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Correlations in the quantum spectra of smooth Hamiltonian systems

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The long-range correlations in the quantum spectra of a smooth Hamiltonian system are shown to be due to classical periodic orbits of the corresponding classical system. This correspondence exists whether the physical system is mostly regular, mixed, or mostly chaotic.

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The energy levels of a bound quantum Hamiltonian system $H(\hat{q},\hat{p})$ exhibit both short-range and long-range correlations [1]. These correlations can be explained with the help of the corresponding classical Hamiltonian system $H(q,p)$ when $\hbar$ is small [2]. The short-range correlations are generic in nature and depend on whether the underlying classical dynamics is regular or chaotic. For example, the nearest-neighbor spacing distribution (NNS) of the energy levels obeys Gaussian orthogonal ensemble (GOE) statistics if the classical phase space is chaotic and obeys Poisson statistics if it is regular [3]. A GOE behavior of the NNS statistic is commonly used as a definition of quantum chaos when only experimentally determined energy levels are available.

In contrast to the short-range correlations in the spectra, the long-range correlations are nongeneric in nature and depend on the particular form of the Hamiltonian under study. Gutzwiller's trace formula [4] describes semiclassically these long-range correlations in terms of classical periodic orbits:

$$d_{osc}(E)=(1/\pi\hbar)\sum_{po}\mathscr{A}\cos[(1/\hbar)\,S-(\pi/2)\,\mu], \tag{1}$$

where $d_{osc}(E)$ is the oscillating part of the density of states. The sum is over all the classical periodic orbits, S is the action of a particular orbit, μ its Maslov index, and the amplitude $\mathscr{A}$ depends on its stability. To demonstrate these long-range correlations in given spectra, one usually takes the Fourier transform of the oscillating part of the density of states $d_{osc}(E)$ with respect to E [5–8]. The success of this approach depends on how fast the period of the orbits change as a function of the energy—this can be seen from Eq. (1) by expanding the classical action S about some energy E^*:

$$S(E)=S(E^*)+\tau(E^*)(E-E^*)+\cdots \tag{2}$$

so that the Fourier transform of $d_{osc}(E)$ over an energy interval about E^* should give a distinct peak at $\tau_j(E^*)$ if the period of the jth orbit is approximately constant on that energy interval. The widths of these peaks about the periods of classical orbits are, however, inversely proportional to the energy interval under consideration and consequently the resolution of these peaks is poor for generic, nonscalable systems. For special systems for which the action S scales with energy, other Fourier transforms are usually more informative [9–14].

In this paper we demonstrate the influence of classical periodic orbits on the quantum spectra by Fourier transforming $\hbar d_{osc}(E;\hbar)$ with respect to $1/\hbar$. According to Eq. (1) this must give peaks at the classical actions of the periodic orbits. This has recently been done for the hydrogen atom in a strong magnetic field [15–18]. They found that only the periodic orbits that start and end at the nucleus gave peaks. We shall demonstrate in this paper that for a more generic Hamiltonian system all short periodic orbits are important semiclassically. We studied the following Hamiltonian system [6,8,19–21]:

$$H(\mathbf{q},\mathbf{p};\alpha)=p_x^2/2+p_y^2/2+\mu x^2/2+(y-\alpha x^2/2)^2, \tag{3}$$

where $\mu=0.1$ and α is the coupling strength. A simple scaling argument shows that a variation of the coupling strength can be interpreted as keeping the coupling strength fixed and varying $\hbar$:

$$E_n[\hbar;\alpha]=(1/\alpha^2)\,E_n[\hbar\alpha^2;1], \tag{4}$$

where $E_n[\hbar;\alpha]$ is the nth eigenvalue of $H(\mathbf{q},-i\hbar\partial_{\mathbf{q}};\alpha)$. We henceforth fix the coupling constant at $\alpha=1$ and vary $\hbar$.

Our system has the reflection symmetry $x\leftrightarrow -x$. We therefore restrict our quantum calculations to the even eigenvalues. For a given $\hbar$ we obtain the exact even quantal eigenvalues by using the basis $\phi_m^{(x)}(x)\phi_n^{(y)}(y-x^2/2)$, where $\phi_m^{(x)}$ and $\phi_n^{(y)}$ are harmonic oscillator wave functions appropriate for the bottom of the well [20]. We used 31 oscillator states for the y direction and 101 even oscillator states for the x direction.

The energy-smoothed even density of states is given by

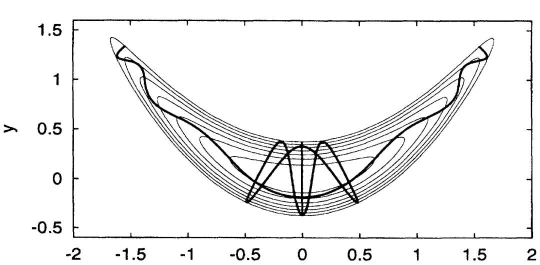

FIG. 1. Equipotential energy contours for $E=0.02$ to 0.14 in steps of 0.02. The vertical orbit, a symmetric rotation, and a symmetric libration at $E=0.14$ are also shown.

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$$d^{(+)}(E;\hbar)=\sum_{i} f_{\epsilon}(E-E_i^{(+)}), \tag{5}$$

where the smoothing function $f_{\epsilon}(E)$ is taken to be of the Lorentzian type:

$$f_{\epsilon}(E)=(\epsilon/\pi)\ [1/(E^2+\epsilon^2)] \tag{6}$$

and $\epsilon=\hbar/T^*$, with T^* fixed. The oscillating part of the even density of states is defined as

$$d_{osc}^{(+)}(E;\hbar)=d^{(+)}(E;\hbar)-d_{avg}^{(+)}(E;\hbar). \tag{7}$$

We calculated the average even density of states $d_{avg}^{(+)}(E;\hbar)$ semiclassically [20,22]. This has the advantage of telling us when the actual numerical diagonalizations fail. We obtained [20]

$$d_{avg}^{(+)}(E)=\frac{1}{2\sqrt{2\mu}}\frac{E}{\hbar^2}\left(1+\frac{\sqrt{\mu}\hbar}{2E}-\frac{\hbar^2}{12\mu E}+O(\hbar^3)\right). \tag{8}$$

The first term is the usual Thomas-Fermi density of states.

Gutzwiller's trace formula for the oscillating part of the even density of states contains three parts:

$$2\pi\hbar d_{osc}^{(+)}(E)=\sum_{ppo}\sum_{n=1}^{\infty}\tilde{f}(n\tau)\frac{\tau}{\sqrt{|tr(\mathscr{M}^{(n)})-2|}}\cos\left[n\left(\frac{\bar{S}}{\hbar}-\frac{\pi}{2}\mu_m\right)\right]\Bigg|_{\substack{periodic\\ orbits}}+\sum_{ppo}\sum_{n\ \mathrm{odd}}\tilde{f}(n\tau/2)\frac{\tau}{\sqrt{|tr(\tilde{\mathscr{M}}^{(n)})-2|}}$$
$$\times\cos\left[\frac{n}{2}\left(\frac{\bar{S}}{\hbar}-\frac{\pi}{2}\mu_m\right)\right]\Bigg|_{\substack{symmetric\\ librations}}+\sum_{n=1}^{\infty}\tilde{f}(n\tau)\frac{\tau}{\sqrt{|tr(\mathscr{M}^{(n)})+2|}}\cos\left[n\left(\frac{\bar{S}}{\hbar}-\frac{\pi}{2}\mu_m\right)\right]\Bigg|_{\substack{vertical\\ orbit}}, \tag{9}$$

where τ is the period of the primitive periodic orbit and $\tilde{f}(t)=e^{-t/T^*}$, the Fourier transform of $f_{\epsilon}(E)$. The first term is the usual sum over all primitive periodic orbits and their repetitions. The amplitude term is written out explicitly in terms of the stability matrix $\mathscr{M}$ of the periodic orbit. The second term is a sum over all the symmetric librations [23] except for the orbit that lies on the symmetry line $x=0$. This last orbit is a boundary orbit and its contribution [24] is the third term in Eq. (9). The Fourier transform in $1/\hbar$ of the oscillating part of the even density of states must therefore show additional peaks at odd multiples of half the action of symmetric librations. Physically, these additional peaks can be understood if we look at the classical motion in the fundamental domain [24], where it is seen that half of a symmetric libration becomes a full periodic orbit.

The classical dynamics and periodic orbits of the Hamiltonian given in Eq. (3) have been studied extensively [19–21]. Figure 1 shows a contour plot of the potential $V(x,y)=H-\frac{1}{2}p^2$ for energies from 0.02 to 0.14 in steps of 0.02. The vertical orbit, a symmetric rotation, and a symmetric libration are also shown. The periodic orbits come in one-parameter families. In Fig. 2 we plot the energy E as a function of the energy-scaled action S/E for periodic orbit families. A solid line indicates where a family is stable and a dashed line when it is unstable. In Fig. 3 we plot E as a function of half of the energy-scaled action of periodic orbit families that are also symmetric librations. In Fig. 4 we plot the percentage of the Poincaré surface of section $x=0$ that is regular as a function of energy. We see that the phase space is mostly regular for energies up to about 0.04 and is mostly chaotic for energies above 0.13. This transition from regular to chaotic manifests itself quantum mechanically in the NNS distribution. In Fig. 5 we plot the NNS distribution for $\bar{E}=0.02$ (top) and $\bar{E}=0.14$ (bottom). For the top figure we considered all energy levels with energies between 0.019 and 0.021 with $\hbar$ values ranging from $1/\hbar=500$ to $1/\hbar=1000$ in steps of 2. The resulting histogram fits the Poisson curve well and this implies that the underlying classical phase space at this energy is mostly regular. For the bottom figure we considered all levels with energies between 0.139 and

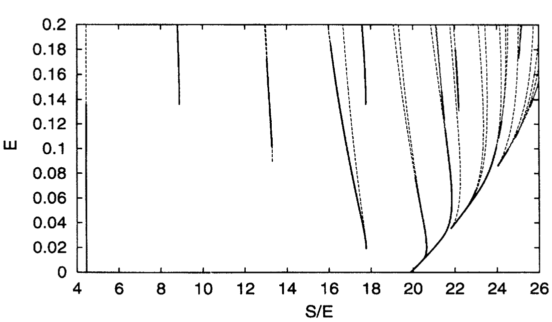

FIG. 2. Energy E vs energy-scaled action S/E for periodic orbit families. A solid line indicates where a family is stable and a dashed line when it is unstable.

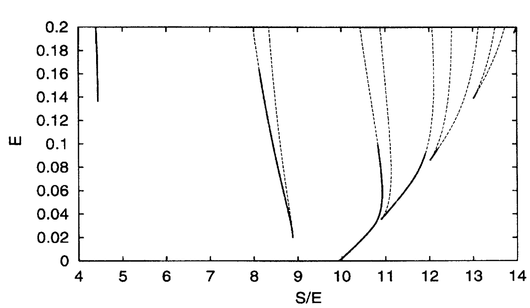

FIG. 3. E vs half of the energy-scaled action of symmetric librations.

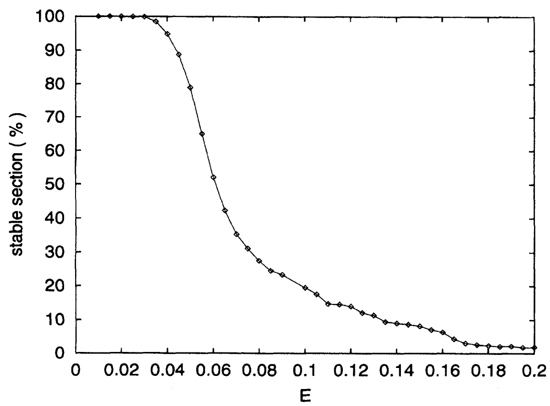

FIG. 4. Percentage of the Poincaré surface of section $x=0$ that is regular as a function of energy.

0.141 with $\hbar$ values ranging from $1/\hbar=100$ to $1/\hbar=300$ in steps of 0.5. Here the GOE curve fits best, indicating that the classical motion at these energies is mostly chaotic.

In Figs. 6–8 we show the results of the finite Fourier transform in $1/\hbar$ of $\hbar d_{osc}(E;\hbar)$ for different values of E. The maximum amplitude in each of the frames has been set to unity. The location of a periodic orbit's contribution at multiples of its energy-scaled action S/E is denoted by a vertical line of height 1 and the location of a symmetric libration's extra contribution at odd multiples of half of its energy-scaled action is denoted by a vertical line of height 0.8. In Fig. 6 we considered values of $\hbar$ ranging from

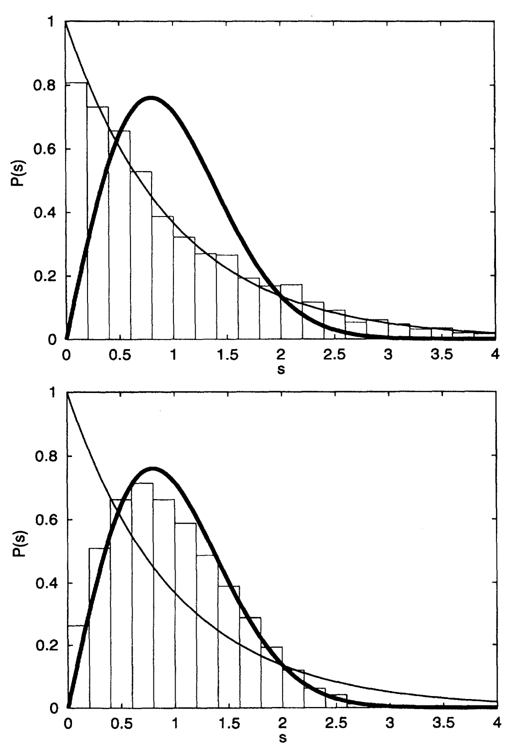

FIG. 5. Distribution of nearest-neighbor spacing for $\bar{E}=0.02$ (top), and $\bar{E}=0.14$ (bottom). Chaotic spectra should follow GOE statistics (thick line) and regular spectra should follow Poisson statistics.

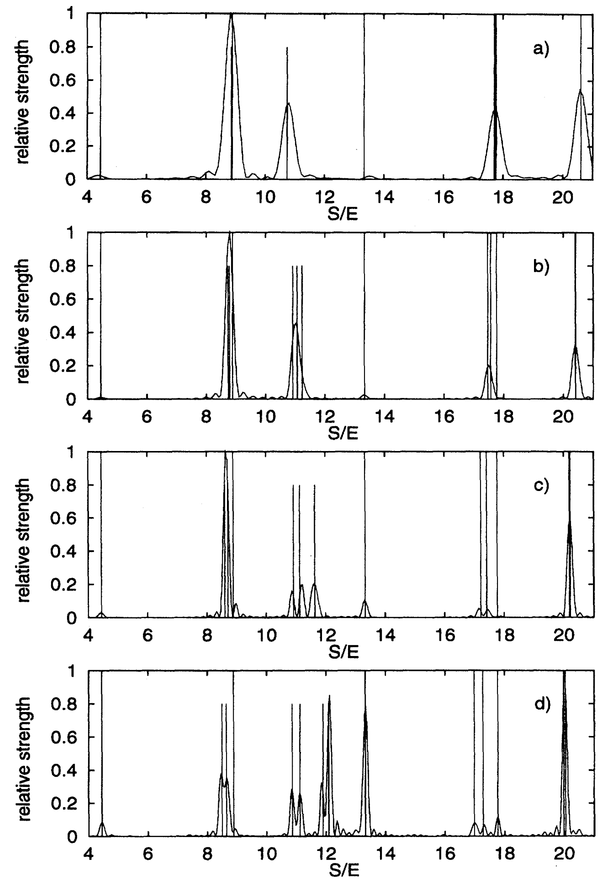

FIG. 6. Fourier transform in $1/\hbar$ for (a) $E=0.03$, (b) $E=0.05$, (c) $E=0.07$, (d) $E=0.09$.

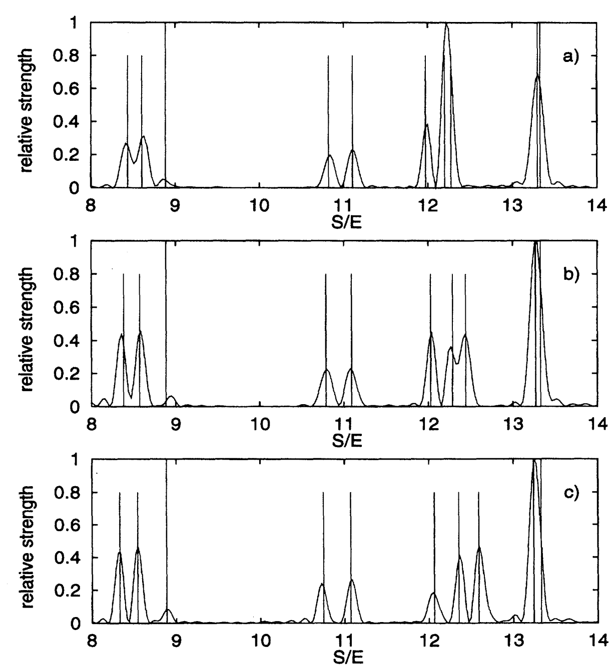

FIG. 7. Fourier transform in $1/\hbar$ for (a) $E=0.10$, (b) $E=0.11$, (c) $E=0.12$.

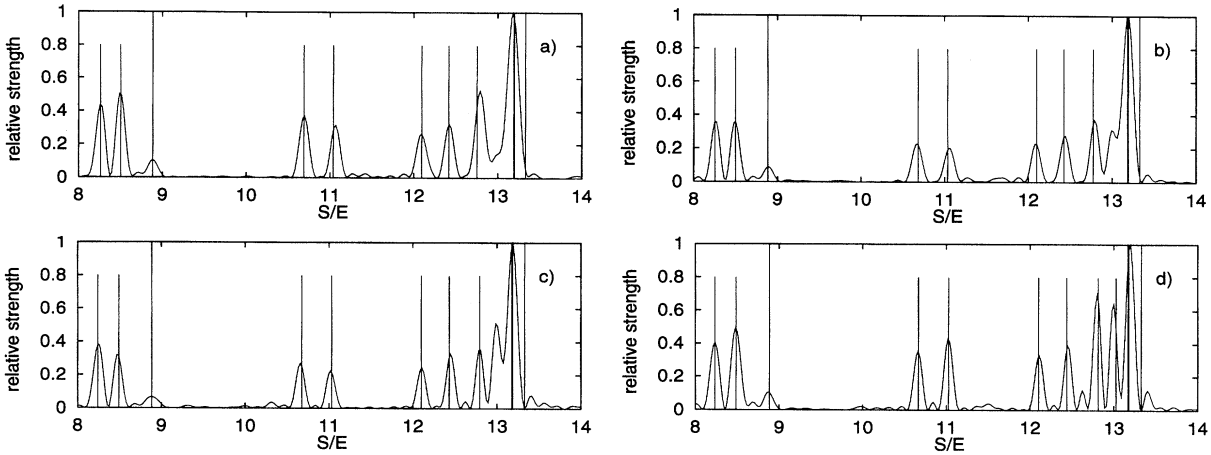

FIG. 8. Fourier transform in $1/\hbar$ for (a) $E=0.134$, (b) $E=0.136$, (c) $E=0.138$, (d) $E=0.140$.

$1/\hbar=100$ to $1/\hbar=400$ in steps of 0.5, and we set $T^*=40$. In Figs. 7 and 8 $\hbar$ ranged from $1/\hbar=10$ to $1/\hbar=240$ in steps of 0.5, and we set $T^*=20$. Whether we were in the mostly regular, mixed, or mostly chaotic regime, the influence of the periodic orbits on the spectra is clearly seen. The signature of bifurcations of periodic orbits in the quantum spectra is also evident. In Fig. 8 we show the occurrence of a peak at around $\bar{S}/E\simeq 13.0$ before a bifurcation actually occurs. This premature peak is attributable to the occurrence of a ghost periodic orbit [11,13]. The periodic orbit that finally appears is a symmetric libration with energy-scaled action $\bar{S}/E\simeq 26.0$ and is depicted in Fig. 1. The large peak at $\bar{S}/E\simeq 13.2$ is due to the symmetric rotation shown in Fig. 1.

In conclusion, we showed that the spectra of a smooth Hamiltonian system contain information about the periodic orbits of the underlying classical system. This correspondence is shown to exist whether the classical phase space is mostly regular, mixed, or mostly chaotic. We also showed that the quantum spectra reflect, through the NNS statistics, whether the classical dynamics is regular or chaotic.

[1] Short-range means of the order of the mean level spacing, whereas long-range means of the order of several mean level spacings.

[2] By $\hbar$ small we mean the dimensionless quantity formed from a combination of physical parameters with $\hbar$ in the numerator. For an introduction to semiclassical mechanics see, for example, A. M. Ozorio de Almeda, *Hamiltonian Systems: Chaos and Quantization* (Cambridge University Press, Cambridge, England, 1988); M. C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer-Verlag, Berlin, 1991).

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