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ABSTRACT

New distribution laws for the energy level spacings and the eigenvector amplitudes, appropriate for systems with a few degrees of freedom in the chaotic regime, are derived by conveniently deforming the GOE. The cases of 2×2 and 3×3 matrices are fully worked out. Suggestions concerning the general case of matrices with large dimensions are made.

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It is well known that the GOE (Gaussian Orthogonal Ensemble) provides a realistic description of statistical properties of complex quantal systems with a large number of degrees of freedom[1)]. In particular, the energy level spacings distribution obtained from GOE approximates very well the Wigner distribution[2)] (W), which describes quite well data. Independently of the spacing distribution, the GOE predicts a Porter–Thomas (PT) law[3)] for the distributions of eigenvectors. Nuclear resonance data systems lends support to the correctness of the PT law[1)].

The statistical independence of the eigenvector and eigenvalue distributions, a characteristic of the GOE, must however, be revised for cases involving systems with a few degrees of freedom in the chaotic regime[4)].

The purpose of this letter is to develop a theory for a mixed eigenvector and eigenvalue distribution which should describe situations intermediate between chaos and order. For this purpose we employ the maximum entropy technique subjected to several physically motivated constraints[4)]. The GOE results will alway be used as a guideline, the case of 2×2 matrices are worked out fully analytically whereas the 3×3 matrices are developed semi–analytically supplemented by numerical evaluation. The general case is then obtained from inference.

Using the maximum entropy technique the GOE distribution is obtained as follows. First we define the entropy as

$$S = -\int dHP(H) \ln P(H) \quad , \tag{1}$$

subject to the constraint

$$\langle \mathrm{Tr}\, H^2 \rangle = dHP(H)\, \mathrm{Tr}\, H^2 = \mu \tag{2}$$

and the normalization condition

$$\int dHP(H) = 1 \quad . \tag{3}$$

Maximizing S subject to (2) and (3) one immediately obtains the GOE distribution

$$P(H) = e^{-\lambda_0 - 1 - \alpha_0 \mathrm{tr} H^2} \tag{4}$$

$$\alpha_0 = \frac{N(N+1)}{4\mu} \quad , \quad e^{-\lambda_0 - 1} = 2^{-\frac{N}{2}} \left[\frac{\pi}{2\alpha_0}\right]^{-\frac{N(N+1)}{4}}$$

where λ and α are Lagrange multipliers determined by the constraints (2) and (3).

From (4) one can construct the joint distribution function, $P(E_1,...,E_N ; C_1,...,C_N)$ using already well known procedure[5),6)], and obtain

$$P^{(GOE)}(E_1,...,E_N ; C_1,...,C_N) = 2 \left[\frac{\pi^{N/2} N}{\Gamma(\frac{N}{2}+1)}\right]^{-1}$$

$$\delta\left[1 - C_1^2 - C_2^2 - C_2^2 - \cdots - C_N^2\right] \cdot \left[N!\, 2^{-1/4N(N-1)} \prod_{g=1}^{N} \Gamma(\tfrac{1}{2} g)\right]^{-1} \tag{5}$$

$$\prod_{i<j} |E_i - E_j| \; e^{-\alpha(E_1^2+E_2^2+\cdots+E_N^2)}$$

where the C_is are the component amplitudes of an eigenvector.

Integrating (5) over all the C,s and all the $E_i - E_j$,s , except one s , one obtains in the $N \to \infty$ limit the Wigner distribution

$$P_W(s) \cong \frac{\pi}{2D^2}\, s \exp\left[-\frac{\pi}{4}\frac{s^2}{D^2}\right] \tag{6}$$

where D is $<s> = \left[\frac{8\pi}{\alpha}\right]^{1/2}$.

Similarly integrating all the E,s and all the C,s except one c , one finds in the limit $N \to \infty$ limit the Porter–Thomas distribution

$$P_{PT}(c) \cong \left[\frac{N}{2\pi}\right]^{1/2} \exp\left[-\frac{N}{2} C^2\right] . \tag{7}$$

As seen from 5, the E and C distributions are completely independent, $(P_E(E,s;C,s) = = P_E(E,s)\, P(C,s))$, which is a consequence of GOE, namely P(H) is invariant under arbitrary rotation of the basis.

To generalize (4) and thus eventually make the joint distribution non–separable, we have to impose further constraints in the construction of P(H) from the maximum entropy principle. We thus redo the calculation with Eq. (1) with the additional condition

$$<\mathrm{Tr}(PHQHP)> = \nu \;, \tag{8}$$

where P is a projecton operator that projects onto a given vector in the basis space, e.g. $P = |i><i|$, and $Q = 1-P$. The new distribution function P(H) constructed from

$$\delta \int P\left[-\ln P - \lambda - \alpha\, \mathrm{Tr}\, H^2 - \beta\, \mathrm{Tr}(PHQHP)\right] dH = 0 \tag{9}$$

is thus given by

$$P(H) = \exp\left[-\lambda - 1 - \alpha\, \mathrm{Tr}\, H^2 - \beta\, \mathrm{Tr}(PHQHP)\right] ,$$

$$= P^{GOE}(H)\, e^{-\beta\, \mathrm{Tr}(PHQHP)} \cdot \left[1 + \frac{\beta}{2\alpha}\right]^{\frac{N-1}{2}} , \tag{10}$$

where the Lagrange multipliers α and β are related to the μ and ν as follows

$$\nu = \frac{N-1}{4\alpha(1+\frac{\beta}{2\alpha})} \equiv \langle \mathrm{Tr\ PHQHP} \rangle \qquad (10.a)$$

$$\mu = \frac{N(N+1)}{4\alpha} - \frac{N-1}{(1+\frac{\beta}{2\alpha})}\frac{\beta}{4\alpha^2} \equiv \langle \mathrm{Tr}\ H^2 \rangle \ . \qquad (10.b)$$

The symmetry inherent in the GOE is now broken because of the favoring of a particular vector spanned by P. This guarantees that the joint distribution $P(E_1,\dots,E_N ; C_1,\dots,C_N)$ is not any more separable, and accordingly significant deviations from both the Wigner and the Porter–Thomas distributions are expected. Since the Jacobian that takes us from P(H) to P(E,s; C,s) is independent of the particular ensemble of real matrices under consideration we conjecture that the joint probability distribution corresponding to Eq. (10) is

$$P(E,s;C,s) = P^{(GOE)}(E,s;C,s)\left[1+\frac{\beta}{2\alpha}\right]^{\frac{N-1}{2}} \cdot \exp\left[-\beta\left[\sum_{\alpha} C_\alpha^2 E_\alpha^2 - \sum_{\alpha,\beta} C_\alpha^2 C_\beta^2 E_\alpha E_\beta\right]\right] \qquad (11)$$

where Tr(PHQHP) has been represented explicitly in terms of the eigenvalues and the amplitudes of the eigenvector which is projected by P.

From the joint distribution, Eq. (11) one can then calculate the spacing and amplitude distributions upon integration. For 2×2 matrices we obtain

$$P(s) = \alpha\left[1+\frac{\beta}{2\alpha}\right]^{1/2} \cdot s\exp\left[-\left[\frac{\alpha}{2}+\frac{\beta}{8}\right]s^2\right] I_0\left[\frac{\beta}{8}s^2\right] \qquad (12)$$

and

$$P(\mathbf{C}) = \frac{\alpha}{\pi}\left[1+\frac{\beta}{2\alpha}\right]^{1/2} \frac{1}{\sqrt{1-C^2}} \frac{1}{[\frac{\alpha}{2} + \beta\, C^2(1-C^2)]} \qquad (13)$$

Eq. (12) represents a spacing distribution which still shows level repulsion but deviates from a pure Wigner one. It is interesting to note that when $\beta = 0$, the Wigner surmise is fully recovered. On the other hand, P(C), Eq. (13), is necessarily different from the Porter–Thomas distribution even when $\beta = 0$, owing to the small dimension of the matrices. For 3×3 matrices the spacing and amplitude distributions are given by

$$P(s) = \frac{8\alpha^3}{3\pi^2}\sqrt{\frac{6\pi}{\alpha}}\left[1+\frac{\beta}{2\alpha}\right] s\exp\left[-\frac{2}{3}\alpha s^2\right]\cdot\int_0^1 dc\,\exp\left[-\beta(1-C^2)C^2s^2\right]$$

$$\int_0^{\pi/2}\frac{d\psi}{Q}\left\{\frac{2B^2s^2 + Q(1-2Bs^2)}{4Q^{3/2}}\sqrt{\pi}\exp\left[B^2\frac{s^2}{C}\right]\cdot\mathrm{erfc}\left[\frac{Bs}{\sqrt{Q}}\right] + s\frac{(Q-B)}{2Q}\right\} \qquad (14)$$

and

$$P(\mathbf{C}) = \frac{\alpha^3}{\pi\sqrt{6\alpha}}\left[1+\frac{\beta}{2\alpha}\right]\int_0^{\pi/2} d\psi \frac{\frac{1}{\sqrt{A}}+\frac{1}{\sqrt{Q}}}{(\sqrt{AQ}+B)^2} \qquad (15)$$

where $A = \frac{2}{3}\alpha + \beta(1-C^2)\, C^2$

$$B = \frac{\alpha}{3} + \beta\, C^2\, C'^2$$

$$Q = \frac{2}{3}\alpha + \beta(1-C'^2)\, C'^2$$

$$\psi = \sin^{-1} \frac{C'}{\sqrt{1-C^2}} .$$

In Figures 1, 2 and 3 we show our results for $P(s)$, $P(c)$ and $P(y \equiv c^2)$ for the 2×2 and 3×3 matrices cases discussed above. An important result which deserves a special attention is that the spacing distribution $P(s)$ for small s dives to zero as fast as $\left[0.86\left[1+\frac{\beta}{2\alpha}\right]^{1/2} + 0.64\right]s$ for 3×3 matrices and as $\left[1+\frac{\beta}{2\alpha}\right]^{1/2} s$ for 2×2 matrices, as β is increased further (α was kept constant $= 1$). In the limit $\beta \to \infty$, which should represent the regular (non–chaotic) limit, the $P(s)$ and $P(c)$ distributions attain the following form

$$P_\infty(s) = \sqrt{\frac{2\alpha}{\pi}} \exp\left[-\frac{\alpha s^2}{2}\right] , \qquad N = 2 \tag{16}$$

$$P_\infty(s) = 2\sqrt{\frac{3\alpha}{8\pi}} \left\{1 + \sqrt{\frac{\pi\alpha}{6}}\, s\, e^{\alpha s^2/6} \operatorname{erfc}\left[\sqrt{\frac{\alpha}{6}}\, s\right]\right\} \exp\left[-\frac{2\alpha}{3} s^2\right] , \quad N = 3 \tag{17}$$

$$P_\infty(c) = \frac{1}{2}\left[\delta(c) + \delta(c-1) + \delta(c+1)\right] , \qquad N = 2 \tag{18}$$

$$P_\infty(c) = \frac{1}{4}\left[3\delta(c) + \delta(c-1) + \delta(c+1)\right] , \qquad N = 3 . \tag{19}$$

Our results above for $N=2$ agree fully with those of Robnik[7] and Alhassid and Levine[8] and disagree with Berry and Robnik[9] who claim to have seen no level repulsion

even for moderately small values of β (the chaoticity parameter is defined differently in Ref. 9)). At this point we would like to point out that our work is very similar in spirit to that of Alhassid and Levine. In fact, the case fully calculated by Ref. 8), namely the 2×2 matrix, agree completely with our Eqs. (12) and (13) with the important identification of their parameter ε by the following relation

$$\varepsilon = \frac{1}{\sqrt{1+\frac{\beta}{2\alpha}}} . \tag{20}$$

Thus the GOE limit obtains by setting $\beta = 0$ and/or $\varepsilon = 1$. Similarly the fully regular case corresponds to $\beta = \infty$ and $\varepsilon = 0$.

We sould, however, point out two major advantages that our theory carries in relation to Alhassid and Levine's namely, first, we deform the GOE by merely favoring one particular vector in the basis space spanned by P and accordingly introduce just one more Lagrange multiplier in the maximum entropy calculation, whereas they introduce $N-1$ Lagrange multipliers to go beyond the GOE. Secondly, our chaoticity parameter, β, could take the full range of values from 0 (fully chaotic) to ∞ (fully regular). Thus, interpreted as an inverse of a "temperature", one may use knowledge in statistical mechanical studies of phase transition phenomena, to better understand the transition from chaos (high–"temperature" behaviour) to order (low–"temperature" behaviour).

Finally, for the general case of $N\times N$ matrices, a large body of numerical calculation would be required in order to pin down the structure of the distribution functions $P(s)$ and $P(c)$. However, one may get a feel for this structure through perturbation expansion in β. It is clear that, from Eq. (11), higher order terms β (arising from the expansion of $\exp(-\beta \operatorname{Tr} PHQHP)$), contain terms of the form $\sum_\alpha C_\alpha^n E_\alpha^n$ as well as more complicated combinations of the C,s and the E,s. If we ignore the latter combinations, then the integrations over the E,s or the C,s can be straightwardly performed[5]. The resulting series would involve higher–order derivatives, with respect to α, of the GOE distribution function.

From the above we are tempted to conclude that the amplitude distribution P(c), would look like, in the limit $N \to \infty$,

$$P(c) \propto C^{\delta(\beta)} \exp\left[-\frac{C^2}{2/N + B(\beta)}\right] \tag{21}$$

where $\delta(0) = 0$ and $B(0) = 0$.

The functions $\delta(\beta)$ (which could be negative!) and $B(\beta)$ can be evaluated with the perturbation expansion discussed above, in conjunction with pade approximant as usually done in phase transition studies using the method of high temperature expansion[10].

In conclusion, we developed in this paper a theoretical scheme through which the transition from regular to chaotic quantum behaviour can be conveniently studied by conveniently deforming the GOE, we were able to derive closed and semi–closed expressions for 2×2 and 3×3 matrix Hamiltonian respectively, for the distributions of level spacings and eigenvector amplitudes. The transition from chaos to order is then studied in a very convenient manner. The general case of N×N matrices is also discussed briefly.

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FIGURE CAPTIONS

Fig. 1 — Calculated energy level spacing distributions P(S); **a)** for 2×2 matrices and **b)** for 3×3 matrices. The value of α was equal to unity (see text for details).

Fig. 2 — Same as figure 1 for the amplitude distribution P(C).

Fig. 3 — Same as Figure 1 for the transition strength distribution $P(y=C^2)$. See text for details.

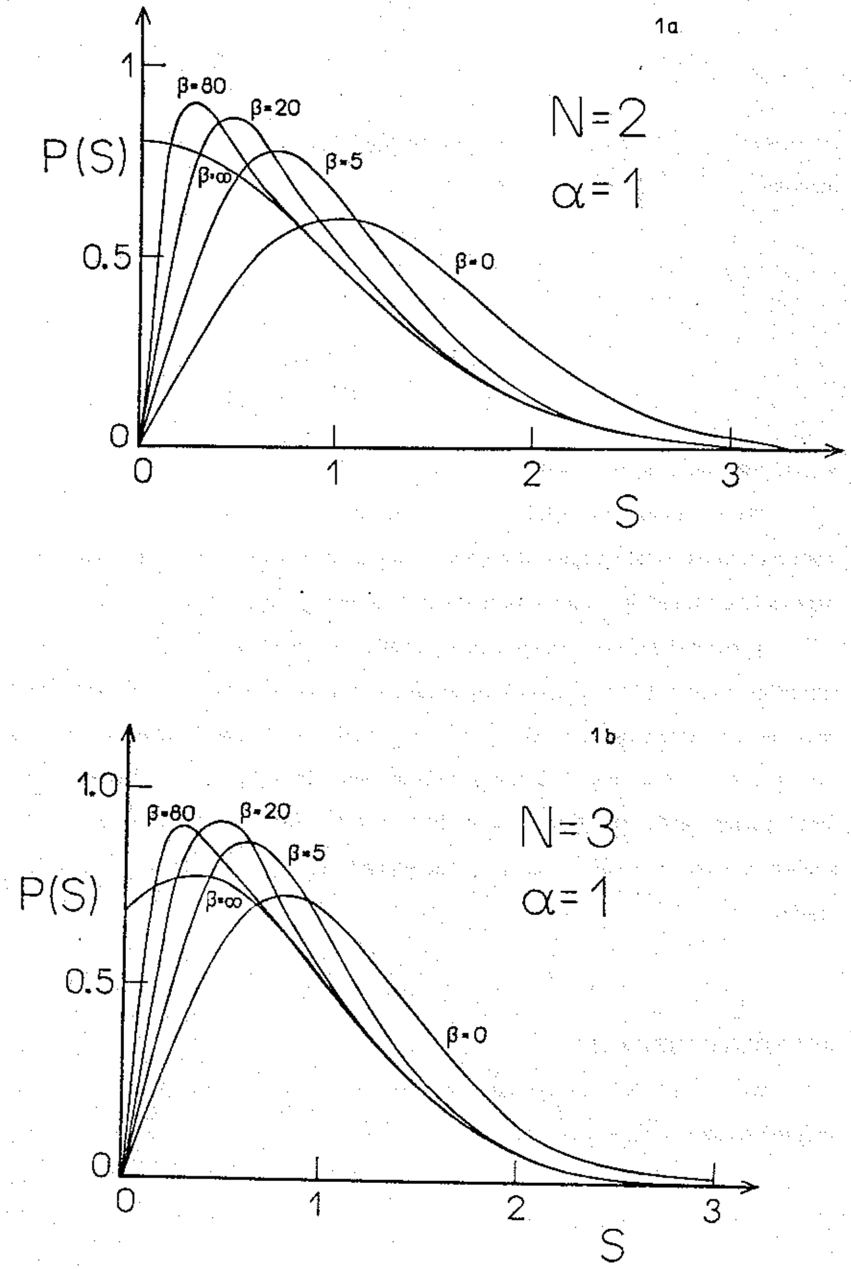

Fig.1

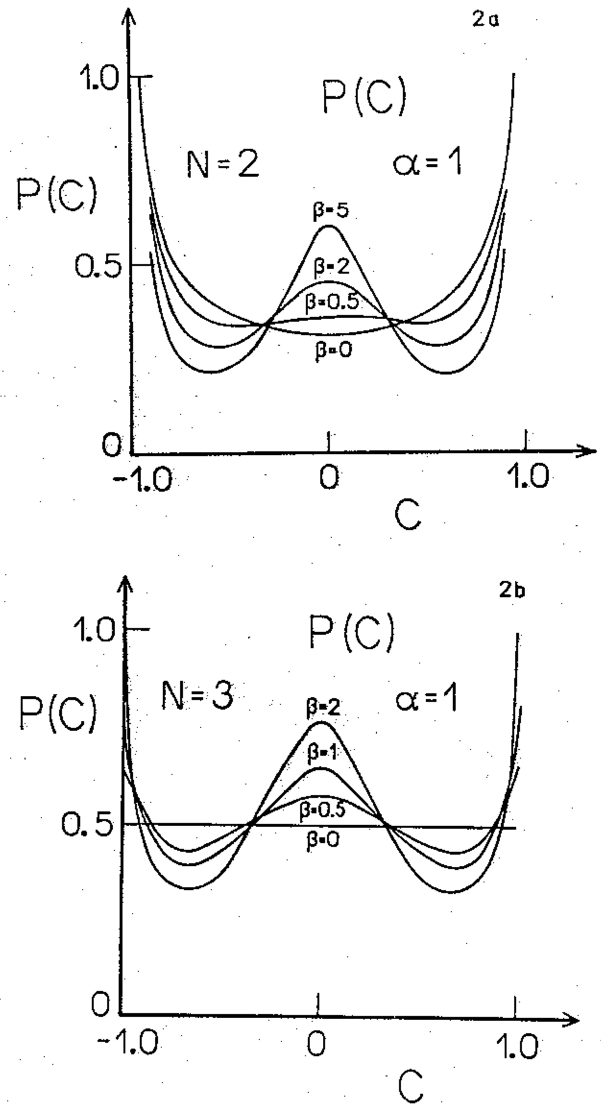
2a
P(C)
N = 2
α = 1
P(C)
β=5
β=2
β=0.5
β=0
1.0
0.5
0
-1.0
0
1.0
C
2b
P(C)
N = 3
α = 1
P(C)
β=2
β=1
β=0.5
β=0
1.0
0.5
0
-1.0
0
1.0
C

Fig. 2

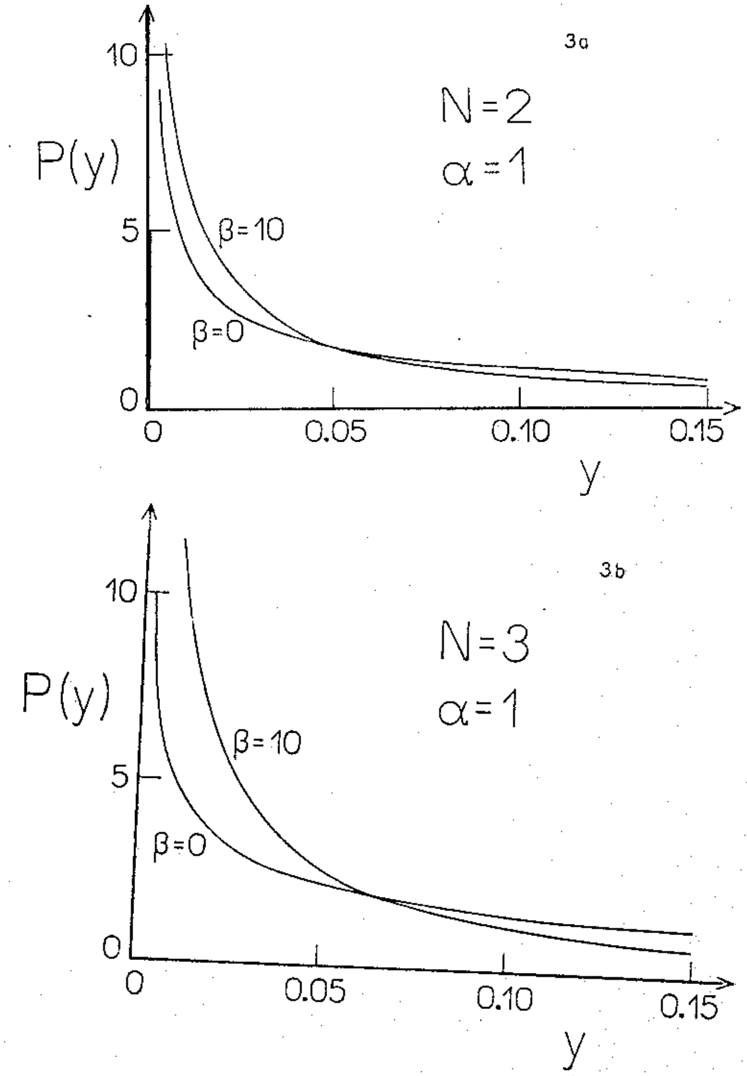
3a
N = 2
α = 1
P(y)
β = 10
β = 0
10
5
0
0
0.05
0.10
0.15
y
3b
N = 3
α = 1
P(y)
β = 10
β = 0
10
5
0
0
0.05
0.10
0.15
y

Fig. 3