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Level Statistics of a Quantized Cantori System

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We study the significance of a pronounced Cantori structure in classical phase space for the level statistics of the associated quantum system. As an example we choose the anisotropic Kepler problem. For high excitations, we find that the level statistics tend to the predictions of random matrix theory, but the convergence is rather slow.

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The many theoretical works on nonlinear theories show that bounded classical (Hamiltonian) systems often exhibit deterministic chaos.[1] It is natural to ask how this behavior emerges from the quantized version of the classical system. The answer is not straightforward, because the necessary condition for chaos is absent in quantum mechanics: The Schrödinger equation is linear. Furthermore, the finiteness of $\hbar$ prevents the applicability of the tools which were so successful in describing classical dynamics.

Systems studied so far belong to three categories: integrable, fully chaotic, and generic systems. Generic systems have mixed phase-space structure and often display a smooth transition between regularity and irregularity as a parameter is varied.[2] Two procedures have been proposed to identify the influence of classical chaotic motion in quantum spectra: an analysis of level fluctuation properties[3] and the study of long-range correlations of energy levels.[4] Most of the work to date has been devoted to the former case and was strongly influenced by the results of random-matrix theory (RMT).[5,6] However, in spite of the success of RMT in predicting fine-scale structures of quantal level fluctuations, the physical mechanisms underlying this behavior are not well understood. The main difficulty is to extract the precise necessary conditions for application of RMT and no rigorous proofs concerning this issue exist.[7] In such a situation numerical "experiments" often enable one to approach the problem from a better starting point, e.g., the question of the level statistics of generic systems (for a recent discussion see Robnik[8]) or "false" level statistics of hyperbolic billiards.[6]

In this Letter we present results and conclusions concerning a new class of systems which has not been considered before. This class consists of systems displaying an abrupt transition between integrability and ergodicity. Generally the Kol'mogorov-Arnol'd-Moser theorem prevents such an abrupt transition in that most of the invariant surfaces in phase space (the tori with irrational winding numbers) survive under small perturbations.[7] However, the Kol'mogorov-Arnol'd-Moser theorem does not apply to the pure Coulomb system, where all the bound orbits are periodic and lie on resonant tori. Hence, all kinds of behavior may occur by addition of a small perturbation to a pure Coulomb potential; the system may remain regular (e.g., Stark effect), it may display a smooth transition to chaos (e.g., atomic diamagnetism[9]), or it may become ergodic at once, independent of how small the perturbation is. There is strong evidence that the anharmonic Kepler Hamiltonian[10] (atomic units used)

$$H=\tfrac{1}{2}p_\rho^2+\tfrac{1}{2}\gamma p_z^2-r^{-1} \qquad (1)$$

belongs to this latter class.[10] Note that the Hamiltonian (1) has a real physical background; it describes very accurately donor impurity levels in a semiconductor,[11] $1-\gamma$ being the mass anisotropy. We will show that for small departures from the integrable case $\gamma=1$ the phase space of this system is densely filled with remnants of tori (Cantori), which makes the system only very weakly

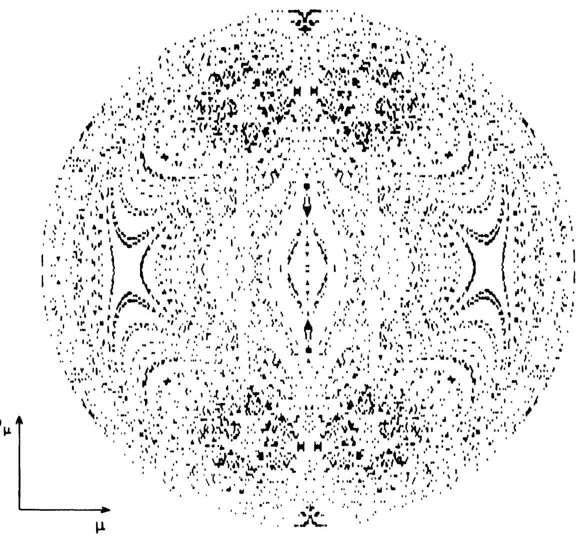

FIG. 1. Typical Poincaré surface of section for the anisotropic Kepler problem generated by a single trajectory ($\gamma=0.8$, $m=0$).

chaotic (small Kolmogorov entropy). The level statistics of the quantized system show a pronounced $\hbar$ dependence.

Since the z component of angular momentum is conserved the problem can be reduced to a two-dimensional but nonintegrable one. A convenient method to visualize the phase-space structure is to study Poincaré surfaces of section.[1] For this we solved the classical equations of motion. As coordinate set we used semiparabolic coordinates $\mu=(r+z)^{1/2}$, $\nu=(r-z)^{1/2}$, which regularize the Coulomb singularity at the origin (for $\gamma=1$). Numerical calculations were performed by use of a fifth-order Runge-Kutta method with variable step size. Because of classical scaling properties the phase-space structure is independent of energy and it is sufficient to calculate surfaces of section for one single negative value of the energy.[10]

A typical surface of section plot obtained by integration of a single trajectory is shown in Fig. 1 (for $\gamma=0.8$). It is easy to make out remnants of tori, which are present everywhere in phase space. Once the orbit is trapped on such a torus, the trajectory remains on it (or at least in its neighborhood) until it passes through chaotic regions and reappears on a different approximate torus, on which it remains for some further time. As a result of this diffusion process the motion becomes ergodic, although (different) constants of motion exist for finite time intervals. Remnants of tori as shown in Fig. 1 are called vague tori[12] or Cantori,[13,14] because the invariant part of such a remnant with irrational winding number may form a Cantor set.[1]

To study energy-level statistics for highly excited states of the anisotropic Kepler problem we developed an efficient quantization scheme. The method is based on

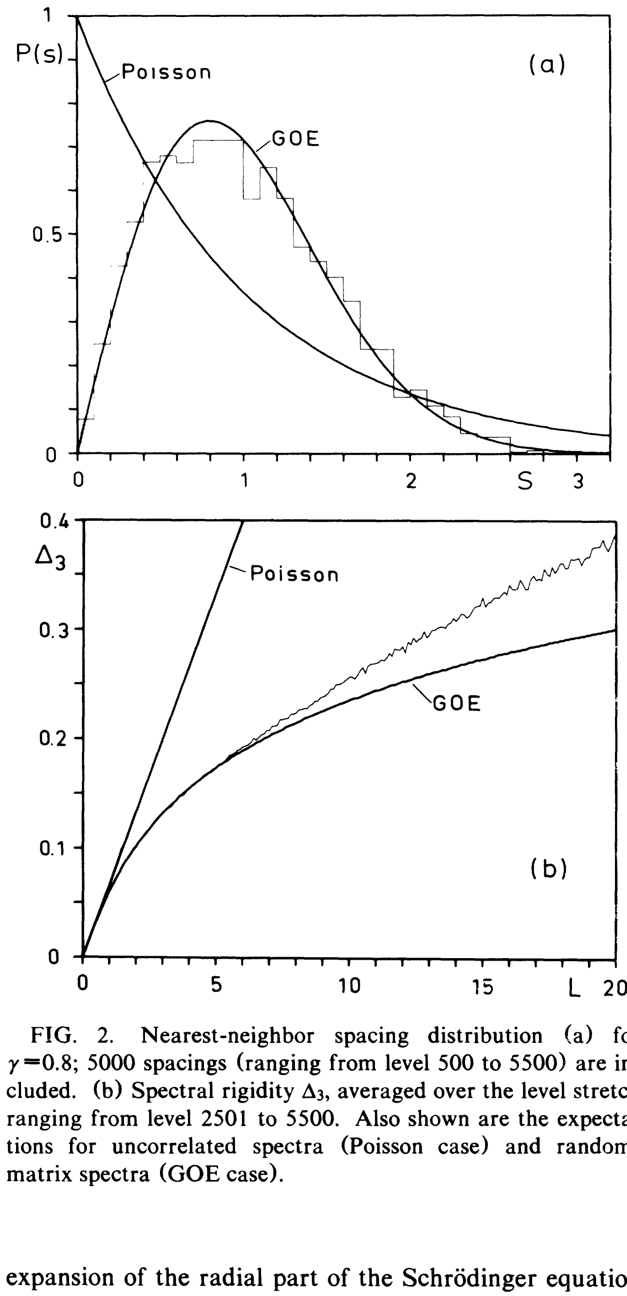

FIG. 2. Nearest-neighbor spacing distribution (a) for $\gamma=0.8$; 5000 spacings (ranging from level 500 to 5500) are included. (b) Spectral rigidity Δ_3, averaged over the level stretch ranging from level 2501 to 5500. Also shown are the expectations for uncorrelated spectra (Poisson case) and random-matrix spectra (GOE case).

expansion of the radial part of the Schrödinger equation in a complete set of Sturmian functions and the angular part in spherical harmonics with fixed azimuthal quantum number m and parity π (the only good quantum numbers). The Hamiltonian matrix can be ordered to have band structure. Using scaling properties, we have achieved convergence of most of the eigenvalues for small mass anisotropies $1-\gamma$. This allows us to calculate eigenvalue sequences which are an order of magnitude larger than in previous quantum calculations on nonintegrable systems. Details of the method can be found in Wintgen, Marxer, and Briggs.[15]

Calculations were done on a Cray 2 computer for $\gamma=0.8$, $m=0$, and even parity. Matrices with dimension up to $\simeq 8000$ were diagonalized giving a converged stretch $\{E_i\}$ of 5500 levels. We applied various statistical measures to the data[5,6]: nearest-neighbor spacing distribution, spectral rigidity Δ_3, and higher moments of the number statistic $n(L)$ (variance Σ_2, skew γ_1, excess γ_2). All these measures apply to a spectrum with unit mean level spacing, that is to the spectrum $\{\mathcal{E}_i\}$ obtained by $\{\mathcal{E}_i\}=\{N(E_i)\}$. $N(E)$ is the cumulative mean level density and is given by a Thomas-Fermi formula[5]:

$$N(E)=-\Gamma/E+A/\sqrt{E}+B. \qquad (2)$$

$\Gamma=1/4\sqrt{\gamma}$ characterizes the volume of phase space; the quantities A and B were fitted numerically to the data. We analyzed the stretch $\{\mathcal{E}_i\}$ in steps of 1000 levels (beginning at level 500) to test stationarity of the fluctuation properties along the spectrum.

Figure 2 shows the nearest-neighbor spacing distribution and the spectral rigidity Δ_3 together with the predictions for uncorrelated spectra (Poisson case) and for random matrices [Gaussian orthogonal ensemble (GOE) case]. The moments of the distribution are shown in Fig. 3. We found that all short-range fluctuation measures tend to the GOE case. However, convergence is rather slow except for the nearest-neighbor spacing distribution, which is stationary over the spectrum and agrees very well with the Wigner distribution (GOE). The other statistics are averages of stretches of length L along the spectrum between levels 2501 and 5500. Systematic departures from RMT predictions are still visible. The largest deviations are present for the spectral rigidity Δ_3. This is not surprising since Δ_3 measures spectral correlations on a wider range. Up to $L=7$ the rigidity follows RMT predictions accurately but differs significantly otherwise. In this case the convergence with the excitation regime is so slow that the observed deviations eventually persist even in the semiclassical limit. Moreover, the deviations cannot be accounted for by periodic orbit theory, which predicts asymptotic saturation of the spectral rigidity.[7]

Finally we summarize and discuss some implications of the present results.

The anisotropic Kepler problem is an ideal system with which to study the abrupt transition between integrability and chaos in Hamiltonian systems. We gave numerical evidence that for small perturbation parameters the classical phase space is densely filled with pronounced remnants of tori, which makes the system only very weakly chaotic. Quantum-level statistics of such systems may help to pin down the necessary conditions for applicability of statistical theories such as RMT.

The present results for short-range fluctuations are in full agreement with RMT. Einstein-Brillouin-Keller quantization of the remnants of tori, as proposed by various authors,[12,13] yields Poisson distributions and hence must fail to give reliable energy eigenvalues in the excitation regime studied here. We found very slow convergence indicating strong $\hbar$ dependence of the statistical measures, except for the nearest-neighbor distribution. The spacing distribution is therefore the most sensitive measure when one comes from the integrable side but the most insensitive one when one comes from the fully chaotic side. Level fluctuations on an intermediate scale

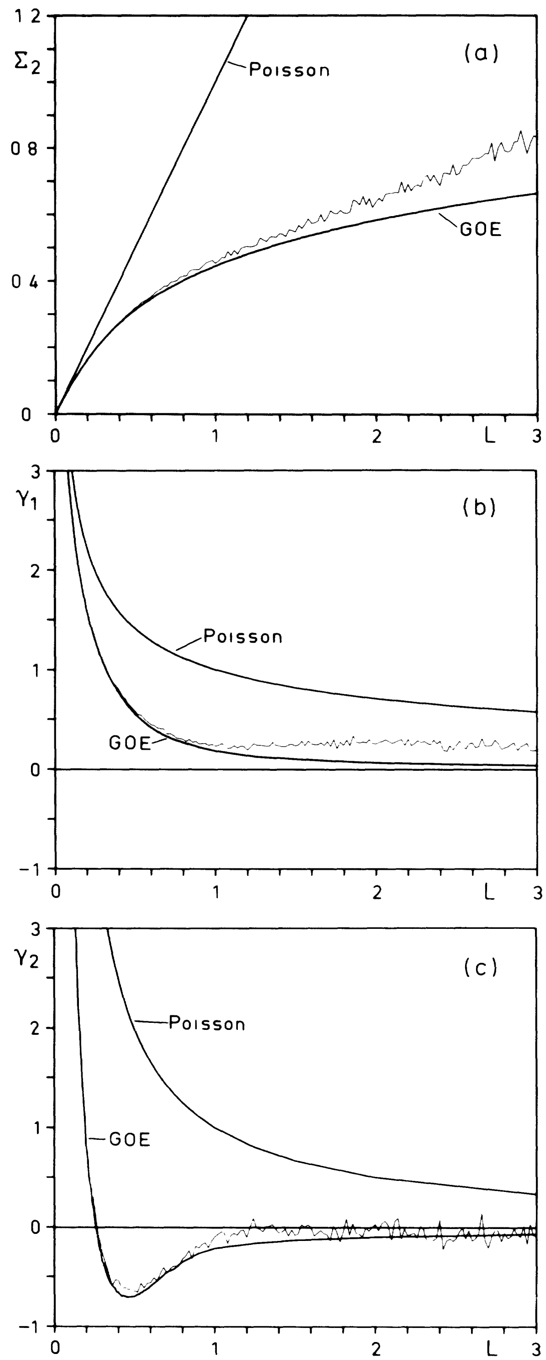

FIG. 3. Higher moments of the number statistics $n(L)$ obtained by averaging over the level stretch ranging from level 2501 to 5500 ($\gamma=0.8$): (a) variance Σ_2, (b) skew γ_1, and (c) excess δ_2, together with the expectations for uncorrelated spectra (Poisson case) and random-matrix spectra (GOE case).

show significant deviations from RMT predictions even in an excitation regime extending as high as the 5500th level. From the numerical evidence we conjecture that both, intermediate-scale deviations and slow convergence to RMT predictions, are connected to the pronounced Cantori structure of the classical phase space.

A (yet nonexisting) theory which would account for the "convergence speed" or $\hbar$ dependence of the statistical measures would presumably incorporate the Hamiltonian flow or transport through the gaps of the remnants. Up to now such theoretical classical investigations have been restricted to the case of isolated Cantori.[13,14] The anisotropic Kepler problem offers the opportunity to test these theories when the remnants of tori lie dense in phase space.

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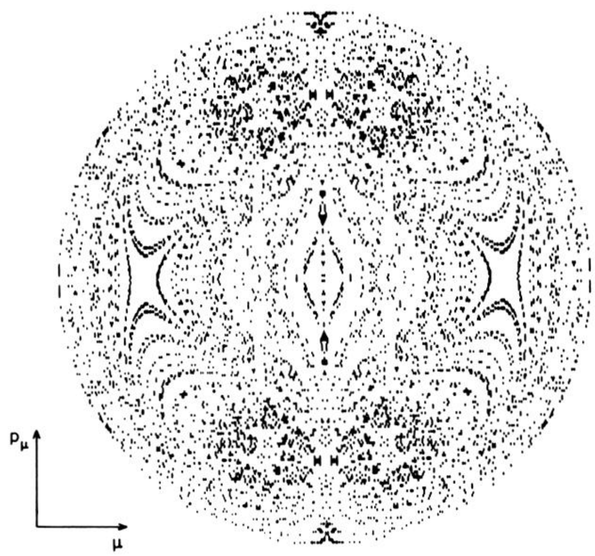

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