RAPID COMMUNICATIONS

PHYSICAL REVIEW A VOLUME 36, NUMBER 10 NOVEMBER 15, 1987

Transition of spectral statistics due to overlap of quantum resonance zones

W. A. Lin and L. E. Reichl
Center for Statistical Mechanics, University of Texas, Austin, Texas 78712
(Received 24 August 1987)

The quasienergy spacing statistics of a particle in an infinite square well perturbed by a monochromatic external field is studied below and above nonlinear quantum resonance overlap. It is found that at small enough perturbations the quasienergies are accurately given by those obtained from a single resonance, integrable Hamiltonian. The quasienergy spacing distribution undergoes a transition from Poissonian toward Wigner-like behavior when quantum resonance zones overlap, indicating the destruction of a quantum local constant of motion.

In classical nonintegrable Hamiltonian systems, the destruction of a local constant of motion, i.e., the destruction of Kolmogorv-Arnold-Moser (KAM) tori, and the subsequent onset of global chaos occurs when nonlinear resonance zones overlap in phase space.[1] In this article, we will show that, in a quantum system, the destruction of a quantum local constant of motion (and its associated quantum number) occurs when quantum nonlinear resonances overlap.

Let us consider a conservative system with two degrees of freedom. If the system is integrable, each energy level can be labeled by two independent quantum numbers.[2] A pure sequence of energy levels[3] is composed of those levels with one of the two quantum numbers the same. The overall spectrum is then a mixed sequence,[3] a superposition of many pure sequences. Mehta has proved that the spacing distribution of a mixed sequence is a Poissonian in the limit when the mixed sequence is composed of an infinite number of pure sequences, whatever the underlying distribution for the pure sequence, based on the assumption that all the pure sequences are uncorrelated.[4] If the system is nonintegrable, the energy is the only global constant of motion, and the overall spectrum is a pure sequence. Extensive work on the spectral statistics of nuclei has shown that a pure sequence exhibits level repulsion leading to a Gaussian orthogonal ensemble (GOE) distribution of nearest-neighbor spacings. Thus, for the two types of systems, one expects to see distinct spectral characteristics. Conversely, the spacing distribution allows us to determine the existence or absence of an additional constant of motion.

Nonlinear quantum resonance zones were first shown to exist by Berman and co-workers for a model system involving two quantum nonlinear resonances.[5] We have shown[6] the existence of external-field-induced quantum resonance zones for a model describing a particle in an infinite square well driven by a monochromatic external field. We shall examine what happens to the spectrum of this system with and without quantum resonance overlap. This system has a time-periodic Hamiltonian. We must study its quasienergy spectrum,[7] because the system can be viewed as a conservative Hamiltonian system with two degrees of freedom and the quasienergy corresponds to the total energy in this two-degree-of-freedom system.[8] Therefore we can apply the technique of spectral statistics to quasienergies.

For the model we are considering, the Hamiltonian inside the walls (at $x=0$ and $x=2a$) is $\hat{H}=\hat{p}^2/2m+\lambda(\hat{x}-a)\cos(\omega_0 t)$, where $\hat{p}$ is the momentum operator, m is the mass of the particle, $\hat{x}$ is the position operator, λ is the amplitude of the external field, ω_0 is the angular frequency of the external field, and t is the time. The wave function vanishes at the walls. In the angle representation, the Schrödinger equation for the state $|\psi(t)\rangle$ that describes this system is

$$i\hbar\frac{\partial\langle\phi|\psi(t)\rangle}{\partial t}=-\hbar\Omega\frac{\partial^2\langle\phi|\psi(t)\rangle}{\partial\phi^2}-\frac{4a\lambda}{\pi^2}\sum_{N=1;\text{odd}}^{\infty}\frac{1}{N^2}[\cos(N\phi-\omega_0 t)+\cos(N\phi+\omega_0 t)]\langle\phi|\psi(t)\rangle\ , \tag{1}$$

where $\Omega=\hbar\pi^2/8ma^2$, with the conditions $\langle-\phi|\psi(t)\rangle=-\langle\phi|\psi(t)\rangle$ and $\langle\phi+2\pi|\psi(t)\rangle=\langle\phi|\psi(t)\rangle$. In the action representation, the Schrödinger equation becomes

$$i\hbar\frac{d}{dt}\langle j;I|\psi(t)\rangle=j^2\hbar\Omega\langle j;I|\psi(t)\rangle-\frac{4a\lambda}{\pi^2}\cos(\omega_0 t)\sum_{N=1;\text{odd}}^{\infty}\frac{1}{N^2}(\langle j-N;I|\psi(t)\rangle+\langle j+N;I|\psi(t)\rangle)\ , \tag{2}$$

with $\langle -j;I|\psi(t)\rangle=-\langle j;I|\psi(t)\rangle$, where $|j;I\rangle$ is an eigenstate of the unperturbed action operator, $\hat{I}=-i\hbar\partial/\partial\phi$, and j is an integer.

Each of the cosine traveling potential wells in Eq. (1) gives rise to a nonlinear quantum resonance zone in action space. The centers of the zones are located at $j=\pm\omega_0/2N\Omega$.[6] The width of each zone has also been estimated.[6] For small enough λ and high enough ω_0, the resonance zones are well separated.[6] If, the initial population [i.e., $\langle j;I|\psi(0)\rangle$] for $j>0$ is nonzero only within or near a given zone, N_0, and far away from any other zone, then one can show[8] that

$\langle j;I|\psi(t)\rangle$ for $j>0$ [the populations for $j<0$ are always understood to follow the condition $\langle -j;I|\psi(t)\rangle = -\langle j;I|\psi(t)\rangle$], to a good approximation, is given by $\langle j;I|\chi_{\updownarrow}^{(\hat{n})}(t)\rangle$ for $j>0$. $\langle j;I|\chi_{\updownarrow}^{(\hat{n})}(t)\rangle$ satisfies the following equation:

$$i\hbar\frac{d}{dt}\langle j;I|\chi_{\updownarrow}^{(\hat{n})}(t)\rangle = j^2\hbar\Omega\langle j;I|\chi_{\updownarrow}^{(\hat{n})}(t)\rangle - \sum_{\substack{N=N_0;\text{odd}\\ \hat{n}\text{ even}}}^{N_0+\hat{n}}\frac{2a\lambda}{\pi^2N^2}[\langle j-N;I|\chi_{\updownarrow}^{(\hat{n})}(t)\rangle e^{-i\omega_0 t}+\langle j+N;I|\chi_{\updownarrow}^{(\hat{n})}(t)\rangle e^{i\omega_0 t}] , \quad (3)$$

for all integer j, and $\hat{n}=0$. In the angle representation Eq. (3) can be written as

$$i\hbar\frac{\partial\langle\phi|\chi_{\updownarrow}^{(\hat{n})}(t)\rangle}{\partial t} = -\hbar\Omega\frac{\partial^2\langle\phi|\chi_{\updownarrow}^{(\hat{n})}(t)\rangle}{\partial\phi^2} - \sum_{\substack{N=N_0;\text{odd}\\ \hat{n}\text{ even}}}^{N_0+\hat{n}}\frac{4a\lambda}{N^2\pi^2}\cos(N\phi-\omega_0 t)\langle\phi|\chi_{\updownarrow}^{(\hat{n})}(t)\rangle , \quad (4)$$

with the condition $\langle\phi+2\pi|\chi_{\updownarrow}^{(\hat{n})}(t)\rangle=\langle\phi|\chi_{\updownarrow}^{(\hat{n})}(t)\rangle$. For $\hat{n}=0$, Eqs. (3) and (4) describe the behavior of a single isolated nonlinear quantum resonance zone. For larger λ, when zones $N=N_0$ and $N=N_0+2$ overlap but zones $N=N_0$ and $N=N_0-2$ do not, generally all $N>N_0+2$ zones will have overlapped with their neighboring zones and they will also be connected with the zones on the negative j side. The most accurate approximation must then maintain all those terms. Computationally, this is not possible. Fortunately, due to the factor $1/N^2$ in the equations, the dominant contributions come from terms with small N. For the purpose of determining whether a quantum local constant of motion exists, it is sufficient to keep only the two largest zones which overlap [take $\hat{n}=2$ in Eqs. (3) and (4)].

Let us consider Eq. (4) for the single resonance approximation ($\hat{n}=0$). Based on our previous work,[6] together with periodicity conditions $\langle\phi|\chi_{\updownarrow}^{(0)}(t)\rangle=\langle\phi+2\pi|\chi_{\updownarrow}^{(0)}(t)\rangle$ and the theory of quasienergy states,[7] the eigenfunctions of the quasienergy Hamiltonian $\mathcal{H}\equiv\hat{H}(t)-i\hbar\partial/\partial t$ are found to be

$$W_{jl}(\phi,t)=U_{a_j}(\theta(\phi,t))\exp\left[i\omega_0\left(\frac{\phi}{2\Omega N_0}+(\nu_j/2+l)t\right)\right] ,$$

where

$$\theta=(N_0\phi-\omega_0 t)/2,\quad \nu_j=(2j-\omega_0/\Omega N_0)/N_0 ,$$

and j and l are any integers.[8] U_{a_j} satisfies a Mathieu equation

$$d^2U_{a_j}(\theta)/d\theta^2+a_jU_{a_j}(\theta)+2\rho\cos(2\theta)U_{a_j}(\theta)=0$$

with $\rho=8a\lambda/\hbar\Omega\pi^2N_0^4$, and must be of the form of a Floquet solution, namely, $U_{a_j}(\theta)=\exp(i\nu_j\theta)Q_j(\theta)$ and $Q_j(\theta)=Q_j(\theta+\pi)$. For each j, there is a corresponding characteristic exponent, ν_j, and therefore a corresponding a_j. The corresponding quasienergy is

$$\mathcal{E}_{jl}=\frac{1}{4}N_0^2a_j\hbar\Omega-\frac{\hbar\omega_0^2}{4\Omega N_0^2}+\left(\frac{j}{N_0}+l\right)\hbar\omega_0 . \quad (5)$$

This describes the complete quasienergy spectrum. The corresponding quasienergy state is $\langle\phi|\chi_{\updownarrow}^{(0)}(t)\rangle = W_{jl}(\phi,t)\times\exp(-i\mathcal{E}_{jl}t/\hbar)$. This proves that the quasienergy spectrum is discrete for a system satisfying Eq. (4) with $\hat{n}=0$.

We are interested in the effect of resonance overlap. We must construct a wave function which is dominantly composed of quasienergy states which are responsible for the resonance zones. The quasienergy spectrum is then the Fourier spectrum of the wave function (for $\hbar=1$). Therefore we compute the spectrum numerically by initially populating a single level inside the resonance zone and obtain solutions to Eq. (3) over a long period of time. We then compute the discrete Fourier transform of the resulting $\langle\phi=O|\chi_{\updownarrow}^{(\hat{n})}(t)\rangle$. Due to the condition $\langle -j;I|\psi(t)\rangle = -\langle j;I|\psi(t)\rangle$, it contains the same spectrum as $\langle\phi=O|\psi(t)\rangle$ when we retain in Eq. (1) the appropriate resonances. In terms of atomic units (see Ref. 6), we choose $a=10$, $m=1$, and ω_0 is chosen to correspond to a resonance transition between $|150;I\rangle$ and $|151;I\rangle$ for specific computations. Thus we are probing the full quantum domain.

We have computed the quasienergy spectra for $N_0=1$ for both the single resonance case ($\hat{n}=0$) and the double resonance case ($\hat{n}=2$) with the same initial condition. The single resonance case is classically integrable and the double resonance case is classically nonintegrable. At $\rho=25$ (which corresponds to $\lambda\approx0.03805$), we obtain identical power spectra for both cases. The spectra form clusters of discrete peaks. For each peak, there is a corresponding peak in the adjacent clusters at a distance of ω_0. The peak locations are found to be in complete agreement with Eq. (5), to six significant figures. Due to a relatively small number of quasienergy states involved, we did not attempt to obtain its spacing distribution. At higher λ, we have computed the Fourier spectra for λ small enough that no overlap occurs ($\lambda=4$), and for λ above overlap ($\lambda=9,15$) (the overlap occurs near $\lambda=7$,)[6] for three different input data windows, $t\in[8.192,2105.344]$, [2105.344,4202.496], and [8.192,4202.496]. The interval [8.192,4202.496] corresponds to about 2479 oscillations of the external field. The spectra are discrete to within numerical accuracy. For these spectra, we compute spacing distributions and then compare them with a theoretical distribution to measure the degree of spectral repulsion. For the theoretical distribution, we will use the Brody distribution,[9]

$$P_q(S)=(1+q)\beta S^q\exp(-\beta S^{1+q}) ,$$

where

$$\beta=\{\Gamma[(2+q)/(1+q)]/D\}^{1+q} ,$$

D is the local average spacing, q is the Brody parameter, S is the nearest neighbor spacing defined in the range $S\in[0,\infty)$. It interpolates between the Poisson distribution ($q=0$) and the Wigner distribution ($q=1$) (the

Wigner distribution is only very slightly different from the GOE distribution).[4] The Brody parameter measures the degree of spectral repulsion in the spectrum. We first eliminate the edges of spectra to obtain "good spectra."[10] They are then unfolded with cubic splines to remove the secular behavior.[11] Because of the finite resolving power of the discrete Fourier transform together with the unfolding procedure, at the edge of small spacings, there are generally less spacings than one could detect with infinite resolving power. We have determined that the spacing distribution for $y < y_c = 4\pi/(TD'_{\min})$ cannot be obtained accurately (y is the unfolded spacing, T is the length of input data window, and $D'_{\min}$ is the minimum of local average spacing in the original spectrum). Therefore the spacing distributions are computed starting from y_c. To take into account this factor, we must construct a truncated distribution[12] from the Brody distribution. We define the corresponding truncated distribution as

$$P'_q(S) \equiv P_q(S) / \int_{S_c}^{\infty} P_q(S) dS, \quad S \in [S_c, \infty) ,$$

where S_c is the minimum spacing to be observed. We obtain, after a change of variable $y = S/D'$, the following truncated Brody distribution:

$$P'_q(y) = A^{1+q}(1+q)B(q)y^q \times \exp[-A^{1+q}B(q)(y_c^{1+q} - y^{1+q})] ,$$

where $A = D'/D$, $B(q) = \{\Gamma[(2+q)/(1+q)]\}^{1+q}$, and $y \in [y_c, \infty]$. $D(D')$ is the average spacing over the range $(0,\infty)([S_c,\infty))$. The computed distributions are then fitted with the truncated Brody distribution by a nonlinear least-square method to obtain the best fit parameters, A and q. For larger S, the distribution changes qualitatively as q changes from 0 to 1 so that even for larger S we obtain considerable information about the value of q.

Figure 1 presents the results for $\lambda = 4$, 9, and 15 using the data window $t \in [2105.344, 4202.496]$. For the single resonance approximation, we see that the distributions are close to the Poisson type for all λ's (the q for $\lambda = 4$ is slightly large; this appears to be due to the smaller number of spacings involved and the resulting poorer statistics). This is consistent with our expectation, since the single resonance approximation is integrable. For the

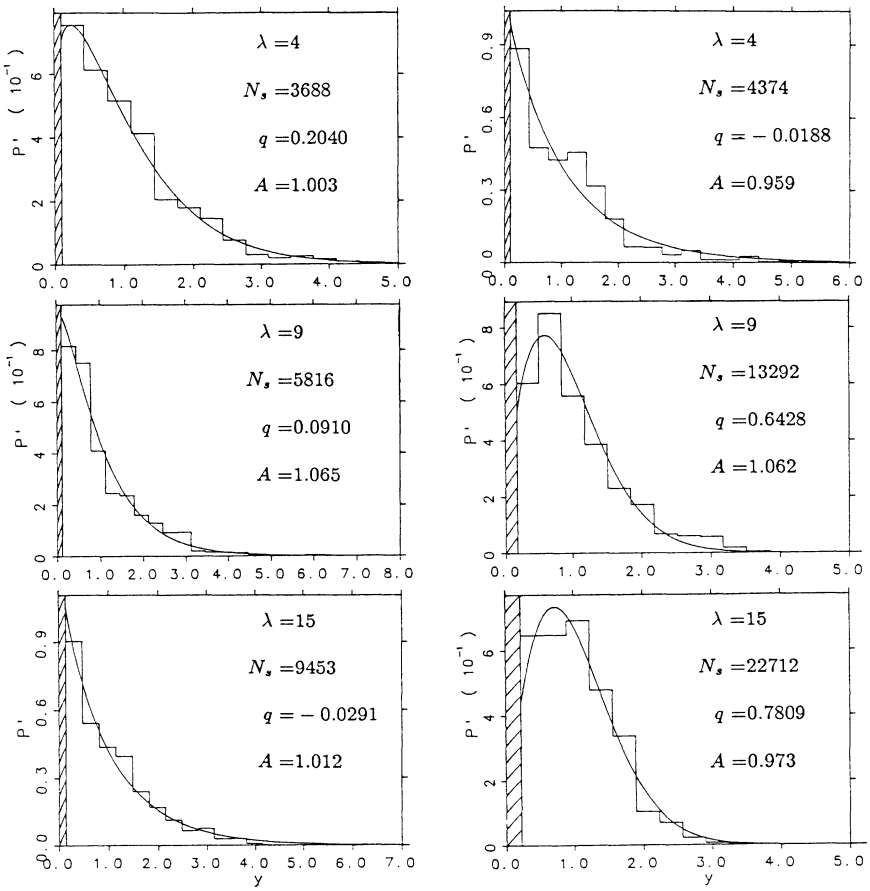

FIG. 1. Spacing distributions from numerical experiments (curve of steps) and best-fit truncated Brody distributions (smooth curve). The slashed part corresponds to the unobserved region $[0, y_c)$. N_s is the total number of spacings involved in the experimental distribution. The left column is for the single resonance approximation and the right column is for the double resonance approximation.

double resonance approximation, the distribution is close to Poisson type at $\lambda=4$. As λ is increased to 9 and 15, the distributions are strongly deviated from the Poisson type and tend toward the Wigner type with large spectral repulsions. Thus the spectrum in the region of the resonance zones undergoes a change in its characteristic from a predominantly mixed sequence to a predominately pure sequence through resonance overlap. Figure 2 gives the best-fit Brody parameters for the three data windows we have computed. At longer data windows, the Brody parameter decreases for the double resonance approximation at $\lambda=9$ and 15. This appears to occur because for the initial condition chosen, the wave function is composed not only of quasienergy states responsible for the resonance zones but also of those which are responsible for the nonresonant region, although with much smaller amplitudes. When the length of data window is increased, one is seeing more contributions coming from the nonresonant regions because of the reduction in leakage in the discrete Fourier transform. But still, the repulsion in the spectrum is nonnegligible.

In conclusion, at very small λ ($\lambda\approx 0.03805$) the system is accurately described by a single resonance Hamiltonian. At larger λ ($\lambda=4$), but below resonance overlap, we find that the spectrum is a predominately mixed sequence. These facts indicate that at small enough λ the quasienergy levels can be labeled by two quantum numbers. This is a quantum version of KAM theorem[13] in the sense that the system behaves like an integrable system at small enough perturbations. There appear to be two constants of motion. One is global and the other is local. Classically, the existence of a local constant of motion forms the basis of KAM theorem. We have here seen the manifestation of this phenomenon in a microscopic quantum domain. At larger perturbations when the resonance zones overlap, the predominately pure sequence observed signifies the destruction of the local constant of motion. This is a quantum manifestation of classical resonance overlap where the destruction of all the nonresonant tori between the two resonance zones implies the destruction of the local constant of motion in a large part of phase space. We hope to present more details of this work in a forthcoming paper.

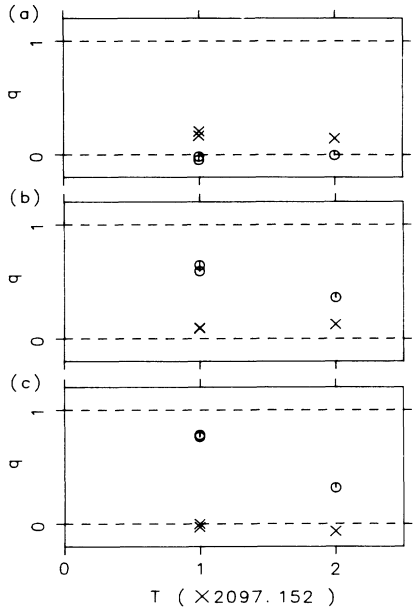

FIG. 2. The Brody parameter measured vs the total length of the data window. The x corresponds to the single resonance approximation and the circle corresponds to the double resonance approximation, (a) $\lambda=4$, (b) $\lambda=9$, (c) $\lambda=15$.

The authors wish to thank the U.S. Naval Air Systems Command (Contract No. MDA 903-85-C-0029) for partial support of this work. The authors also wish to thank the Welch Foundation of Texas for partial support, in particular, Grants No. F-1051 (W.A.L. and L.E.R.) and No. F-365 (W.A.L.).

[1]A. J. Lichtenberg and M. A. Lieberman, *Regular and Stochastic Motion* (Springer, New York, 1983).

[2]I. C. Percival, J. Phys. B **6**, L229 (1973).

[3]T. A. Brody, J. Flores, J. B. French, P. A. Mello, A. Pandey, and S. S. M. Wong, Rev. Mod. Phys. **53**, 385 (1981), and references therein; R. U. Haq, A. Pandey, and O. Bohigas, Phys. Rev. Lett. **48**, 1086 (1982).

[4]M. L. Mehta, *Random Matrices and the Statistical Theory of Energy Levels* (Academic, New York, 1967).

[5]G. P. Berman and G. M. Zaslavskii, Phys. Lett. **61A**, 295 (1977); G. P. Berman, G. M. Zaslavskii, and A. R. Kolovsky, *ibid.* **87A**, 152 (1982); G. P. Berman and A. R. Kolvsky, *ibid.* **95A**, 15 (1983); G. P. Berman, G. M. Zaslavskii, and A. R. Kolovsky, Zh. Eksp. Teor. Fiz. **81**, 506 (1981) [Sov. Phys. JETP **54**, 272 (1981)]; G. P. Berman and A. R. Kolovsky, Physica D **8**, 117 (1983).

[6]L. E. Reichl and W. A. Lin, Phys. Rev. A **33**, 3598 (1986).

[7]Ya. B. Zel'dovich, Zh. Eksp. Teor. Fiz. **51**, 1492 (1966) [Sov. Phys. JETP **24**, 1006 (1967)]; Ya. B. Zel'dovich, Usp. Fiz. Nauk **110**, 139 (1973) [Sov. Phys. Usp. **16**, 427 (1973)]; H. Sambe, Phys. Rev. A **7**, 2203 (1973).

[8]W. A. Lin, Ph.D. thesis, University of Texas at Austin, 1986 (unpublished).

[9]T. A. Brody, Lett. Nuovo Cimento **7**, 482 (1973). The semiclassical formula of Berry and Robnik [J. Phys. A **17**, 2413, (1984)] does not appear to apply in what we are considering since our potential does not have scaling behavior, the system is in a full quantum regime, and the spectra cover wide ranges.

[10]F. J. Dyson and M. L. Mehta, J. Math. Phys. **4**, 701 (1963).

[11]E. Haller, H. Köppel, and L. S. Cederbaum, Phys. Rev. Lett. **52**, 1665 (1984).

[12]E. Abramson, R. W. Field, D. Imre, K. K. Innes, and J. L. Kinsey, J. Chem. Phys. **80**, 2298 (1984).

[13]G. Hose and H. S. Taylor, Phys. Rev. Lett. **51**, 947 (1983); L. E. Reichl and W. A. Lin, Found. Phys. **17**, 689 (1987).