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Effect of interactions on the integrability and level statistics of two particles in an infinite quantum well

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Abstract

We determine the energy spectrum of a system consisting of two particles which interact through a screened Coulomb potential. The spinless particles are confined in a one-dimensional infinite well. The integrable bouncing-ball limit and the bare potential cases, the latter one for different strengths, are considered. In both cases, the level of distribution for the integrable limits do not follow a Poisson distribution. In the second case, however, a transition from the singular distribution of free particles to a Wigner-like form takes place as the strength of the bare potential increases. This is similar to the transition for typical systems with mixed dynamics.

Keywords: Chaos; Level statistics

Classical chaotic systems and their quantum counterparts have been extensively studied in recent years. Billiards, in particular, have shown generic manifestations of chaoticity in both eigenfunctions and eigenvalues [1,2]. A typical billiard consists of a particle moving in a region limited by hard walls. Experimental realizations of these systems can be found in the quantum dots [3]. The usual theory applied to these mesoscopic systems is that of the typical billiard and emphasis has been put mainly on shape effects. However, more than one particle is expected to be simultaneously present in 'nearly isolated' dots (weakly coupled to the leads) and the interactions among them should be considered in a more complete description. In fact, some experimental [3], and theoretical [3,4] results in these systems have pointed out effects attributed to the interactions between the particles.

To get a better understanding of interaction effects on the properties of quantum dots, we study a Hamiltonian system consisting of two particles moving along a line and interacting through a screened Coulomb potential, i.e., a Yukawa potential with screening length λ^{-1}. The particles are confined in an infinite-wall potential well. We have recently analyzed the classical system [5]. We observed a mixed dynamical behavior (with both chaotic and integrable regions in phase space), which is

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determined by the inverse of the screening length λ and the total energy E. The integrable case corresponds to $\lambda \to \infty$. Then the potential goes to a ∂ function and the particles behave as bouncing balls. Notice that the transition to integrability is not smooth but rather singular. Only in the case of infinite λ (or energy) the system becomes integrable. On the other hand, the limit $\lambda = 0$ corresponds to the bare Coulomb potential for which the problem is well behaved (except for infinite kinetic energy). Secondary stability islands which correspond to correlated motion of the particles are prevalent. Intermediate values of λ and E determine a much more complex dynamics. We now study the quantum analog of this system in both regimes, by also considering a varying bare potential. Our analysis focuses here on the level spacing distribution.

Level statistics analysis has become an important tool to analyze the manifestations of chaos in the semiclassical regime. Thus, for the integrable case the energy levels are uncorrelated, and the distribution $P(s)$ of nearest-neighbor spacing s is Poisson-like [6], while in the extreme regime of ergodicity a Wigner distribution is well approximated. Previous works have found that the quantum analog of mixed dynamical systems have a generic behavior [7,8]. As the chaos increases, a transition from the Poisson (PD) to the Wigner (WD) distribution is observed. Moreover, an analytical expression for the transition distribution has been derived in the semiclassical limit [7]. However, numerical results showed that this expression is valid only for $s > 1$ [9]. Instead, a Brody distribution (BD), $P^{B}_{\beta}(s) = as^{\beta}\exp(-bs^{\beta+1})$, where a and b are related to the parameter β, describes more properly the transition between PD ($\beta = 0$) and WD ($\beta = 1$) [9].

When taking $\hbar^2/2m = 1$, the Schrödinger equation to be solved is

$$-(\nabla_1^2 + \nabla_2^2) + V(x_1, x_2)\Psi = E\Psi, \qquad (1)$$

where $V(x_1, x_2) = \alpha e^{-\lambda|x_2 - x_1|}/|x_2 - x_1|$, and α is the potential strength. The subindex 1(2) refers to the position of each particle $x_{1(2)}$. Here, we focus our attention on the cases $\lambda \to \infty$, for which $V(x_1, x_2) = \alpha\delta(x_2 - x_1)$, with $\alpha \gg 1$, and the bare potential $\lambda = 0$, $V(x_1, x_2) = \alpha/|x_2 - x_1|$. These cases allow analytical expressions for the Hamiltonian matrix elements.

The quantum well is defined by x_1, x_2: $[-a, a], a = \frac{1}{2}$ in such a way that its width is $L = 1$. The wave function must satisfy the usual boundary conditions on the infinite walls $\Psi(x_1 = \pm a) = \Psi(x_2 = \pm a) = 0$, and we have chosen a basis set of n products of plane waves $\{\phi_{k_1}(x_1)\phi_{k_2}(x_2)$: $\phi_k(x) \propto \cos(kx), \sin(kx), k = 1, 2, \ldots\}$, with k in units of π. Each wave number pair k_1, k_2 has to be properly chosen in order to satisfy the boundary conditions. Because of the singularity in the bare potential at $x_1 = x_2$, a cutoff $\varepsilon = 10^{-3}$ is introduced. Thus, for the case of spinless particles the wave function is expanded as

$$\Psi_E(x_1, x_2) = \sum_{k_1, k_2} A_{k_1, k_2}\phi_{k_1}(x_1)\phi_{k_2}(x_2). \qquad (2)$$

A diagonalization procedure is performed numerically for $n = 900$, and in general about 700 levels are considered in the statistics below.

Before presenting our results, some remarks are important. First of all, we can transform our system to that of a *single particle* with coordinates (x_1, x_2) moving in a two-dimensional *hyperbilliard*. For the integrable bouncing balls, the *hyperbilliard* is an isosceles right triangle, whose eigenvalues are given by $E = (k_1 + k_2)^2 + k_2^2$, with k_1 and k_2 as above [10]. On the other hand, when the bare potential is considered, the integrable case corresponds to the limit of independent noninteracting particles whose *hyperbilliard* is a square. The eigenvalues are well known, $E = k_1^2 + k_2^2$. The nongeneric level sequence for the rectangular billiard has been pointed out by Berry and Tabor [6]. Instead of the PD, they suggested $P(s) = (1 - e^{-X})e^{-Xs}$, $X = \pi/4$ for the square. The triangle spectrum is a subset of the square levels so a nongeneric spectrum is also expected.

Following Prosen and Robnik [9], the cumulative level spacing distribution $I(s) = \int_0^s P(s)\,ds$ is transformed properly to linearize the BD. Under the transformation $\sigma = \log(s)$, one defines the distribution $T(\sigma) = \log(-\log(1 - I(\exp\sigma)))$, which for the BD becomes $T^{B}(\sigma) = (1 + \beta)\sigma + \log b$. Fig. 1 shows $T(\sigma)$, the transformed distribution of 4500 levels as obtained by the sequences given before, for both the triangle and the square. The straight lines

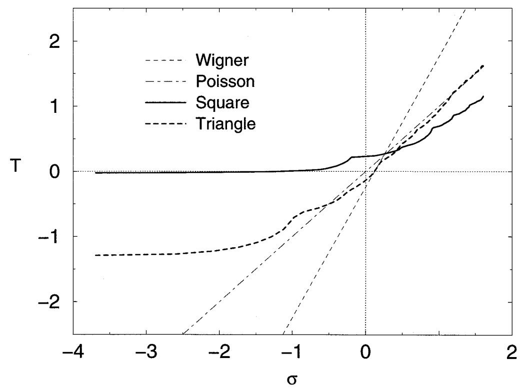

Fig. 1. The transformed distribution $T(\sigma)$ for the analytical spectra of the triangle and the square, as well as for PD and WD functions.

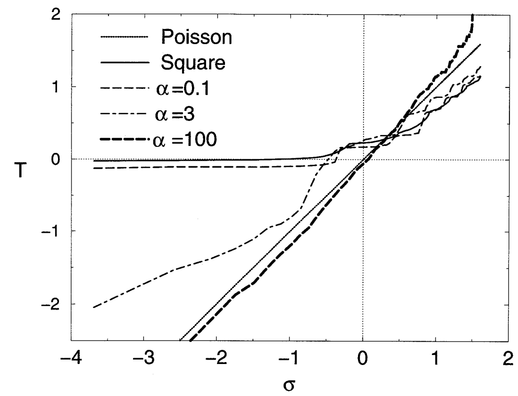

Fig. 3. The transformed distribution $T(\sigma)$ for the bare Coulomb potential. Different strengths α and fixed $n = 900$ are shown.

correspond to PD and WD and are shown for comparison. It is clear that a linear fit to a BD is not possible, which confirms the singularity of these sequences.

Fig. 2 shows our numerical results for the bouncing balls, i.e., the δ function potential for the strengths $\alpha = 10^4$ and 10^{12}. The former value with $n = 2500$ basis functions is also shown. Since both the 'height' of the δ function potential and the basis set are finite, we do not expect to obtain the exact sequence of values for the triangle, which is also included for comparison. This behavior is a signature of the expected singular nature of the pure δ potential limit. Nevertheless, notice that the overall behavior is well reproduced and it improves slightly as the number of functions in the expansion increases. The bare potential case below is however well behaved.

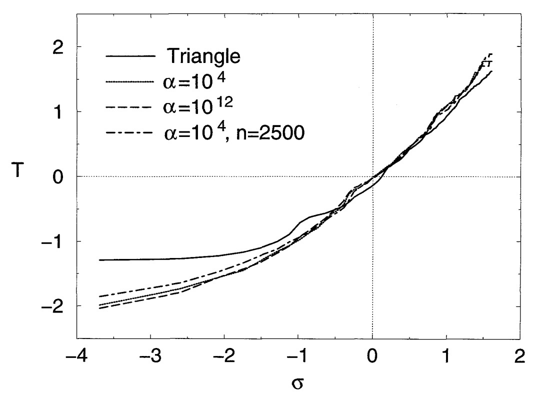

Fig. 2. The transformed distribution $T(\sigma)$ for the bouncing balls as obtained numerically. Different strengths α are shown for $n = 900$ basis functions, and $n = 2500$.

We now consider the bare Coulomb potential. Fig. 3 shows the sequence of different values of α. The presence of a weak potential ($\alpha = 0.1$) can be considered a rather small perturbation of the square billiard ($\alpha = 0$). Then, the T-distribution curves are very similar. However, as α increases, a transition to the PD occurs ($\alpha = 3$) and the trend towards a WD is observed ($\alpha = 100$). In fact, the histogram of $P(s)$ in that case (not shown here) is rather Wigner-like.

To conclude, we have analyzed the level of statistics of two systems consisting of two interacting particles in an infinite quantum well. The first case, of simple bouncing balls, does not show the PD of generic integrable systems. In the other regime, as the Coulomb potential is switched on, the integrable limit is singular. However, as the strength of the potential increases, the distribution becomes more and more Poisson-like and eventually crosses over towards a Wigner-like distribution. These results suggest a transition towards a generic mixed-dynamics system, where the level distribution will be provided by a growing WD component, in qualitative agreement with the observed classical behavior [5]. As for particles moving in a higher-dimensional quantum well, the same conclusions are expected to apply, at least qualitatively. More quantitative statements require closer analysis of the semiclassical regime, as described by Berry and Robnick [7]. This is in progress and will be presented elsewhere.

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