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Kramers' Degeneracy and Quartic Level Repulsion.

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Abstract. – An elementary technique, based on almost degenerate perturbation theory, is used to establish the association between (unitary and antiunitary) symmetries and universality classes of level repulsion for autonomous and periodically driven quantum systems. For one such class, characterized by Kramers' degeneracy and quartic level repulsion, we present a simple example, a periodically kicked top with half-integer angular momentum, which has one antiunitary symmetry (a generalized time reversal) but no unitary symmetry; in the classical limit that top behaves chaotically.

Four universality classes of random Hermitian and unitary matrices have proven relevant for the quantum dynamics of nuclei, atoms, nonlinear oscillators etc. Matrices of one of these classes have eigenvalues with a tendency to clustering; the remaining three classes display level repulsion of different degrees (linear, quadratic and quartic) [1-3].

Hermitian random matrices can serve as models of Hamiltonians H of autonomous systems. Unitary random matrices play an analogous role for periodically driven systems, as models of the unitary evolution operators U describing the change of the quantum state during one cycle of the driving; their powers U^n with $n = 1, 2, 3, \ldots$ yield a stroboscopic description of the driven dynamics in question.

It is well established that operators H or U pertaining to one of the classes with level repulsion yield, in the classical limit, chaotic dynamics dominating the phase space [4-6]. Level clustering, on the other hand, can be the quantum signature of either classically regular motion [7] or classical chaos. Indeed, a quantum system exhibiting, in some suitable representation, Anderson localization tends to have degeneracies with respect to eigenvectors (of H or U) sufficiently disjoint in their supports, even if its classical counterpart has its phase space dominated by chaos [8, 9].

Realistic operators H or U often do not have universal spectral properties according to one of the four classes mentioned. It is not untypical, though, to find a transition from level

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clustering to level repulsion, parallel to the classical transition from dominantly regular to dominantly chaotic motion, as a parameter in H or U is varied [10-14].

The three universal degrees of level repulsion can be characterized by symmetries. To find the potential universality class for a given operator H or U the unitary symmetries S obeying $[S, H] = 0$ or $[S, U] = 0$ must be identified. Even more importantly, it must be known whether or not there is an antiunitary symmetry T such that (1,2)

$$T^2 = \pm 1 \quad \text{and} \quad THT^{-1} = H \quad \text{or} \quad TUT^{-1} = U^+. \tag{1}$$

The cases $T^2 = +1$ and $T^2 = -1$ arise for systems with, respectively, integer and half-integer values of the total angular momentum; obviously, the latter case is possible only if the number of fermions in the system is odd. $T^2 = -1$ implies the double degeneracy of all eigenvalues of H or U known as Kramers' degeneracy.

An example of an antiunitary symmetry is conventional time reversal [1, 2, 15] T_0 (which leaves coordinates invariant and reverses the sign of all momenta as well as angular momenta). That symmetry is broken by magnetic fields; in such situations a generalized time reversal invariance may still hold [14, 16] with TT_0^{-1} some unitary operator (3).

The association of symmetries with universality classes is the same for Hermitian and unitary operators. It can be summarized as follows. *Linear level repulsion* is typical in either of two situations. i) One or several antiunitary symmetries exist, *all* with $T^2 = +1$. Only levels within a subspace defined by fixed eigenvalues of geometric symmetries S must be considered. ii) There is a T with $T^2 = -1$ in addition to sufficiently high geometric symmetries (like two anticommuting parities both squaring to -1 or full rotational symmetry). *Quadratic level repulsion* results when i) there is no antiunitary symmetry at all or ii) there is one such with $T^2 = -1$ in addition to one parity S with $S^2 = -1$, $[T, S] = 0$. *Quartic level repulsion* obtains for systems with Kramers' degeneracy (*i.e.* T with $T^2 = -1$ holds) lacking any geometric symmetry.

Using Wigner's theory of co-representations we have recently worked out the association just sketched for unitary operators U [17]; the extension to time-independent Hamiltonians is trivial. Technically easier than the group-theoretical procedure is an argument based on almost degenerate perturbation theory [18]. We shall now illustrate that technique for unitary evolution operators with an antiunitary symmetry T, $T^2 = -1$.

Imagine a close encounter of two eigenphases (quasi-energies) of U such that their spacing is smaller than the distance of either to all other levels. To find out how strongly the two levels resist a true crossing, we choose a quadruple of orthonormal vectors as approximants to the four relevant eigenstates of U (due to Kramers' degeneracy there are two states for each level). We incorporate $T^2 = -1$ by requiring the four vectors to obey

$$T|1\rangle = |2\rangle, \qquad T|2\rangle = -|1\rangle, \qquad T|3\rangle = |4\rangle, \qquad T|4\rangle = -|3\rangle. \tag{2}$$

In the space so arranged the operator U is represented by a four-by-four matrix. Due to the

(1) The «covariance» of U with T is a natural extension of the invariance of H to periodically driven systems whose Hamiltonians obey $H(t) = H(t + \tau)$ and $TH(t)T^{-1} = H(-t)$; an appropriate shift of the zero of time may be necessary to make the latter symmetry manifest.

(2) Antiunitary operators anticommuting with H or commuting with U lead to conclusions similar to the ones given in the text; the main difference to (2) is that these cases exclude the possibility of Kramers' degeneracy and thus of quartic level repulsion.

(3) A constant magnetic field $\boldsymbol{B}$ leads to a unitary operator TT_0^{-1} describing a rotation by π around an axis perpendicular to $\boldsymbol{B}$.

T covariance that matrix takes the form (4)

$$U = \begin{bmatrix} \alpha + i\beta & 0 & \sigma + i\gamma & \delta - i\varepsilon \\ 0 & \alpha + i\beta & \delta + i\varepsilon & -\sigma + i\gamma \\ -\sigma + i\gamma & -\delta + i\varepsilon & \alpha - i\beta & 0 \\ -\delta - i\varepsilon & \sigma + i\gamma & 0 & \alpha - i\beta \end{bmatrix}. \tag{3}$$

By unitarity the six parameters α, β, γ, δ, ε, σ are all real (5) and their squares sum up to unity.

A lowest-order approximation for the two almost degenerate levels is given by the eigenvalues of (3). Due to $T^2 = -1$ the quartic secular equation of (3) is biquadratic and has the two double roots

$$e_\pm = \alpha \pm i\sqrt{\beta^2 + \gamma^2 + \delta^2 + \varepsilon^2 + \sigma^2}. \tag{4}$$

The discriminant in (4) being the sum of five nonnegative terms there would have to be five free parameters in the operator U to make the level crossing $e_+ = e_-$ a generic possibility rather than an unlikely exception. Quartic level repulsion results [19].

In the foregoing discussion, we have tacitly barred unitary symmetries which could make some of the real amplitudes β, γ, δ, ε, σ vanish and thereby lessen the resistance to level crossing. To illustrate the effect of such symmetries we assume one parity S with $S^2 = -1$, $[T, S] = 0$, $[S, U] = 0$. The four basis vectors can then be built so as to obey (2) as well as

$$S|1\rangle = -i|1\rangle, \qquad S|2\rangle = i|2\rangle, \qquad S|3\rangle = i|3\rangle, \qquad S|4\rangle = -i|4\rangle. \tag{5}$$

It follows that $\langle 1|U|3\rangle = -\langle 1|SUS|3\rangle = -\langle 1|U|3\rangle$, *i.e.* $\gamma = \sigma = 0$. The number of nonnegative terms in the discriminant in (4) is thus reduced to three and the degree of level repulsion to quadratic.

To conclude our discussion of the influence of symmetries on the resistance of levels to crossings, we allow for a second parity $\tilde{S}$ as a symmetry of U with $\tilde{S}^2 = -1$, $[\tilde{S}, T] = 0$, $S\tilde{S} + \tilde{S}S = 1$. Beyond (2) and (5) our basis vectors now also obey (2) with T replaced by $\tilde{S}$. We, therefore, have $\langle 1|U|4\rangle = -\langle 1|\tilde{S}U\tilde{S}|4\rangle = -\langle 2|U|3\rangle$, *i.e.* $\delta = 0$. With only two nonnegative terms in the discriminant in (4) surviving level repulsion is diminished to linear.

The argument given goes through similarly for a Hermitian Hamiltonian H. The antiunitary symmetry gives to H the structure (3) as well, but by Hermiticity the five parameters β, γ, δ, ε, σ are all purely imaginary, while α remains real.

While there is ample experimental evidence for linear level repulsion in highly excited nuclei, atoms, and molecules [20-24], we do not know of any observation of the quadratic nor the quartic case. Systems without any antiunitarity T are hard to realize and so are systems with Kramers' degeneracy and no or sufficiently low geometric symmetry.

As regards numerical results for model systems, the literature abounds with examples of linear repulsion. The quadratic case has been found in billiards [25, 26], in nonlinear oscillators [27], for a modified kicked rotator [28], and for kicked tops, in the latter system

(4) The structure (3) is easily verified by, *e.g.*, $U_{21}^* = (U^+)_{12} = -\langle 1|TUT|2\rangle = \langle 1|TU|1\rangle = \langle T1|T^2U|1\rangle^* = -\langle 2|U|1\rangle^* = -U_{21}^*$.

(5) Apart from an arbitrary common phase factor which can be set equal to unity by a proper choice of the reference point of the eigenphases of U.

both with $T^2 = -1$ [17] and without any T [14]. We have also realized quartic repulsion for kicked tops [29, 30].

Periodically kicked tops have evolution operators

$$U = \exp[ikV] \exp[iH_0] \tag{6}$$

with H_0 and V polynomials in angular-momentum operators J_i such that the squared angular momentum is conserved,

$$[U, \boldsymbol{J}^2] = 0 , \qquad \boldsymbol{J}^2 = j(j+1) . \tag{7}$$

Provided $[H_0, V] \neq 0$ and U does not simply correspond to a rotation, the classical limit $j \to \infty$ yields, for sufficiently large kick strengths k, chaos dominating the classical sphere $\boldsymbol{J}^2/j^2 = 1$. By appropriate choice of H_0 and V all three universality classes of level repulsion can be obtained.

Our first realization [29] of the so-called symplectic case of quartic repulsion was done for $j = 249.5$, $H_0 = 5J_z^2/j$ and V a 500 by 500 matrix randomly chosen so that one generalized time reversal was respected but no geometric symmetry. Such a V corresponds to a polynomial

$$V = \sum_{m,n=0}^{2j} v_{mn} (J_+^m J_z^n + J_z^n J_-^m) , \tag{8}$$

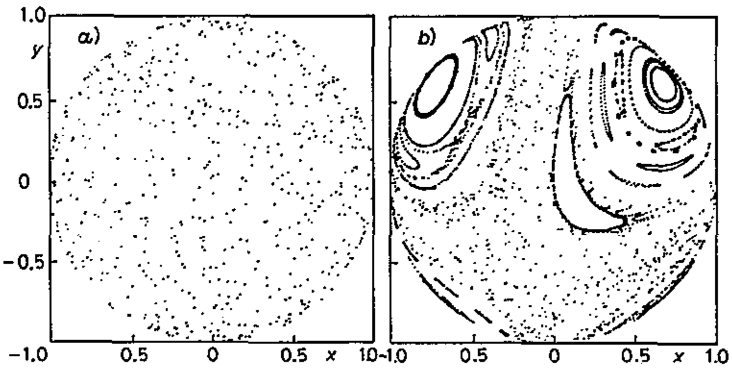

Fig. 1. – Portraits of classical trajectories for the map (6, 9) with $p = k = 2.5$, $A = 2$, $B = 3$ (*a*)) and $p = 0.05$, $k = 0.5$, $A = 2$, $B = 3$ (*b*)). The classical phase space is the sphere $(J/j)^2 = x^2 + y^2 + z^2 = 1$. Depicted are trajectories on the half-sphere $z \geq 0$, projected on the plane $z = 0$. In contrast to *b*), *a*) shows only a single trajectory.

the coefficients v_{nm} of which are uniquely determined by the matrix elements of V. Quartic repulsion was obtained but due to the technical difficulty of calculating the coefficients v_{nm} we refrained from investigating the corresponding classical behaviour.

We now present a more satisfactory example of the symplectic case ([6]),

$$\begin{cases} H_0 = p J_z^2/j , \\ V = J_z^4/j^3 + (A/j)\{J_x J_z + J_z J_x\} + (B/j)\{J_x J_y + J_y J_x\} . \end{cases} \tag{9}$$

([6]) The same results arise with $J_z^4/j^3 \to J_z^2/j$ in V.

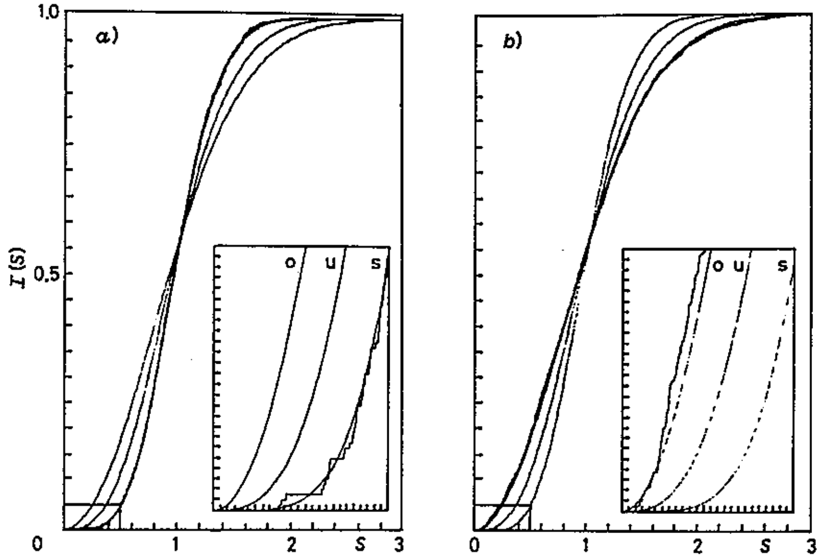

Fig. 2. – Integral $I(S)$ of the density of level spacings S for the map (6, 9) with k, A, B as in fig. 1*a*); to smoothen the distribution, data for $2p = 5.0$, 5.1, 5.2, 5.3 have been superimposed. Figures 2*a*) and *b*) show our numerical results for $j = 249.5$ and $j = 250$, respectively. As a reference, in both cases the three theoretical curves pertaining to Dyson's ensembles of unitary matrices are given (o = = orthogonal, u = unitary, s = symplectic).

The operators (9) share no geometric symmetry. Being even in the J_i, they both respect conventional time reversal T_0. U is, therefore, T covariant with $T = \exp[-iH_0]\,T_0$. The latter T squares to -1 or $+1$ for half-integer j and integer j, respectively.

For $p = k = 2.5$, $A = 2$, $B = 3$ the classical limit of the stroboscopic dynamics (6, 9) yields a sphere $(J/j)^2 = 1$ with no detectable islands of regular motion (fig. 1*a*)), while for $p = 0.05$, $k = 0.5$, $A = 2$, $B = 3$ we find coexistence of chaotic and regular trajectories (fig. 1*b*)).

By diagonalizing U with H_0 and V as in (9) for $j = 249.5$ and $j = 250$, in both cases with $p \simeq k = 2.5$, $A = 2$, $B = 3$, we find the level spacing statistics displayed in fig. 2*a*), *b*). In accordance with our above arguments, level repulsion turns out quartic for the half-integer value of j and linear for the integer value. The agreement of our histograms with the

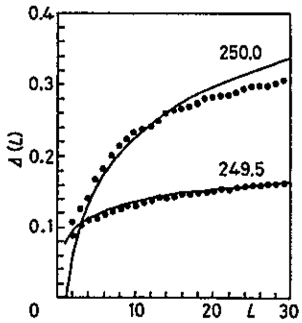

Fig. 3. – Spectral rigidity $\Delta(L)$ for the map (6, 9) with the coupling constants as in fig. 1*a*). Our numerical results for $j = 249.5$ and $j = 250$ agree well with the expectation [16] drawn from random matrix theory.

theoretical curves pertaining to Dyson's circular symplectic (fig. 2*a*)) and orthogonal (fig. 2*b*)) ensembles of random matrices is impressive. Figure 3 depicts the spectral stiffness obtained for $j=249.5$ and $j=250$; there is again beautiful agreement with the theoretical curves [27, 31]

$$\begin{cases} \Delta(L) = \dfrac{1}{\pi^2}\ln L - 0.00695\,, & \text{orthogonal,} \\[2ex] \Delta(L) = \dfrac{1}{4\pi^2}\ln L + 0.07832\,, & \text{symplectic,} \end{cases} \tag{10}$$

corresponding to Dyson's respective ensembles. It may be worth noting that no quantity approaching a well-defined classical limit as $j \to \infty$ can be expected to undergo dramatic change when j increases (by 2 p.p.t.) from 249.5 to 250. Indeed, level spacings and their fluctuations are quantities without classical counterparts: they are phenomena of quantum chaology [32].

To our knowledge, the dynamics (6, 9) for half-integer j is the first theoretical realization of quartic level repulsion which has a simple classical limit with chaotic behaviour.

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