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# Dynamical Quasidegeneracies and Separation of Regular and Irregular Quantum Levels

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Dynamical quasidegeneracies may arise in the spectrum of systems having discrete symmetries. They are semiclassically interpreted as quantized congruent-but-distinct tori in phase space. With them the separation of regular and irregular states in the quantum spectrum of some mixed-phase-space systems may be performed in a simple, yet clear fashion. At finite energies ($h$ finite), the frontier between regular and irregular states is not sharp. This is illustrated by the study of two coupled quartic oscillators.

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The recent advances in classical mechanics regarding the coexistence of regular and stochastic motion in low-dimensional generic Hamiltonian systems have not yet been fully translated insofar as the correspondence principle is concerned. In this Letter, we partially address this shortcoming by demonstrating the complete classification of quantum levels in a spectrum, as conceived by Percival[1] more than 15 years ago, in a simple, yet precise manner. He proposed that the quantum energy levels of a system classically possessing a mixed phase space [containing Kol'mogorov-Arnol'd-Moser (KAM) islands and chaotic regions] should belong *either* to a regular *or* an irregular class. To date, the attempts to perform this identification systematically throughout a spectrum have been inconclusive because none of the criteria used, such as the behavior under a slowly changing perturbation, were by themselves exclusive enough. Our technique shall rest on a combination of Einstein-Brillouin-Keller (EBK) quantization and discrete symmetries. We find that Percival's classification scheme works quite well although there exist levels of a somewhat intermediate character. In fact, depending on the nature of the dynamics at the KAM-chaos interface, the frontier between regular and irregular states may be difficult to define.

For some systems the discrete symmetries, when properly understood, provide the key in identifying regular levels. They have the following effect on the classical phase space: An invariant torus of a regular region is transformed by the symmetry-group elements into an invariant torus which is congruent to the initial one and which may or may not coincide with it.[2] In this latter case one expects, and finds, that quantum levels corresponding to torus quantization will appear as quasidegenerate doublets (multiplets in general)—an example of what may be coined *dynamical quasidegeneracies*—belonging to different symmetry classes. The extremely small splittings result from what is termed *dynamical tunneling* by Davis and Heller.[3] This is the generalization of the well-known tunneling in a one-dimensional symmetric double-well potential (quasidegeneracies of parity doublets). Note that no potential-energy barrier is necessary. For those systems whose invariant tori are all duplicated in phase space, yet do not have global symmetries implying exact degeneracies, the resultant quasidegeneracies provide a "filter" for the complete set of regular levels since those levels which are not quantized on tori do not appear quasidegenerate except for random coincidences (assuming a single significant chaotic region). This filter is made even more stringent by realizing that EBK (torus) quantization results in the regular levels appearing *locally* as though they fit into a series of nearly uniform (harmonic-oscillator-like) subspectra. The occasional fake quaside-

generacy almost never fits into one of these sequences. The great simplicity of this method is that it does not rely at all on the eigenfunctions or statistical assumptions about their morphology.

Let us first briefly describe what is expected on the basis of standard EBK quantization. As is well known, the EBK scheme can only be performed when there exist invariant tori. For two-degrees-of-freedom systems each torus is specified by the values of its actions $\{J_1,J_2\}$ and usually one chooses $J_1$ as the area interior to the intersection of the torus with a Poincaré section. If one restricts one's attention to a single KAM island at fixed energy $E$, $J_2$ can be expressed as a function of $J_1$: $J_2=g^E(J_1)$. However, the actions $\{J_1,J_2\}$ are not directly accessible by classical propagation of trajectories. It is thus convenient to first introduce the function $J=f^E(\alpha)$, where $\alpha$ is the winding number of the torus $(J_1, J_2=g^E(J_1))$, and $J=J_2+\alpha J_1$. $J$ can be interpreted as the action integral along a trajectory between two successive intersections of a Poincaré section $\theta_2=$const at energy $E$ ($\theta_1,\theta_2$ are the angle variables associated with the actions $J_1,J_2$). It is easily shown that $\alpha=-dg^E/dJ_1$. The transformation from $g^E$ to $f^E$ (and the reverse) is therefore a Legendre transformation.

To construct $f^E$, one follows an orbit many times around the torus until it nearly closes on itself while counting the number of times $\{r,s\}$ it has traveled around the primitive cycles corresponding to the actions $\{J_1,J_2\}$. This is easily done by numerically integrating and watching the Poincaré section. The action integral along the orbit may then be written approximately as a linear combination of $\{J_1,J_2\}$,

$$S=\int_{\text{orbit}}\mathbf{p}\,d\mathbf{q}\simeq rJ_1+sJ_2=sJ^E. \tag{1}$$

This gives $J$ and $\alpha$ through $\alpha\simeq r/s$. From $f^E$, one then deduces the curve $g^E$. Although the function $g^E$ is, strictly speaking, generally (in nonintegrable cases) nowhere continuous, this calculation provides a smoothed $g^E$ except where there exist large resonances which show up as gaps in the curves $J=f^E(\alpha)$ and $J_2=g^E(J_1)$.

The gist of the semiclassical quantization rules for the spectrum is to construct, in the $(J_1,J_2)$ space, the one-parameter family $g^E$ for the energy range of interest. Then, the Bohr-Sommerfeld conditions imply that when $E$ is such that the curve $g^E$ lies on a point of the grid

$$\begin{pmatrix}J_1\\J_2\end{pmatrix}=\begin{pmatrix}2\pi\hbar(n_1+l_1/4)\\2\pi\hbar(n_2+l_2/4)\end{pmatrix}\quad(n_1,n_2=0,1,2,\ldots) \tag{2}$$

[where $(l_1,l_2)$ are Maslov indices], then $E=E_{n_1,n_2}$ is a quantum eigenenergy with quantum number $n_1,n_2$.

The system we investigate[4] is governed by the Hamiltonian

$$H(\mathbf{q},\mathbf{p};\lambda,b)=\tfrac{1}{2}(p_1^2+p_2^2)+a(\lambda)(q_1^4/b+2\lambda q_1^2q_2^2+bq_2^4). \tag{3}$$

The multiplicative factor $a(\lambda)>0$ is there for convenience, $b$ is chosen near but different from 1, reducing the symmetry from $C_{4v}$ to $C_{2v}$ (thus no exact degeneracies are expected), and the coupling parameter $\lambda\geq 1$ determines the relative degree of regular to stochastic motion. This $H$, previously investigated by several authors,[5] is well suited here for several reasons. (i) $\lambda$ may be chosen such that a considerable fraction of phase space is covered with resonant tori all of which are duplicated. (ii) The symmetries are simple, time-reversal and $q_1,q_2$ reflections, so there are four representations labeled by $(\epsilon_1,\epsilon_2)(\epsilon_i=\pm 1,\ i=1,2)$. (iii) The classical study can be performed at a single energy (which we do at $E_0=1$) since all actions $S$ and periods $T$ scale as (the dynamics are otherwise unchanged) $S^E=(E/E_0)^{3/4}S^0$, $T^E=(E/E_0)^{-1/4}T^0$ (rescaled quantities are denoted by a 0 superscript). One main consequence is that, since $g^E(J_1)=E^{3/4}g^0(E^{-3/4}J_1)$, it is sufficient to construct only the curve $g^0$ to obtain the one-parameter family $g^E$. (iv) Long accurate spectral sequences are obtainable[6] (20000–30000 levels) with errors $<10^{-5}$ of a mean spacing $D$ (this we find by calculating an upper and lower bound on each level).

It is sometimes convenient to reexpress the quantization conditions (2) in terms of $\{\alpha,J\}$. Using (1) and (2) for this system,

$$E^{3/4}_{n_1n_2}=(2\pi\hbar/J^0_{n_1n_2})[(n_2+1)+\alpha(n_1+\tfrac{1}{2})] \tag{4}$$

which is not a harmonic-oscillator spectrum because there is an outer edge, $J_1(\max)$, to the KAM islands and $\{\alpha,J^0\}$ are not constant. Usually, however, $J^0$ varies little for resonant KAM islands and so

$$\Delta E^{3/4}_{n_1n_2}\equiv E^{3/4}_{n_1n_2+1}-E^{3/4}_{n_1n_2}\simeq 2\pi\hbar/J^0_{n_1n_2} \tag{5}$$

is locally approximately constant in $E^{3/4}$. Therefore, long uniform sequences of quasidoublets (going to infinite energy) found by changing $n_2$ will appear in the spectrum considered. For the rescaled tori (to an energy surface $E=1$, say), increasing $n_2$ ($n_1$ fixed) is associated with moving toward the center of the KAM island and the energy splittings tend to zero (though not necessarily uniformly). Increasing $n_1$ ($n_2$ fixed) does the opposite and the sequences cut off in $n_1$ as one exits from the KAM island.

From which sequences the quasidegenerate levels are found depends on the symmetry properties of the tori. With the convenient choice $(\lambda,b)=(-0.35,\pi/4)$, 12% of the phase space is covered by KAM islands and each of the quantizing tori, to an energy of approximately the 22000th state, has only one duplicate. They all reside in one of four main islands; see Fig. 1. One element of the reflections $\{P_1,P_2,P_1P_2\}$ leaves the tori of a given island invariant. Thus, for a given torus associated with a wave function $\Psi$, among the four functions

$$\Psi_{\epsilon_1\epsilon_2}=\tfrac{1}{4}(1+\epsilon_1P_1)(1+\epsilon_2P_2)\Psi, \tag{6}$$

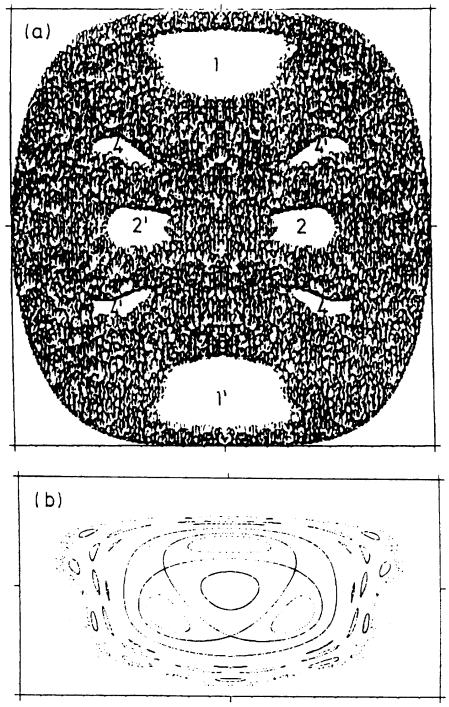


FIG. 1. (a) Poincaré section $q_1=0$ for $(\lambda,b)=(-0.35,\pi/4)$ showing the different KAM islands. (b) Enlarged view of the largest KAM island (island 1).

which belongs to states labeled by $(\epsilon_1,\epsilon_2)$, two are nonzero and associated with quasidegeneracies and the two remaining ones vanish; see Table I.

The first step in the analysis of the quantum levels is to compare two symmetry-related spectra, searching for all quasidegeneracies. From this list of candidates, fixed-$n_1$ sequences are constructed. One finds that almost all of the best quasidegeneracies, splittings $\sim 10^{-3}D$ to $\sim 10^{-8}D$, do reside in sequences. The quantum number assignments are then relatively straightforward to make even without constructing the curve $g^0$, since the $n_1=0$ sequence comes lowest in the spectrum, then $n_1=1$, etc., and usually only one integer $n_2$ gives a value of $J_2^0$ in the right range. Next, a quantum-derived curve $g_{\rm qm}^0$ is constructed via the computed quantum energies, the scaling relations, and the quantization conditions. The classical and quantum results for island 1 are given in Fig. 2. We find that (i) the two curves coincide to a very high precision where the

TABLE I. Symmetries of quasidoublets (see Fig. 1).

| Island | $n_2$ even | $n_2$ odd | Symmetry |
|---|---|---|---|
| 1,1′ | (++),(−−) | (+−),(−+) | $P_1P_2$ |
| 2,2′ | (++),(+−) | (−+),(−−) | $P_1$ |
| 3,3′ 4,4′ | (++),(−+) | (+−),(−−) | $P_2$ |

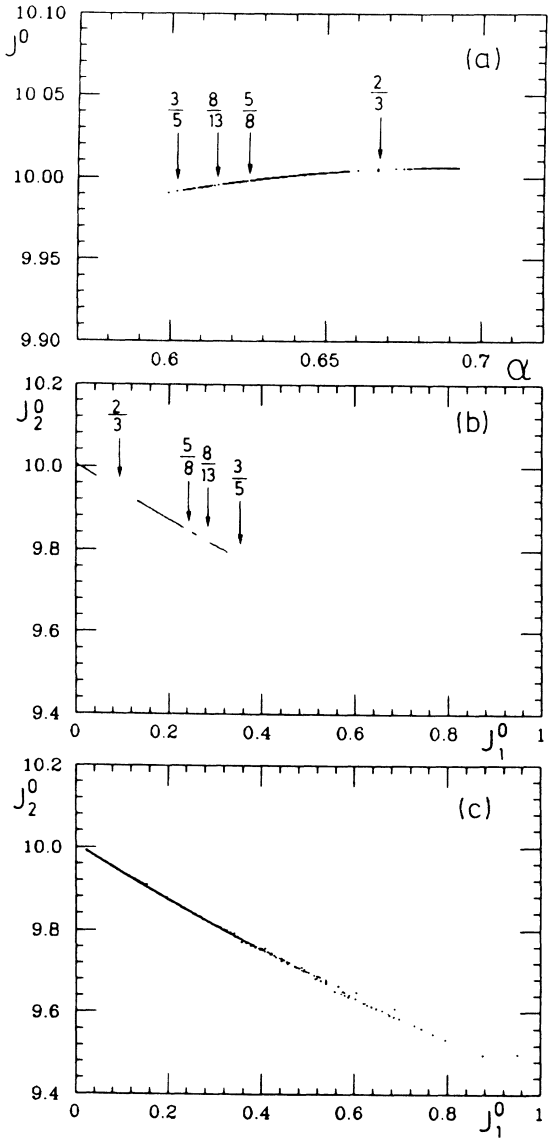


FIG. 2. Regular states in island 1 (see Fig. 1). (a) Plot of the curve $f^0$ relating $J^0$ and $\alpha$. (b) Curve $g^0$ relating the scaled actions $J_1^0$ and $J_2^0$; (a) and (b) come from the classical motion. (c) Curve $g_{\rm qm}^0$ obtained from the quantum spectrum.

classical one is defined, (ii) the quantum curve interpolates through the gaps, and (iii) the quantum curve extrapolates beyond the edge of the island $J_1^0(\max)=0.37$. Remark (i) is not surprising, nor is (ii) when $\hbar$ is too large to resolve the resonant structures (the $\frac{2}{3}$ resonance is an exception here [Fig. 1(b)], which will be treated elsewhere[4]); remark (iii), however, deserves further comment.

Up to $J_1^0=0.40$ the continuation of $g^0$ quantum mechanically by $g_{\rm qm}^0$ is almost perfect. One expects to find exactly 1112 quasidoublets and 1088 are found with quantum number assignments. Beyond 0.40 one still locates 202 quasidoublets with sometimes dubious quantum number assignments. They rather gently continue

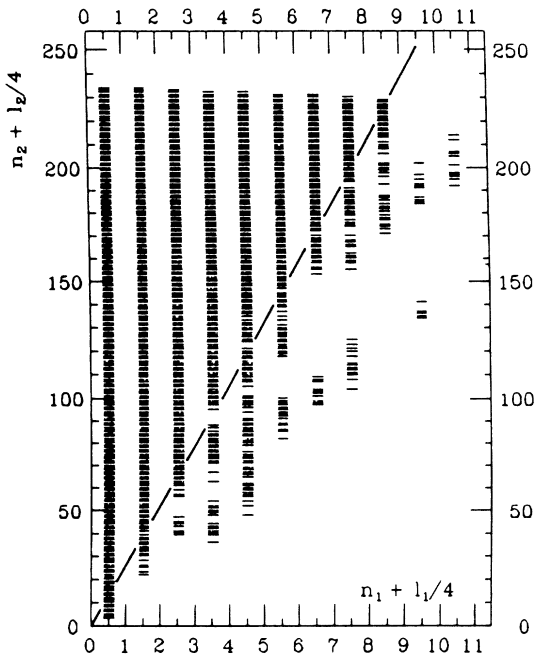


FIG. 3. Quantum numbers $n_1,n_2$ of the regular states identified in and around island 1 as quasidoublets among the first $\simeq$22000 levels. The straight line locates the border of the KAM island. The lower right represents the exterior.

the curve $g^0$ but their splittings tend to be larger and they no longer form (almost) complete sequences (for instance, for $0.40 \leq J_1^0 \leq 0.50$ one finds only 103 quasidoublets instead of 271). What happens is further illustrated in Fig. 3, where the points which give rise to identified quasidoublets on the grid $(n_1,n_2)$ are plotted. One sees that the quasidoublets on the lower right have extended beyond the classical boundary. The regular-chaotic interface is such that the regular region, as "viewed" quantum mechanically, is larger than the classical regular region. But this is not always so. For the case of islands 2, 3, and 4 [see Fig. 1(a)], for instance, the opposite happens; fewer quasidoublets than expected semiclassically can be identified. In fact, depending on the nature of the regular-chaotic interface as described by classical dynamics (i.e., fast mixing beyond the border or, on the opposite extreme, presence of partial barriers), reduction or extension of the signatures of regularity interior to or beyond the boundary may result.

To conclude, let us start by emphasizing that Percival's scheme works well. Only a few percent of the levels appear to be of an intermediate nature and EBK works remarkably well as a guide. Despite this, one could not necessarily select eigenvalues based solely on the quantized energies derived from $g^0$ because of ambiguities with close-lying levels and displacements due to tunneling. The dynamical quasidegeneracies are essential. Furthermore, their existence, resulting from a conspiracy of discrete symmetries and classical dynamics (structure of phase space showing different congruent tori) is not exceptional but, on the contrary, rather conspicuous and they may exist in regular as well as mixed systems. Examples are provided by models of the $H_2O$ molecule,[7] the $H_2^+$ molecule (regular system),[8] the elliptic billiard (regular system),[9] the Hénon-Heiles potential (mixed system),[3] and the hydrogen atom in a constant magnetic field (mixed system).[10] A distinctive feature of the quasidegeneracies, in contrast to statistically expected near degeneracies, is that even when varying a parameter over large ranges (the $\lambda$ coupling in our case) they persist, at differing energies, as long as the classical dynamics still preserves the existence of the tori on which they are built. The splittings of the quasidegeneracies (dynamical tunneling) are ideally suited for studies of tunneling in the presence of chaos, a subject still in its infancy.[11] For systems showing scaling properties, as the coupled quartic oscillator case, one can study the approach to the semiclassical limit without ambiguities, using the fact that each rescaled torus quantizes an infinite number of times, giving rise to an infinite sequence of dynamical quasidegeneracies. Work along these lines is in progress.

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