle 2 is at the right edge of the billiard. Notice that the available region of space decreases for smaller $\lambda$, as the total energy is fixed and the inter-particle potential energy has a stronger confining effect.

The results using the map described before are now presented. Figure 3 shows the PS for $\lambda = 0$ obtained by solving (a) the differential Hamilton equations in $q$-space, and (b) the algebraic Eq. (3). The graph obtained by means of the latter has been reflected about $q_2 = \frac{1}{2}$ for easy comparison. The two $\lambda = 0$ PS are topologically identical (if traversed in different sequences). The agreement is excellent even for $\lambda \approx 1$, while the computation time is substantially reduced ($\sim 10^3$ times) if the map is used.

Using the map, we have calculated the Lyapunov exponent $\sigma$ for $\lambda \leq 1$, following the procedure of Ref. [3]. Figure 4 shows that, as $\lambda$ increases, the fraction of phase space filled by the chaotic sea increases also. This is reflected in the Lyapunov exponent (not shown), which for a constant energy ($E = 1.56$) increases monotonically (from 0.34 to 0.59) with the inverse screening length $\lambda$ (0 to 1). Increasing energy produces similar curves with ever larger values of $\sigma$.

A general formalism for two interacting particles in a $d$-dimensional billiard has been presented. The one-dimensional case with a screened Coulomb potential was shown to exhibit soft chaos. Only in the case of infinite screening length (or energy), the particles can be considered as bouncing balls. These results suggest that the effects of electrostatic interaction between electrons in quantum dots, for example, may play a very important role in the quantum-classical correspondence and they should be considered when these systems are studied. The analysis of the quantum mechanical analog of the billiard system described in this work is now in progress.

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FIG. 1. The closest approach between the particles, \( r_m \), as a function of the inverse screening length \( \lambda \), for different energies \( E \).

FIG. 2. Poincaré sections for \( E = 1.56 \). a) \( q_1 = -\frac{1}{2}, \lambda = 20 \), b) \( q_2 = \frac{1}{2}, \lambda = 0.6 \). Crosses (×) indicate the symmetric periodic motion.

FIG. 3. Poincaré sections for the selected energy \( E = 1.56 \), \( \lambda = 0 \) and \( q_1 = -\frac{1}{2} \). a) Solving the Hamilton equations and b) using the map.
Fig. 1
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\[ r_m \] vs. \( \lambda \)

- \( E = 1 \)
- \( 1.56 \)
- \( 5 \)
- \( 100 \)
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