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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 nonintegrability with resonant islands of stability. [S1063-651X(97)51006-3]

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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 [1]. However, once the translational symmetries are broken, as when the system is placed inside a billiard, the center-of-mass (c.m.) 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 [2,3], have allowed the study of the quantum manifestations of well-known classical nonintegrability in some billiards [4,5]. In the case of quantum dots, disagreement between theory and experiment has been attributed to geometrical factors [3]. A considerable amount of theoretical work exists on the effect that geometry has on the integrability of dynamics in billiards [4,6–8], as well as on their quantum analogs [5,9]. 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 interactions on various features observed in such mesoscopic systems [10]. 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 (1D) 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 [6], being regularizable for a particle mass ratio of 1 and 3 (or $\frac{1}{3}$) [7].

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 ith particle. The motion takes place in a d-dimensional billiard, a compact simply connected region of $\mathbb{R}^d$ whose boundary is denoted by Γ. We assume that Γ is piecewise smooth and defined by ν surfaces, $\Gamma_j=\{\mathbf{q}: f_j(\mathbf{q},\alpha_j)=0\}$, $j=1,\ldots,\nu$, where f_j and α_j denote the function and the set of constants which characterize the jth 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 λ^{-1} is the screening length. Notice that this potential goes to a δ function when $\lambda\to\infty$. In this limit, the particles behave as bouncing hard-core balls, i.e., noninteracting impenetrable point particles, for which the dynamics can be integrable, as described above. Hence, for a given energy, λ plays the role of the perturbation parameter. Due to the interaction, a finite value of λ 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

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

where the function $U(f_j(\mathbf{q}_i,\alpha_j))$ represents the infinite repulsion potential exerted by the jth hard wall on the ith 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 $\dot{\mathbf{q}}_i=\mathbf{p}_i$ and $\dot{\mathbf{p}}_i=-\nabla_{q_i}V(\mathbf{q}_1,\mathbf{q}_2)+\Sigma_{j=1}^{\nu}\mathbf{A}_j(\mathbf{p}_i)\,\delta(f_j(\mathbf{q}_i,\alpha_j))$, where $i=1,2$ and the vector function $\mathbf{A}_j$ represents the change of momen-

tum due to the bounce on the jth 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 ρ space.

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

$$\dot{\mathbf{p}}=-\nabla_r V(r)+\sum_{j=1}^{\nu}\mathbf{A}_j(\mathbf{p},\mathbf{P})\,\delta(F_j(\mathbf{r},\mathbf{R},\alpha_j)),$$

$$\dot{\mathbf{P}}=\sum_{j=1}^{\nu}\mathbf{B}_j(\mathbf{p},\mathbf{P})\,\delta(F_j(\mathbf{r},\mathbf{R},\alpha_j)). \qquad (2)$$

As before, $\mathbf{A}_j$ and $\mathbf{B}_j$ represent the change of the momenta $\mathbf{p}$ and $\mathbf{P}$, respectively, due to the bounce on the jth wall.

Notice that these equations describe the motion of *one particle* in the ρ 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 [6,7,12]. Usually, the hyperspace is constructed without introducing transformations of the coordinates. Here, however, the change to the c.m. 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 c.m. momentum is no longer a constant of motion. In the case of noninteracting and equal-mass particles, the changes in the c.m. momentum are determined only by the geometry of the billiard. In our case, however, the interaction couples the c.m. 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 ρ space indicate that *between* bounces the *particle* moves freely along the c.m. 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 E constant. We take advantage of this fact: Consider that the *particle* at the nth bounce has the coordinate $\rho_n=(\mathbf{r}_n,\mathbf{R}_n)$. The condition that the time spent by the *particle* until the next bounce at ρ_{n+1} on the jth wall be the same along the $\mathbf{r}$ and $\mathbf{R}$ coordinates,

$$\tau_r(\rho_n,\rho_{n+1})=\tau_{R_k}(\rho_n,\rho_{n+1}),\quad k=1,\ldots,d, \qquad (3)$$

represents an interesting opportunity. Here, τ_r (τ_{R_k}) refers to the time along the relative (k component of c.m.) coordinate. The times τ_{R_k} for the free motion between collisions can be calculated easily. The left-hand-side (LHS) in Eq. (3) can be obtained by noting that the motion along $\mathbf{r}$ becomes separable between bounces and the time τ_r can then be calculated by quadratures, as illustrated below. Equation (3) and the equation corresponding to F_j result in a set of nonlinear algebraic equations for ρ_{n+1}. We call this set the *map* of the billiard since it indeed expresses ρ_{n+1} in terms of ρ_n. The momenta are changed and the next bounce can be determined. This iterative 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 [11], but rather as an extension of Benettin and Strelcyn'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 two ($\nu=2$) 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 $f_1(q_1)=q_1+\frac{1}{2}$ and $f_2(q_2)=q_2-\frac{1}{2}$. Moreover, A_j, here associated with bounces *on* the jth wall, will describe bounces of the jth particle only. The Hamilton equations for the $r-R$ coordinates are then $p=\mu\dot{r}$, $P=M\dot{R}$, and

$$\dot{p}=-\frac{dV(r)}{dr}+A_1\delta\left(R-\frac{r}{2}+\frac{1}{2}\right)+A_2\delta\left(R+\frac{r}{2}-\frac{1}{2}\right),$$

$$\dot{P}=B_1\delta\left(R-\frac{r}{2}+\frac{1}{2}\right)+B_2\delta\left(R+\frac{r}{2}-\frac{1}{2}\right). \qquad (4)$$

According to the arguments of the δ functions, the point boundaries are transformed into lines in ρ space ($F_1=R-r/2+\frac{1}{2}$, $F_2=R+r/2-\frac{1}{2}$), which define a billiard with an isosceles-triangle shape, similar to the case of noninteracting hard-core particles [6], although here the billiard is in the r-R space. The base of this triangle in our case acts as a repulsive wall of potential $V(r)$. The motion inside this billiard can be determined as follows.

After the bounce on (r_n,R_n), the *particle* describes a trajectory, in general towards the base, under the action of the potential. The closest approach to the repulsive base (the turning point) depends on the energy associated with the relative motion for that trajectory, $\epsilon=E-P^2/2M$. The *particle* will then move away from the base, until the next bounce takes place at (r_{n+1},R_{n+1}), this latter one satisfying any of the lines F_i, i.e., at the intersection of the trajectory and the boundary of the hyperbilliard. Then, the momenta are changed and the procedure is repeated iteratively. The functions giving the change of momentum are simple. For example, for bounces of the ith particle (on the ith wall) we have $A_i=-p\pm 2\mu P/M$, where P and p are the momenta immediately *before* the collision, and the $+(-)$ sign refers to $i=1$ (2).

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

$$\tau\{T_\epsilon(r_n),T_\epsilon(r_{n+1})\}=\left|\frac{R_{n+1}-R_n}{P/M}\right|, \qquad (5)$$

where τ is the time elapsed going from r_n to r_{n+1}, expressed in terms of the time T spent by the particle from the turning point to r,

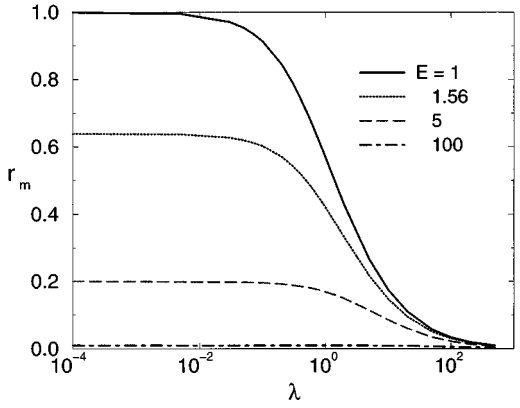

FIG. 1. The closest approach between the particles, r_m, as a function of the inverse screening length λ, for different energies E.

$$T_\epsilon(r)=\frac{rp}{2\epsilon}+\left(\frac{\mu}{2\epsilon^3}\right)^{1/2}\cosh^{-1}(r\epsilon)^{1/2}. \tag{6}$$

For $\lambda\leqslant 1$ we can expand $V(r)$ to first order and obtain the same expression for T, except that E is shifted to $E-\lambda$. For all different initial conditions there are only a few possible trajectories (the *particle* bounces either on the same or different wall, and reaches or not the turning point), which can be determined by analyzing the momenta. A simple algorithm can then be obtained to solve Eq. (5) for r_{n+1} and determine the Poincaré surfaces of section [e.g., when the *particle* reaches the turning point, $\tau=T_\epsilon(r_n)+T_\epsilon(r_{n+1})$]. 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. Because of the indistinguishability of the particles, the topology of the PS does not depend on which mass is selected. In fact, the surfaces are identical, except for left-right exchange symmetry.

Between bounces on the walls, the masses approach each other a distance given by their relative energy. The shortest distance of approach, r_m, can be considered as twice the minimum effective radius of the particles (for zero c.m. energy). This effective radius is a characteristic of the system and its dependence on the total energy E and the inverse screening length λ is shown in Fig. 1, as obtained from the condition $E=V(r_m)$. When $\lambda\gg 1$, the interaction is short ranged, which results in nearly free particles for some moments. Note that for all values of E and λ, the initial condition $q_1^{(0)}=-\frac{1}{2}$, $q_2^{(0)}=\frac{1}{2}$, $p_1^{(0)}=[E-V(1)]^{1/2}$, $p_2^{(0)}=-p_1^{(0)}$ corresponds to a periodic orbit and we call it the *symmetric* motion.

We now fix $E=1.56$ and change λ. Figure 2(a) shows the PS for the ''short-range potential'' case $\lambda=20$. These results were obtained by direct numerical integration of the equations of motion. Here $q_1=-\frac{1}{2}$, which means that we are plotting the position and momentum of the particle 2 as particle 1 is at its (left) edge of the billiard. According to the

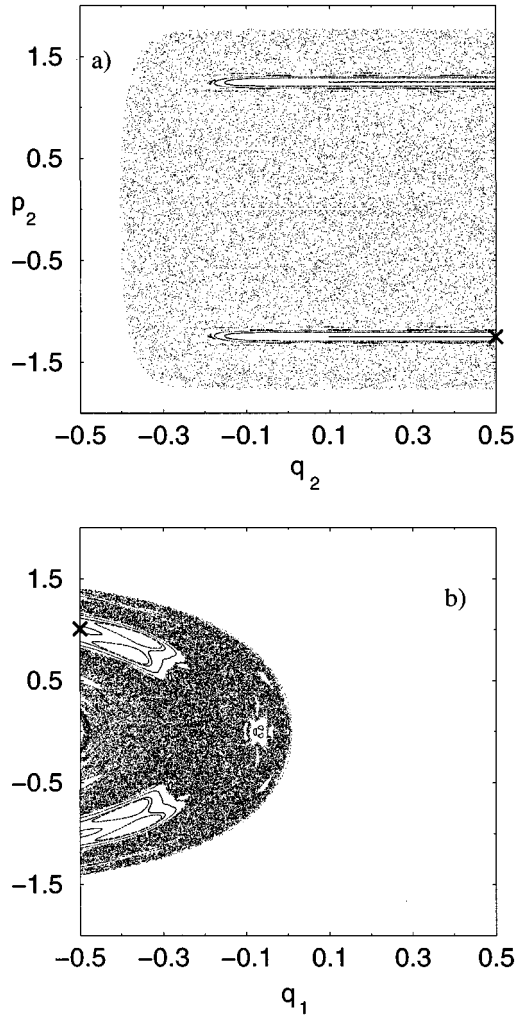

FIG. 2. Poincaré sections for $E=1.56$. (a) $q_1=-\frac{1}{2}$, $\lambda=20$, and (b) $q_2=\frac{1}{2}$, $\lambda=0.6$. Crosses ($\times$) indicate the symmetric periodic motion.

Kolmogorov-Arnold-Moser theorem [1], some invariant tori will be preserved under the interaction, although they are somewhat deformed. These periodic or quasiperiodic orbits lie inside the *primary islands of stability*, which in our case are situated around the fixed point corresponding to the symmetric motion, the latter one represented by means of $\times$. Higher values of λ present a similar PS, but the chaotic region fills more and more of the available space consistent with E fixed. It is clear that only for the case of point particles, i.e., zero screening length ($1/\lambda=0$), is the bouncing-ball behavior observed. It is also possible that the infinite-energy limit (with $r_m=0$) would be similar, as Fig. 1 also suggests.

Secondary islands appear for $\lambda\approx 1$. These islands are due to the interparticle interaction [11] and correspond to correlated motion, as when, for example, particle 1 bounces twice and the other once. For each pair of values (λ, E) there is a specific island structure. The orbits 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 λ decreases [Fig. 2(b)], the number of stability islands increases. In this case $q_2=\frac{1}{2}$, so that the PS shows the

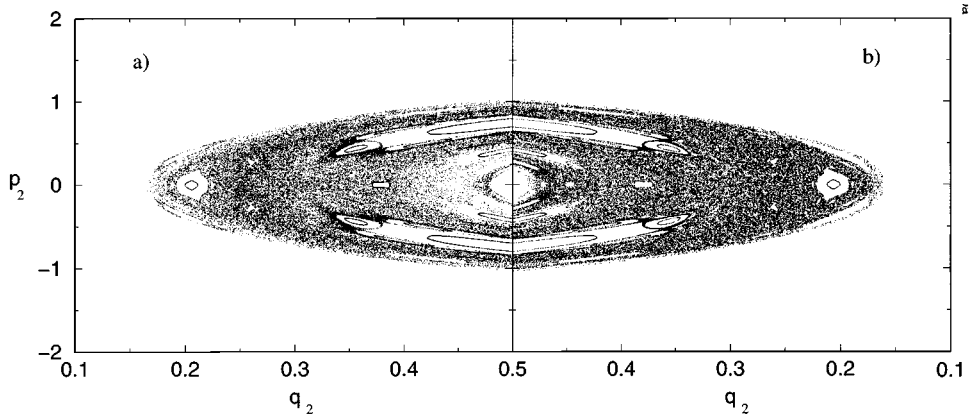

FIG. 3. Poincaré sections for the selected energy $E=1.56$, $\lambda=0$ and $q_1=-\frac{1}{2}$. (a) Solving the Hamilton equations and (b) using the *map*.

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 λ, as the total energy is fixed and the interparticle 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 equation (5). 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's 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 σ for $\lambda\leqslant 1$, following the procedure of Ref. [13]. Figure 2 shows that, as λ 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 λ (from 0 to 1). Increasing energy produces similar curves with ever larger values of σ.

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) can the particles be considered as bouncing balls. These results suggest that the effects of the 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. An analysis of the quantum-mechanical analog of the billiard system described in this work is now in progress.

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