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# Joint densities of secular coefficients for unitary matrices

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**Abstract.** We determine the joint density of secular coefficients and of the traces of powers for random unitary matrices from Dyson's circular ensembles. A byproduct are workable 'unitarity conditions', necessary and sufficient for all roots of a polynomial to be unimodular and different. These findings will be useful for combinations of random-matrix theory with semiclassical approximations in calculating spectral properties of quantum systems whose classical limit is globally chaotic. In a first such application we show that reasonable quasi-energy spectra result by throwing dice *à la* random-matrix theory to complement restricted knowledge (rigorous or from short periodic orbits) of the secular polynomial of a unitary Floquet matrix.

There is growing interest in the interrelation of semiclassical information and random-matrix theory (RMT) for quantum systems whose classical phase space is dominated by chaos. Both approaches are complementary in as much as spectral fluctuations on the scale of a mean level spacing tend to be universal and faithful to RMT, while short periodic orbits usually suffice to determine system specific properties of the (quasi)energy spectrum on larger scales. Numerous attempts at explaining the success of RMT have been made, some based on level dynamics [1–4], others more recently on superanalytic [5] (Efetov's nonlinear $\sigma$-model) and semiclassical [6–8] methods. The more recent ones among these even predict certain corrections to RMT, due to system specific properties such as the rate of equilibration of a (coarse grained) classical phase-space density.

This paper joins such efforts but takes up a different chain of thought. We propose to clarify what help RMT can offer, as a complement to semiclassical information, in calculating, for example, quasienergy spectra.

Correlations between secular coefficients of unitary time evolution operators $U$ were recently proposed [9, 10] as an indicator of quantum signatures of classical chaos. The coefficients in question are defined through the secular determinant $\det(\lambda - U) = \sum_{n=0}^{N} \lambda^n a_{N-n}$ where $N$ is the dimension of the Hilbert space; the $a_n$ are related to the traces of powers of the operator $U$, $t_n = \operatorname{tr} U^n$, by Newton's famous formulae [11]. Semiclassically, the $n$th trace $t_n$ can be constructed from properties of classical periodic orbits of period $n$. This fact allows us to interpret the index $n$ as a dimensionless time counting the number of iterations of the quantum map defined by the unitary operator $U$ or the corresponding classical map. The investigations in [10] were based on RMT and motivated by the universality of certain spectral properties of quantum systems [4] with chaos in their classical limit.

Concentrating on semiclassical aspects Smilansky and coworkers [7] then showed that correlations of secular determinants are related to the classical Frobenius Perron operator and the Ruelle zeta function. They treated the traces $t_n$ with $1 \leqslant n \leqslant N/2$ as independent Gaussian random quantities. In fact, the $t_n$ do behave that way [10] when $U$ is allowed to range within any one of Dyson's circular ensembles [12, 13], provided the matrix dimension

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$N$ is large and the trace index $n$ is small, $n \ll N$. An interesting dilemma remained for the semiclassical treatment of dynamical systems with classical chaos: the Gaussian character as well as the independence of the $t_n$ get lost when $n$ becomes of order $N$, i.e. precisely where one would like to replace semiclassical information from classical periodic orbits by information from random-matrix theory. Indeed, large $n$ means large times and these in turn reveal spectral information on small (quasi)energy scales; but spectral properties on the smallest (quasi)energy scales tend to be universal and correctly represented by random-matrix theory.

As a first step to resolve the dilemma mentioned we determine the exact joint distributions for the traces $t_n$ and the secular coefficients $a_n$ for Dyson's circular ensembles. As a useful byproduct we find necessary and sufficient conditions for all roots of a self-inversive polynomial [14] to be unimodular and different, conditions rather more practical than previously known ones [15].

We start from the joint density of eigenphases $\varphi_1, \varphi_2, \ldots, \varphi_N$ of Dyson's ensembles [12, 13], $P_\varphi \propto \prod_{j<k} |e^{i\varphi_j} - e^{i\varphi_k}|^\beta$ where $\beta$ is the level repulsion exponent ($\beta = 1, 2, 4$ for the circular orthogonal, unitary and symplectic ensembles: COE, CUE, CSE, respectively). That distribution determines both the joint distribution $P_t$ of the traces through

$$t_n = \sum_{j=1}^{N} e^{in\varphi_j} \tag{1}$$

and the distribution $P_a$ of the secular coefficients $a_n$ through Newton's formulae

$$na_n = -t_n - \sum_{k=1}^{n-1} a_{n-k} t_k. \tag{2}$$

The latter recursion relation can be solved explicitly for the $a_n$ in terms of the $t_m$ with $m \leqslant n$ or vice versa for the $t_n$ as functions of the $a_m$ with $m \leqslant n$. Due to the unitarity of $U$ the coefficients are self-inversive [14],

$$a_{N-n} = a_N a_n^* \tag{3}$$

with $a_0 = 1$. It follows that all secular coefficients as well as the first $N$ traces are determined by $N$ real parameters, like for instance the eigenphases $\varphi_i$.

Let us first assume even $N$ and establish the conditions under which (1) uniquely determines the $\varphi_1, \varphi_2, \ldots \varphi_N$ as functions of the $t_m, t_m^*$ with $1 \leqslant m \leqslant N/2$. Since for one such set any permutation is also a solution we may restrict ourselves to the region

$$0 \leqslant \varphi_1 < \varphi_2 < \cdots < \varphi_N < 2\pi. \tag{4}$$

The outer boundaries $\varphi_1 = 0$, $\varphi_N = 2\pi$ correspond to similar manifolds with one dimension less than (4). Both can be merged and then they belong to the interior of the manifold (4). With this identification understood when referring to the manifold (4), the boundary of that manifold or of any permutation of it appears whenever two eigenphases coincide. Thus the boundary is given by

$$0 = |\prod_{j<k} (e^{i\varphi_j} - e^{i\varphi_k})|^2 \equiv \det(t_{n-m}) \tag{5}$$

where we have introduced the $N \times N$ matrix $t_{n,m} = t_{n-m} = t_{m-n}^*$ with traces (1) as its elements. However, the 'trace matrix' $(t_{n-m})$ contains more than $N/2$ different traces; the elements $t_m$ with $m > \frac{N}{2}$ have to be determined in terms of the 'first' $N/2$ ones through Newton's formulae (2) and the self-inversiveness (3). The identity in (5) is a simple consequence of the properties of the van der Monde determinant whose squared

modulus appears in (5). From (1) we see that the matrix $t_{n,m}$ is Hermitian and positive semidefinite. It follows that the boundary in discussion is reached whenever one or more eigenvalues of the trace matrix vanish. In other words, we may define the interior of the allowed region by requiring that matrix to be positive definite, i.e. the inequalities

$$t_0 = t_0^* = N > 0 \qquad \begin{vmatrix} t_0 & t_1 \\ t_1^* & t_0 \end{vmatrix} > 0$$
$$\begin{vmatrix} t_0 & t_1 & t_2 \\ t_1^* & t_0 & t_1 \\ t_2^* & t_1^* & t_0 \end{vmatrix} > 0 \qquad \cdots \qquad \begin{vmatrix} t_0 & \cdots & t_{N-1} \\ \vdots & & \vdots \\ t_{N-1}^* & \cdots & t_0 \end{vmatrix} > 0. \tag{6}$$

It follows that $|t_n| \leqslant N$ for all $n$, i.e. that all $t_n$ lie in a compact region.

We can now refine the question in pursuit: With the conditions (6) met, do we upon solving (1) find unique phases in the interior of the region (4)? To find the affirmative answer we propose showing that the transformation (1) from phases to traces (i) is essentially one to one and (ii) maps the region (4) *onto* rather than only just into the region (6). The strategy of proof will be, roughly speaking, to make sure that the boundary of (4) maps *onto* the boundary of (6); by continuity, the interiors must then map onto one another as well. It might be helpful to note that the obvious mapping of the boundary of (4) *into* the boundary of (6) is much less than the 'onto' we need to establish.

Let us look at the self-inversive polynomial of degree $N$ constructed from the traces $t_m$ with $m \leqslant \frac{N}{2}$ with the help of Newton's formulae (2) and the self-inversiveness (3). We know [14] that its zeros $\lambda$ lie on the unit circle or appear in pairs $(\lambda, \frac{1}{\lambda^*})$. It follows that the full $N \times N$ trace matrix can be written as

$$t_{n-m} = \sum_{j=1}^{N} \mathrm{e}^{\mathrm{i}(n-m)(\varphi_j + \mathrm{i}\varepsilon_j)} \tag{7}$$

with either $\varepsilon_j = 0$ or pairwise $\varepsilon_j = -\varepsilon_k$ and $\varphi_j = \varphi_k$; complex 'phases' thus come in complex conjugate pairs. Its determinant generalizes the one defined in (5) as

$$\begin{aligned} \det(t_{n-m}) &= \prod_{j<k} [(\mathrm{e}^{\mathrm{i}(\varphi_j + \mathrm{i}\varepsilon_j)} - \mathrm{e}^{\mathrm{i}(\varphi_k + \mathrm{i}\varepsilon_k)})(\mathrm{e}^{-\mathrm{i}(\varphi_j + \mathrm{i}\varepsilon_j)} - \mathrm{e}^{-\mathrm{i}(\varphi_k + \mathrm{i}\varepsilon_k)})] \\ &= \prod_{j<k} [2\sin((\varphi_j - \varphi_k + \mathrm{i}\varepsilon_j - \mathrm{i}\varepsilon_k)/2)]^2. \end{aligned} \tag{8}$$

Note that the matrix (7) is still Hermitian, $t_{n-m} = t_{m-n}^*$. It is easy to check that the matrix $t_{n-m}$ (starting with real nondegenerate phases, i.e. with all $\varepsilon_j = 0$) immediately loses positivity when two phases collapse into degeneracy, say $\varphi_1 = \varphi + \eta, \varphi_2 = \varphi - \eta$ with $\eta \to 0$, and proceed to becoming a complex conjugate pair ($\eta \to \mathrm{i}\epsilon$). The generalized trace matrix (7) is then given by

$$t_{n-m} = \mathrm{e}^{\mathrm{i}(n-m)\varphi} 2\cos(\eta(n-m)) + \sum_{j=3}^{N} \mathrm{e}^{\mathrm{i}(n-m)\varphi_j} \tag{9}$$

and the determinant (8) can be written as

$$\det(t_{n-m}) = (2\sin\eta)^2 \prod_{k=3}^{N} \left[ 4\left( \sin^2\left(\frac{\varphi - \varphi_k}{2}\right) - \sin^2\left(\frac{\eta}{2}\right)\right)\right]^2 \prod_{l<m}^{3\cdots N} \left[ 2\sin\left(\frac{\varphi_l - \varphi_m}{2}\right)\right]^2. \tag{10}$$

As $\eta = \mathrm{i}\varepsilon$ becomes imaginary this determinant becomes negative, since it is $\propto -\sinh^2\varepsilon$ and it never changes sign again as $\varepsilon$ goes to infinity. The lowest eigenvalue of the matrix

$t_{n,m}$ thus changes sign at $\eta = 0$ and is negative for $\varepsilon \neq 0$. Equations (9) and (10) together show that this eigenvalue behaves $\propto -\varepsilon^2$ for small $\varepsilon$. It is also easy to see from (9) that the $2 \times 2$ determinant $t_0^2 - |t_1|^2$ becomes negative at least for sufficiently large $\varepsilon$. From this fact and the nonvanishing of (10) we may already conclude that the lowest eigenvalue is negative. The foregoing argument can be generalized: let us look at a second coalescence of two phases going into complexity. Then the determinant (10) changes sign again and it may contain two or no negative eigenvalues. Again one sees that the determinant preserves its sign as the second pair moves further away from the real axis of the complex 'phase' plane. The preserved sign together with the eventual negativity of $t_0^2 - |t_1|^2$ implies that there is at least one negative eigenvalue. The same reasoning works for any number of separated coalescences, for which we conclude that the lowest eigenvalue is negative, as long as separated pairs of phases have moved into the complex plane. All other cases, such as multiple coalescences and coalescences of pairs in the complex plane can be included as limits by continuous changes of the parameters $\varphi_j, \varepsilon_j$, and therefore again the lowest eigenvalue is nonpositive.

We may conclude, at this point, that inequalities (6) secure unitarity up to a similarity transformation, i.e. they ensure that the matrices $U^n$ with traces $t_n$ have unimodular eigenvalues. These conditions might enjoy lots of applications, such as for instance unitarity checks on semiclassically approximated traces.

It remains to find the Jacobian of the transformation (1) with $N/2$ complex traces on the l.h.s. A straightforward calculation shows

$$\frac{\partial\{\mathrm{Re}\, t_1, \mathrm{Im}\, t_1, \ldots, \mathrm{Im}\, t_{\frac{N}{2}}\}}{\partial\{\varphi_1, \ldots, \varphi_N\}} \propto |a_{\frac{N}{2}}|(\det(t_{n-m}))^{\frac{1}{2}}. \tag{11}$$

Due to condition (6) this does not vanish (except on the lower-dimensional manifold $a_{N/2} = 0$ on which the transformation (1) is not one to one; this is in analogy with the transformation from polar to Cartesian coordinates in a plane where the vanishing of the Jacobian in the origin does not matter; compare the example for $N = 2$ discussed below in figure 1). The Jacobian $\partial t/\partial a$ following from (2) is a constant. We thus obtain for the joint densities $P_t$ of the traces or $P_a$ of the secular coefficients for even $N$ using the joint density of the eigenphases and (5)

$$P_t \propto P_a \propto \frac{1}{|a_{N/2}|}(\det(t_{n-m}))^{\frac{\beta-1}{2}} \qquad N \text{ even}. \tag{12}$$

These densities come with the ranges (6) to which the traces or secular coefficients are confined; everything has to be expressed in the desired variables with the help of the self-inversiveness (3) and Newton's formulae (2).

In the case of odd $N$ we have to keep one phase, say $a_N = \mathrm{e}^{\mathrm{i}\hat{\varphi}}$, and transform to $(N-1)/2$ traces or secular coefficients. Now the Jacobian (11) does not contain the factor $|a_{N/2}|$, and the joint densities $P_t$ of traces and the phase $\hat{\varphi}$ or the joint density $P_a$ of coefficients and the phase $\hat{\varphi}$ are given by

$$P_t \propto P_a \propto (\det(t_{n-m}))^{\frac{\beta-1}{2}} \qquad N \text{ odd}. \tag{13}$$

Again conditions (6) define the admissible ranges. Interestingly, in the orthogonal case, $\beta = 1$, the distribution (13) is constant in the region defined by conditions (6). Formulae (12) and (13) extend also to the case $\beta = 0$, which implies in that case a singular (but integrable) behaviour near the boundary of integration.

As a simple example we consider for $N = 2$ the transformation

$$t = \mathrm{e}^{\mathrm{i}\varphi_1} + \mathrm{e}^{\mathrm{i}\varphi_2} \tag{14}$$

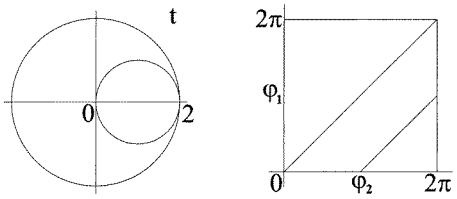


**Figure 1.** Map (12) transforms the diagonal of the square onto the circle with radius 2. The small circle is the image of the identified boundaries $\varphi_1 = 0$ and $\varphi_2 = 2\pi$. The point $t = 0$ is singular and is the image of the line $\varphi_1 = \varphi_2 - \pi$.

which maps the triangle $0 \leqslant \varphi_1 < \varphi_2 < 2\pi$ in a complicated way (see figure 1) to the interior of the circle with radius 2, $|t| < 2$. The distribution $P_t$ is given by $P_t \propto \frac{1}{|t|}(4 - |t|^2)^{\frac{\beta-1}{2}}$, obtained for $\beta = 1, 2$ in [10].

As already mentioned [10], the joint density of the first $n$ traces $t_m$ with large $N$ and small $m \leqslant n \ll N$, is Gaussian. Certainly equations (12) and (13) show that this Gaussian character gets lost when $n$ approaches the order of $N$. Nevertheless, it is interesting to see, for example, that for $\beta = 1$ the Gaussian property follows solely from restrictions given by the boundary (6). This is due to integrating out a large number of remaining variables. An interesting consequence of the transformation (14) is, for example, for the map $t = \mathrm{e}^{\mathrm{i}\varphi_1} + \mathrm{e}^{\mathrm{i}\varphi_2} + \mathrm{e}^{\mathrm{i}\varphi_3}$ the circle from figure 1 is rotated around a boundary point such that $|t|$ covers the whole range $|t| \leqslant 3$. Similarly it follows for the map (1) that each $t_n$ covers the whole range $|t_n| \leqslant N$ (for $N > 1, n > 0$).

We proceed to an application of the statistics of the traces $t_n$ to the determination of quasienergy spectra, considering kicked tops with Floquet operators of the form [4]

$$U = \mathrm{e}^{-\mathrm{i}(\frac{k_x}{2j+1}J_x^2 + p_x J_x)}\mathrm{e}^{-\mathrm{i}p_y J_y}\mathrm{e}^{-\mathrm{i}(\frac{k_z}{2j+1}J_z^2 + p_z J_z)}. \tag{15}$$

Here angular momentum operators $J_i$, $i = x, y, z$ appear as generators of rotations by angles $p_i$ and nonlinear rotations by angles $\propto k_i J_i/(2j+1)$; for the calculations to be presented here we have chosen $p_x = 1.0$, $p_y = 1.0$, $p_z = 1.1$, $k_x \approx 8$, $k_z \approx 6$. These Floquet operators are meant to act in a Hilbert space of dimension $2j+1$ with the latter determined by the integer or half integer quantum number $j$ which fixes the conserved squared angular momentum as $(\boldsymbol{J})^2 = j(j+1)$. The classical limit, $j \to \infty$, yields the sphere $\lim_{j\to\infty}(\boldsymbol{J})^2/[j(j+1)] = 1$ as phase space and that space is dominated by chaos for the chosen values of the $p_i, k_i$. Time reversal invariance is broken since both torsion constants are taken as nonzero [4].

The secular polynomial and thus the $2j+1$ eigenphases are of course determined by the first $j$ traces $t_n$, the determinant $\det U$, and the self-inversiveness (3), assuming integer $j$. One might imagine the required traces and $\det U$ determined semiclassically [16], so as to have $t_n$ expressed in terms of properties of classical periodic orbits of period $n$. While for small values of $n$ such semiclassical evaluation of the $t_n$ is quite feasible [16], the infamous exponential proliferation of periodic orbits makes for trouble quickly as $n$ grows. On the other hand, it is the short periodic orbits which carry the most important system specific information into the traces $t_n$, while orbits with periods near $j$, i.e. periods of the order of the Heisenberg time $2j+1$, tend to influence the quasienergy spectrum on the scale of an inverse level spacing where universal behaviour prevails. One is therefore tempted to combine the semiclassical technique with RMT: the former could be employed in determining periodic orbits with small periods and the thus accessible first few traces, and the latter to fix the remaining traces with $n$ up to $j$ by throwing the dice according to the joint probability density of the traces for the CUE determined above. We have undertaken such a hybrid

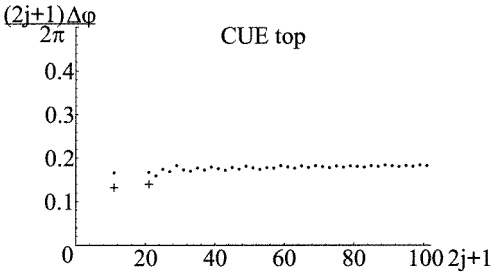


**Figure 2.** The standard deviation between exact and hybrid eigenphases for CUE tops obtained from independent (·) and correlated (+) traces as described in the text.

procedure but, in order to test the random-matrix part of the game by itself, employing exact rather than semiclassical values for the first 60% of the required $j$ traces and the determinant. Every set of traces so fixed yields $2j+1$ approximate eigenphases; by repeatedly throwing dice for the $t_n$ with $0.6j < n \leqslant j$ we obtain $2j+1$ 'clouds' of approximate eigenphases. Once the 'centres of mass' of these clouds have stabilized we stop the game and take those centres as final approximants for the eigenphases. Figure 2 depicts the standard deviation between exact and approximate eigenphases, $\Delta\varphi = (\frac{1}{2j+1}\sum_{i=1}^{2j+1}(\varphi_i - \varphi_i^{\mathrm{appr}})^2)^{1/2}$, versus the dimension $2j+1$. In order to obtain an impression of what typically happens, an average over several Floquet matrices with slightly different values of the $p_i, k_i$ was worked into figure 2. We find the error to be insensitive to the dimension and near 14% of the mean spacing $2\pi/(2j+1)$, somewhat less than the 18% one incurred when the randomly chosen traces are treated as independent Gaussian numbers with the CUE means and variances [10], $\langle t_n\rangle = 0$, $\langle |t_n|^2\rangle = n$. Repeating the game for COE-type tops with time reversal invariance ($k_z = p_z = 0$) we obtained errors about 5% higher while CSE-type tops [4], according to their greater spectral stiffness, yielded errors 4% less than the CUE-type ones referred to in figure 2. We may conclude that Monte Carlo completion of exact or semiclassical information about traces allows meaningful shots at quasienergy spectra.

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