Interaction-induced chaos in a two-electron quantum dot system

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A quasi-one-dimensional quantum dot containing two interacting electrons is analyzed in search of signatures of chaos. The two-electron energy spectrum is obtained by diagonalization of the Hamiltonian including the exact Coulomb interaction. We find that the level-spacing fluctuations closely follow a Wigner-Dyson distribution, which indicates the emergence of quantum signatures of chaos due to the Coulomb interaction in an otherwise nonchaotic system. In general, the Poincaré maps of a classical analog of this quantum-mechanical problem can exhibit a mixed classical dynamics. However, for the range of energies involved in the present system, the dynamics is strongly chaotic, aside from small regular regions. The system we study models a realistic semiconductor nanostructure, with electronic parameters typical of gallium arsenide.

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In a many-body system, it is possible for signatures of quantum chaos to appear due solely to the interactions among its particles. During the last decade, such interaction-induced signatures of quantum chaos have been investigated, for example, in spin-fermion models,[1] in the extended Hubbard model in a ring geometry,[2] in the compound nuclear state with 12 particles in the *sd* shell,[3] and in the heavy rare-earth atom of cerium.[4] In those studies, evidence of quantum signatures of chaos found in level-spacing statistics, the response to arbitrary perturbations, or the statistical properties of the wave functions were considered to be conclusive. This conclusion is not entirely surprising, since all of those systems, having relatively large numbers of particles (>10), are similar to the complex nuclear systems that motivated the introduction of the ideas of random matrix theory (RMT) in the first place.[5] On the other hand, it is not obvious *a priori* whether the inclusion of the interaction in few-body systems, like, for example, currently available semiconductor quantum dots, also leads to signatures of quantum chaos. In a recent study, the effect of electronic interactions was considered in a parabolically confined three-electron system.[9] (It is well known that three is the lowest number of interacting electrons necessary to break the integrability in a parabolic quantum dot.) In that study, the crossover from regular to irregular spectra as a function of the interaction strength was found to be incomplete, possibly due to the existence of hidden symmetries not taken into account in the statistical analysis. Therefore, the question of the emergence of signatures of quantum chaos due to interparticle interactions in systems of very few particles remains open.

Closely related to the issue of characterizing the dynamical properties of simple interacting systems is the problem of quantum control with external fields. The manipulation of a few particles (electrons and holes) in semiconductor quantum dots is a potentially important technological problem that is receiving increasing attention.[6,7] In this context, recent theoretical studies have shown interesting effects of single-electron turnstile behavior, and localization and correlations in systems of quantum dots with two interacting electrons in them.[8] In the present paper we investigate the signatures of quantum chaos in a similar system, i.e., two interacting electrons in a quasi-one-dimensional semiconductor quantum dot. We show that the Coulomb interaction between the electrons induces an unambiguous transition from a regular spectrum to a spectrum that follows closely the predictions of RMT for systems whose classical analog exhibit chaotic dynamics.

In order to fully characterize the emergence of chaos due to interactions in this simple system, we also study the dynamics of its classical analog. The Poincaré maps that describe the classical system show a strongly (albeit mixed) chaotic behavior due to the inclusion of the true Coulomb interaction in the system.

We assume that the quantum dot has a narrow parabolic confinement in the transversal x-y dimensions, so that the energies associated with those modes are high compared to the energies of the remaining degree of freedom (the Born approximation). The two-electron wave function can then be written as

$$\Psi(\mathbf{r}_1,\mathbf{r}_2)=\phi(x_1)\phi(y_1)\phi(x_2)\phi(y_2)\Phi(z_1,z_2), \qquad (1)$$

where $\phi(x)$ is the lowest harmonic-oscillator energy eigenstate. The energy eigenstates satisfy

$$[H_0(z_1)+H_0(z_2)+V_{1D}(|z_1-z_2|)]\Phi(z_1,z_2) = E\Phi(z_1,z_2), \qquad (2)$$

where $H_0(z)=-(\hbar^2/2m^*)\partial^2/\partial z^2+V(z)$ is the single-particle Hamiltonian, with $V(z)$ being the quantum dot defining potential. m^* is the effective mass, and V_{1D} is the Coulomb interaction given by

$$V_{1D}(|z_1-z_2|) = \int dx_1 dy_1 dx_2 dy_2 \frac{e^2\phi^2(x_1)\phi^2(y_1)\phi^2(x_2)\phi^2(y_2)}{\epsilon|\mathbf{r}_1-\mathbf{r}_2|}. \qquad (3)$$

We use the values of the dielectric constant $\epsilon=13.1$ and $m^*=0.067m_e$ corresponding to gallium arsenide. We choose to work with a quasi-one-dimensional semiconductor quantum dot confined in 15 Å in the x-y plane, and a width of 800 Å in the z direction.

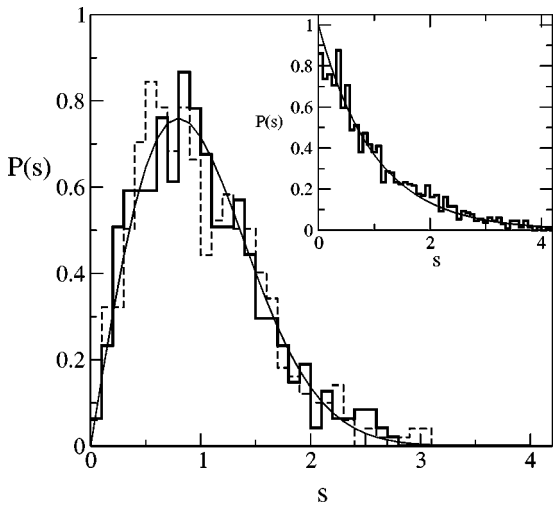

FIG. 1. NNS distribution obtained for the interacting two-electron system described in the text. The solid thick line (dashed line) is $P_{IS}(s)[P_{IT}(s)]$. The Wigner surmise $P_W(s)$ is plotted as a thin solid line in order to compare it to the obtained distributions. Inset: NNS distribution $P_{NI}(s)$ for the noninteracting two-electron system described in the text (thick line), together with the Poisson distribution $P_P(s)$ (thin line).

In the absence of the interaction term in Eq. (2), the Hamiltonian is a sum of two single-particle one-dimensional Hamiltonians, whose classical counterpart is obviously integrable. The main question we seek to answer is whether the Coulomb interaction between the electrons introduces chaos in the system.

In order to look for signatures of quantum chaos, we follow a standard statistical analysis of the energy spectrum, which consists of the following steps. First we calculate the exact spectrum $\{E_n\}$ by diagonalization of the Hamiltonian matrix. The level spectrum is used to obtain the smoothed counting function $N_{av}(E)$ which gives the cumulative number of states below an energy E. In order to analyze the structure of the level-fluctuation properties, one ''unfolds'' the spectrum by applying the well-known transformation $x_n = N_{av}(E_n)$.[10] From the unfolded spectrum one calculates the nearest-neighbor spacing (NNS) distribution $P(s)$, where $s_i \equiv x_{i+1} - x_i$ is the NNS.

We first consider the spectral properties of the noninteracting two-electron problem whose Hamiltonian is $H_0(z_1) + H_0(z_2)$. Its eigenstates can be classified by their total spin in singlets and triplets. To compute the NNS distribution we use eigenstates of a given spin. In the inset of Fig. 1 we show the obtained NNS noninteracting distribution $P_{NI}(s)$ (histogram), which follows a Poisson distribution (characteristic of an uncorrelated sequence of energy levels) given by $P_P(s) = e^{-s}$ and shown for comparison as a solid thin line. Due to the finite dimension of the Hilbert space, $N_{av}(E)$ saturates in the highest-energy region. Therefore, we compute the NNS distribution using the lowest ~ 1000 eigenvalues.[11] The obtained Poisson distribution is an expected signature of most quantum two-dimensional systems whose classical counterparts are integrable.[12]

To analyze the interacting spectrum, we diagonalize Eq. (2) exactly. We also take into account the symmetry of the spectrum due to the parity of the confining potential and the interaction potential. Therefore, in order to compute the NNS distribution we use eigenstates of a given parity and spin. This kind of decomposition is a standard procedure followed in the analysis of spectral properties of quantum systems whenever the Hamiltonian of the system possesses a discrete symmetry.[10] After unfolding the spectrum the NNS distribution is computed for the even-parity states. Again, we consider ~ 1000 eigenstates of the interacting Hamiltonian (whose eigenenergies are lower than the energy of the first transversal mode, for compatibility with the Born approximation).

Since the singlet is the ground state of the two-electron system, we first concentrate on the subspace of spatial wave functions that are symmetric under particle exchange. The interaction affects very clearly the spectrum, resulting in a strong level repulsion: the NNS distribution is in accordance with the predictions of RMT.[13] As a consequence, the obtained NNS distribution $P_{IS}(s)$ (the histogram shown by the thick solid line in Fig. 1) is well described by the Wigner surmise[13] $P_W(s) = \frac{1}{2}\pi s \exp(-\pi s^2/4)$, shown for comparison by the thin solid line.

For the triplet states, due to the antisymmetry of the spatial wave functions, it is reasonable to expect that the tendency of the two electrons to avoid each other results in a weaker level mixing. Nevertheless, although some differences with the singlet case would appear for other statistical measures (that are not possible to perform with the number of levels at hand), those differences are not qualitatively visible on the computed NNS distribution $P_{IT}(s)$, shown as a dashed line in Fig. 1. Again, the obtained histogram fits the predictions of RMT quite well.

We now turn to the dynamics of the classical counterpart of the two-electron quantum dot system. We consider the classical interaction potential given by $V_{cl}(|z_1 - z_2|) = \alpha/\sqrt{(d^2 + |z_1 - z_2|^2)}$, where the parameters α and d have been obtained from the best fit to the Coulomb interaction $V_{1D}(|z_1 - z_2|)$ [Eq. (3)]. (The fit is very good at all distances, down to the resolution of the spatial grid used in our numerical calculations.) The classical single-particle confining potential $V_C(z)$ is a square well of length L, and we restrict the analysis to bounded motion within this box. In this situation, the effect of the confining potential is to reflect the particles elastically off the boundaries in each bounce, breaking the translational symmetry of the problem. As a consequence, the center-of-mass momentum is not preserved. Nevertheless, in the absence of interaction each single-particle energy is a constant of motion, and therefore the classical problem is integrable. On the other hand, the inclusion of the Coulomb interaction breaks the conservation of the single-particle energies, and can induce an irregular dynamics in the confined system.

For a total energy $E = E^* \equiv \alpha/d$ there is a separatrix in the classical dynamics. That is, for $E < E^*$ the particles never cross each other and the sign of the relative coordinate $z_2 - z_1$ never changes, while for $E > E^*$ it can change.

Denoting $\epsilon \equiv E/E^*$, we write

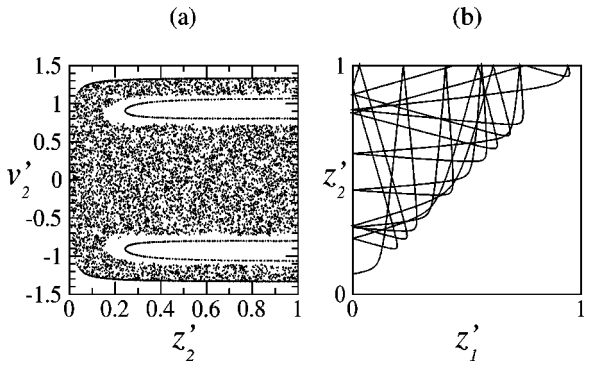

FIG. 2. (a) Poincaré surface of section v_2' vs z_2' for a rescaled energy $\epsilon=0.9$. (b) For the same value of ϵ, a piece of a trajectory in the z_2' vs z_1' plane corresponding to an initial condition in the chaotic region.

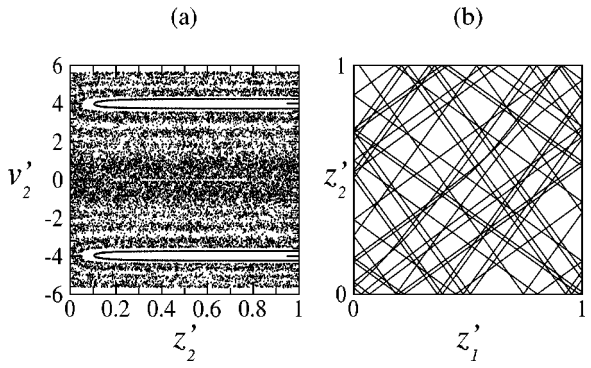

FIG. 3. (a) Poincaré surface of section v_2' vs z_2' for a rescaled energy $\epsilon=16$. (b) For the same value of ϵ, a piece of a trajectory in the z_2' vs z_1' plane corresponding to an initial condition in the chaotic region.

$$\epsilon=\frac{v_1'^2}{2}+\frac{v_2'^2}{2}+V_C(z_1')+V_C(z_2')+\frac{d^*}{\sqrt{d^{*2}+|z_1'-z_2'|^2}}, \tag{4}$$

where we have defined

$$v_i'=v_i\frac{\sqrt{m^*d}}{\sqrt{\alpha}}, \quad z_i'=\frac{z_i}{L}, \quad d^*=\frac{d}{L}, \tag{5}$$

with $i=1$ and 2. In this way, for a given value of the rescaled energy ϵ, the classical dynamics depends only on the parameter d^*. Taking into account that $L=800$ Å and the best fit with the quantum Coulomb term V_{1D} gives $d=8$ Å, we obtain $d^*=0.01$.

In Fig. 2(a), for $\epsilon=0.9$ we show the Poincaré surface of section v_2' versus z_2', for the motion of one of the particles, taken at times when the other particle bounces off the left boundary of the well (the topology of the Poincaré section does not depend on which particle is selected). The motion is chaotic over most of the accessible phase space for the given energy shell. Figure 3(a) shows another Poincaré section for $\epsilon=16$. Again, except for small regions of regular motion, the dynamics is fully chaotic.

Although the two Poincaré sections look qualitatively similar, the trajectories in the plane z_2' versus z_1' are quite different as can be seen in Figs. 2(b) and 3(b). Figure 2(b) [3(b)] shows, for $\epsilon=0.9$ ($\epsilon=16$), a piece of a trajectory in the z_2' versus z_1' plane corresponding to an initial condition in the chaotic region. In Fig. 2(b) the trajectory never crosses the straight line defined by $z_2'=z_1'$, because for $\epsilon=0.9$ $z_2'>z_1'$ always. In Ref. 14 the authors performed a classical analysis of the emergence of chaos due to the inclusion of an interparticle screened Coulomb interaction in an infinite well. The classical motion of such a system is qualitatively similar to our classical model, only for $\epsilon<1$.

From the roughly 1000 eigenstates employed to compute the NNS distribution displayed in Fig. 1, only the lowest 5% have eigenenergies that correspond to $\epsilon<1$. The eigenenergies of the remaining states correspond to values of ϵ ranging from 1 to 16, for which, as we have shown, the classical dynamics is chaotic over most part of the energy shell. Therefore the NNS distribution computed from these states results in a remarkable quantum signature of the underlying classical chaotic dynamics.

For energies $\epsilon\gg1$ the classical regular regions in the Poincaré maps should become predominant over the chaotic ones, because in such a limit the Coulomb term can be considered as a perturbation of the noninteracting two-electron Hamiltonian. Nevertheless, values of $\epsilon\gg1$ are not realistic for quantum wells describing semiconductor nanostructures.

In conclusion, we show that the Coulomb interaction is responsible for the chaotic dynamics in a quasi-one-dimensional two-electron quantum dot, both from quantum and classical points of view. We show a clean Wigner-Dyson statistics for two interacting electrons, arising from the interparticle interaction.[15] We believe that the present results may put constraints to models of semiconductors nanostructures in which the interaction among particles is modeled, for a finite number of particles, as a capacitive term in the form of a constant interaction. The inclusion of a constant interaction gives an interacting Hamiltonian whose spectral properties are those of the noninteracting one. In other words, a Poisson NNS distribution will remain Poissonian after considering the interaction in the constant interaction model.

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