Chaos in double-barrier heterostructures

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We have found chaotic behavior in two classical systems of three particles moving on a one-dimensional ring, where the particles interact via a nonhomogeneous Toda or Coulomb interaction. Chaos appears due to the spatial symmetry breaking induced by the nonhomogeneous interactions. Under certain conditions this system may be considered a classical counterpart of the quantum double-barrier heterostructure, a system for which fingerprints of chaos in its energy spectrum were recently found.

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Recently, interest has arisen in chaotic properties of quantum double-barrier resonant tunneling heterostructures [1]. The energy level spacing distribution was studied in Ref. [2]. When there are no interactions between the electrons in the heterostructure, or these interactions are homogeneous, the energy level spacing distribution follows a Poisson distribution. For nonhomogeneous interactions a Wigner distribution of the energy level spacing was found. It was suggested in Ref. [2] that the barriers are not the crucial factor in the transition between the different types of distribution, and that a classical system which has inhomogeneous interactions (but no barriers) might capture the crucial features in the transition to chaos of the quantum double-barrier system.

Nontrivial relations between classical and quantum chaos are the main motivation of our study [3–8]. One usually studies the deterministic chaos in a classical system, and then the question arises as to the signatures of this chaotic behavior in the quantum system. A fingerprint of the classical deterministic chaos appears in the appropriate quantum system as a change in the energy level spacing distribution from the Poisson distribution for an integrable system in the classical limit to a Wigner Gaussian orthogonal ensembles (GOE) distribution for a system which is chaotic in that limit. The latter phenomenon is usually referred to as "quantum chaos." Recently it has been shown that the appearance of a Wigner distribution of the quantum energy level spacing does not necessarily indicate an underlying classical chaotic dynamics [9–11]. Therefore, it is important to see whether the GOE level spacing observed for the quantum double-barrier system is accompanied by a classical chaotic behavior of this system.

The appearance of deterministic chaos for the classical analog of the quantum double barrier is investigated here using an example of a three particle system moving on a one-dimensional ring with exponential (the Toda lattice) or Coulomb (the Kepler system) interactions between the particles. These systems are known to exhibit a transition to chaos once the particles have unequal masses [12, 13]. In this paper we show that similar chaotic behavior appears once different types of interactions between particles which happen to be in different space regions are introduced. This situation is common for heterostructure electronic devices where different electronic densities may be found at different regions of the device. Since the effectiveness of screening depends strongly on the electronic density the electron-electron interactions at different regions of the heterostructure have different forms. This nonhomogeneous interaction, like transitions from equal to unequal masses, comprises the symmetry breaking factor, which brings qualitative changes in the behavior of the nonhomogeneous systems compared with the appropriate homogeneous ones with or without interactions.

It turns out that deterministic chaos appears for nonhomogeneous interactions while it is absent when the interactions take place everywhere on the ring or when they are completely absent. Hence, for the heterostructure case the transition of the level statistics to a Wigner distribution is indeed an indication for the appearance of "quantum chaos."

As a first example we consider the Toda lattice, which is one of the few known examples of an integrable system (both in classical and quantum cases) with more than two degrees of freedom. We consider the three body one-dimensional Toda lattice with a Hamiltonian of the form

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{p_3^2}{2m_3} + e^{-|q_1-q_2|} + e^{-|q_2-q_3|} + e^{-|q_3-q_1|}. \tag{1}$$

For equal masses $m_1 = m_2 = m_3$ one can construct Lax pairs [14] and find three independent integrals of motion for the Toda lattice [7, 14], which means that the system described by Eq. (1) with equal masses is integrable, i.e., does not exhibit chaotic behavior. The Toda lattice and its continuum limit—the nonlinear Korteweg-de Vries equation with soliton solutions—are examples of integrable nonlinear systems.

Casati and Ford [12] considered the unequal mass symmetry breaking perturbation to the integrable solution. They showed numerically for different energies and mass ratios that for relatively small perturbations, in accordance with the Kolmogorov-Arnold-Moser theorem [7], the system remains nearly integrable while for large perturbations it shows chaotic behavior.

In contrast to Ref. [12] we keep the masses equal, $m_1 = m_2 = m_3 = m$, but rather introduce a nonsymmetric interaction (see Fig. 1). The solid line on the ring

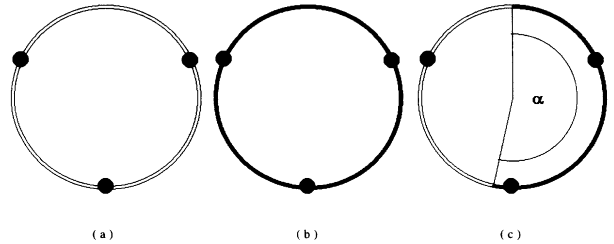

FIG. 1. Schematic drawing of the ring system. The points represent the initial positions of the particles. The angle coordinate α corresponds to the angular portion of the ring in which interactions take place, represented by the dark region of the ring. There are no interactions in (a) ($\alpha = 0$), interactions everywhere in (b) ($\alpha = 2\pi$), and interactions which take place only in a part of the system (c) ($\alpha = 1.1\pi$).

shows the regions where the interactions occur. Hence, Fig. 1(a) corresponds to the noninteracting case, Fig. 1(b) to the homogeneously interacting particles, while Fig. 1(c) represents the case for which interactions between particles exist only when both particles are in the angular region of 1.1π and are absent when any of the particles are outside this region.

As an indication of chaos we will use, as is done in Refs. [12, 15, 16], the phase space separation distance D defined as

$$D = \sqrt{\sum_{i=1}^{3} \left[(p'_i - p_i)^2 + (q'_i - q_i)^2\right]}, \tag{2}$$

where the dotted and undotted quantities belong to two trajectories which initially are very close to each other. For integrable systems D grows as a function of time no more than linearly while for chaotic systems D grows exponentially. This is the well-known sensitivity to initial conditions characteristic of chaos.

We have chosen symmetric initial positions of particles on a ring as shown in Fig. 1, $q_1^0 = \pi/3$, $q_2^0 = \pi$, $q_3^0 = 5\pi/3$, and masses $m_1 = m_2 = m_3 = 1$. The second trajectory is identical to the first one except for changing the initial position of one particle $q\prime_2^0 = q_2^0 + 10^{-4}$. The total energy H of our conservative system is defined by Eq. (1) and remains constant. Each case described in Fig. 1 has different interaction energy; therefore, for the same initial positions of the particles and identical masses one has to consider different initial momenta $\{p_i^0\}$, in order to have the same total energy for all cases. For $H = 10$, we have chosen $p_1^0 = -p_3^0 = 3.162\,28$, $p_2^0 = 0$ for the noninteracting case described in Fig. 1(a), $p_1^0 = -p_3^0 = 3.077\,212\,437$, $p_2^0 = 0$ for the case of Fig. 1(b), and $p_1^0 = -p_3^0 = 3.134\,179\,26$, $p_2^0 = 0$ for Fig. 1(c).

In Fig. 2 we show typical graphs of separation distances D vs time. In the symmetric cases (the noninteracting case or interactions everywhere on the ring) D either does not grow or grows no stronger than linearly as a function of time. On the other hand, when symmetry is broken, as in the case described in Fig. 1(c), it can be seen (Fig. 2) that D grows exponentially as a function of t as is expected in a chaotic case. The process saturates eventually because the separation is restricted by the finite volume of the phase space available for the particle.

For comparison we display in Fig. 2 the separation distance D for the unequal mass case where $m_1 = 1$, $m_2 = 0.5$, and $m_3 = 1.5$. In order to remain on the same energy surface $H = 10$ as for all other curves in Fig. 2 we have chosen $p_1^0 = -p_3^0 = 3.370\,917\,332$, and $p_2^0 = 0$. It turns out that D grows exponentially in this case showing very similar behavior to that of the heterostructure case.

Let us now turn to the second example. Extensive studies were conducted for three particles interacting via Coulomb interactions (the anisotropic Kepler problem). For the case of particles of equal masses such a system is integrable since it has as many conserved quantities as there are degrees of freedom. On the other hand, chaotic behavior has been found for unequal masses of the particles [7, 8].

The Hamiltonian of three particles with Coulomb interactions has the form

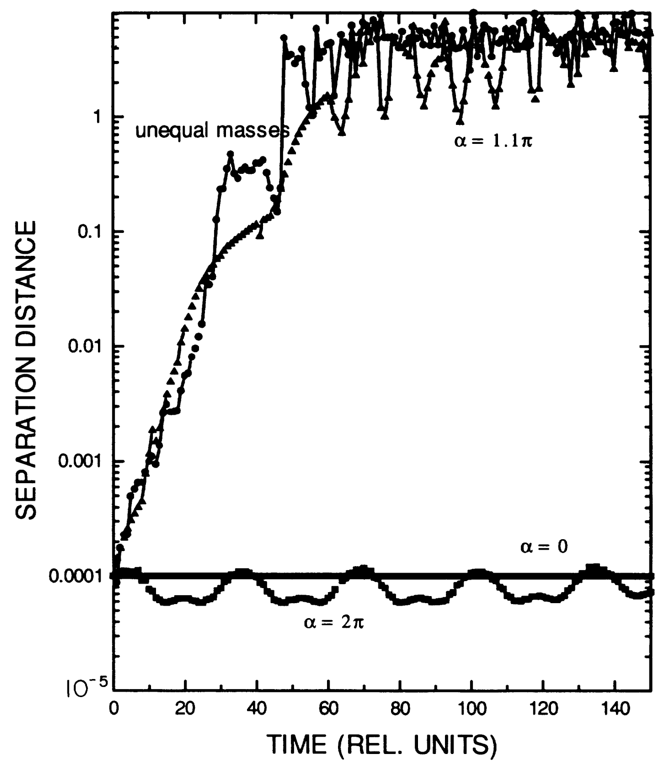

FIG. 2. Separation distance D, as defined in Eq. (2), vs time for two adjacent trajectories in phase space for the Toda system [Eq. (1)]. For the noninteracting case ($\alpha = 0$), D is constant. D moderately changes for particles which interact all over the ring ($\alpha = 2\pi$). On the other hand, for the heterostructure case ($\alpha = 1.1\pi$) D grows exponentially. For all these cases the particle masses are equal. Similar exponential growth of D is observed for an unequal mass case. The exponential growth of D is typical of chaotic behavior.

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{p_3^2}{2m_3} + \frac{1}{|q_1 - q_2|} + \frac{1}{|q_2 - q_3|} + \frac{1}{|q_3 - q_1|}, \quad (3)$$

where the exponential interactions of Eq. (1) are replaced by Coulomb interactions.

As in the preceding section we shall consider the case of equal masses $m_1 = m_2 = m_3 = 1$. The initial positions of the particles are chosen as $q_1^0 = \pi/3$, $q_2^0 = \pi$, $q_1^0 = 3\pi/2$. The noninteracting particles result is obviously identical to that of the Toda lattice. For the homogeneously interacting case we chose $p_1^0 = -p_3^0 = 2.8632$, $p_2^0 = 0$, and for the heterostructure case $p_1^0 = -p_3^0 = 3.069$, $p_2^0 = 0$. Under these initial conditions all these cases have the same energy $H = 10$.

The typical behavior of D vs time is shown in Fig. 3 for all the different cases. These curves bear a strict resemblance to those presented in Fig. 2 for the Toda lattice. As expected, the specific form of interactions has only a minor influence on the generic properties of nonlinear systems.

The behavior of the system for a given total energy and different interactions can be illustrated by a set of Poincaré surfaces of sections. In Fig. 4 we show the Poincaré section for $H = 10$ and the above mentioned initial conditions. Figure 4(a) corresponds to the homogeneously interacting particles, while Fig. 4(b) relates to the heterostructure case shown in Fig. 1(c). The latter case clearly exhibits chaotic behavior. Moreover, the heterostructure system is a mixed one, i.e., its behavior is chaotic or regular depending on the initial conditions. For example, if one chooses the initial condition to be symmetric with respect to the region of interaction the motion is nonchaotic, in contrast to the case presented in Fig. 4(b).

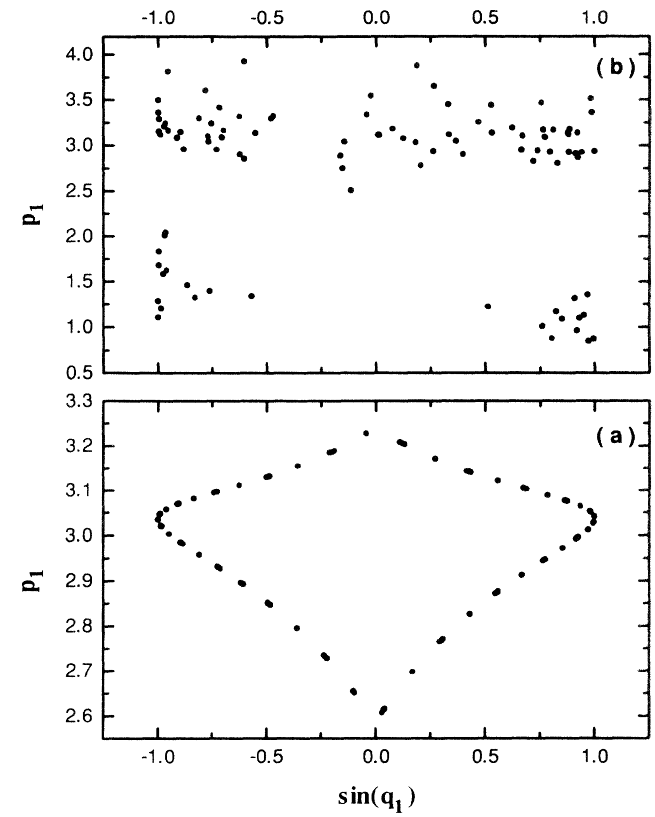

FIG. 4. Poincaré surfaces of sections for homogeneously (a), and nonhomogeneously (b) interacting particles.

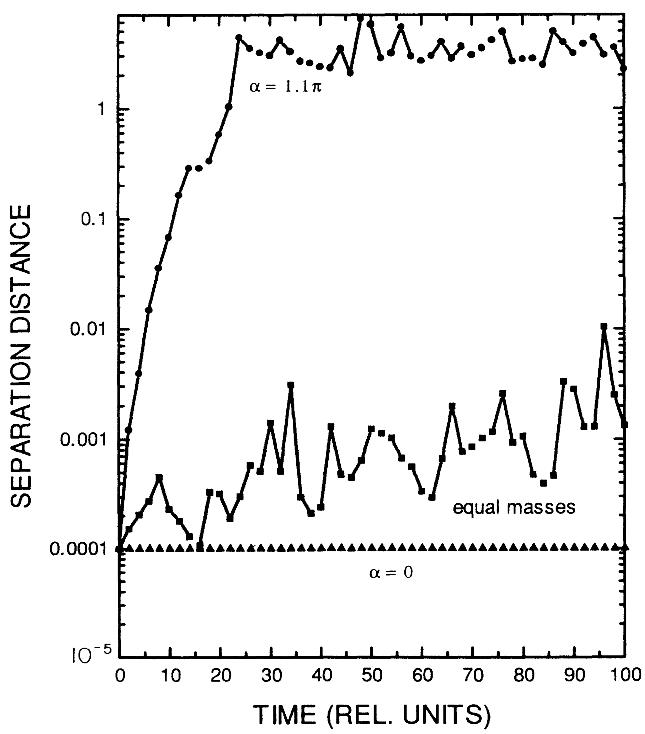

FIG. 3. Separation distance as in Fig. 2 for the Coulomb interaction [Eq. (3)], for equal particle masses.

Let us finally turn to the quantitative analysis in terms of the Lyapunov exponents. Let $\vec{d}(0)$ and $\vec{d}(t)$ denote the separation vectors of two close trajectories at times 0 and t, respectively. Then

$$\vec{d}(t) = J\vec{d}(0). \quad (4)$$

The matrix J is of the order $n \times n$, where n is the dimension of the phase space (in our case of three particles $n = 6$). The matrix J can be diagonalized to the form

$$J = \begin{pmatrix} \Lambda_1(t) & & \\ & \ddots & \\ & & \Lambda_6(t) \end{pmatrix}. \quad (5)$$

Then $\lambda_i = \lim_{t\to\infty} \ln[\Lambda_i(t)]/t$ are called the Lyapunov exponents, and the largest exponent λ_1 will define the convergence (or divergence) of the neighboring trajectories. Using the phase space plus tangent space approach [17, 18] and the standard subroutines for finding eigenvectors in MAPLE V we have found that for the homogeneously interacting particles [Fig. 1(b)] $\lambda_1 = -0.006$ and for noninteracting particles [Fig. 1(a)] $\lambda_1 = 0$, i.e., the systems are nonchaotic. However, if the masses in Fig. 1(b) are nonequal or the interaction is nonhomogeneous as in Fig. 1(c), $\lambda_1 = 0.18$ and 0.176, respectively. Therefore, in the last two cases the motion of the particles is chaotic.

One must consider the question of computer integration accuracy. To solve the Hamilton-Jacoby equations for the Hamiltonians given in Eq. (1) and Eq. (3) we used the Fehlberg fourth-fifth order Runge-Kutta method [19]. The tolerance of the numerical calculation for relative error of convergence was 10^{-10}. Computations were performed with 14 floating point significant digits.

Hence, we have suggested nonhomogeneous interactions as a new possible source for the onset of deterministic chaos in nonlinear systems. It turns out that different interactions between particles in different space regions result in symmetry breaking, and in the appearance of chaos. As an example we have considered three particles moving on a one-dimensional ring, with Toda or Coulomb interactions between them. Our numerical calculations clearly show that the separation between two neighboring trajectories increases exponentially for nonhomogeneous interactions in contrast to the noninteracting case, or the homogeneously interacting case. The detailed form of the heterostructure is of no special importance as long as a spatial symmetry breaking of the interactions exists. Some exceptional cases exist in which particles never reach, or never leave, a region for which the interactions are different. For example, for the case shown in Fig. 1(c) this will happen if the interaction region extends to $0 < \alpha < \pi$. As there are more particles in the systems these exceptional cases become rarer.

Nonhomogeneous interactions as a factor which induces deterministic chaos are similar to unequal masses of the particles. Symmetric cases such as equal masses and homogeneous interactions correspond to integrable systems while unequal masses as well as nonhomogeneously interacting particles result in chaotic trajectories in phase space almost for all initial conditions. Finally, we have established a simple classical counterpart to the interacting quantum double barrier, supporting the claim of Ref. [2] that the decisive factor in the appearance of chaos in the quantum double-barrier resonant tunneling heterostructure is the spatial symmetry breaking due to nonhomogeneous interactions rather than the presence of barriers.

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