Expectation Value Fluctuations in the Unitary Ensemble*

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The random matrix hypothesis is used to derive the expectation value fluctuations for systems which violate time-reversal symmetry. A general expression is derived for the even moments of a complex direction cosine in an N-dimensional unitary space. It is shown that the second and third moments about the mean of the gyromagnetic ratio for the unitary case are obtained from those for the orthogonal ensemble by replacing the dimension N by $2N$ in the case of large dimension.

I. INTRODUCTION

In the consideration of quantal spectra there are four measurable types of quantities: energy-level positions, energy-level widths, potential scattering amplitudes, and energy-level expectation values. This paper is concerned with the statistical properties of the last of the four for systems which violate time-reversal symmetry, i.e., for which the unitary ensemble[1] is relevant. A preliminary discussion[2] of expectation value statistics for systems which have rotational symmetry and time-reversal symmetry, i.e., for which the orthogonal ensemble is relevant, has already been published, and a more detailed treatment of those results will be reported in the future. In this paper similar considerations are developed for the unitary ensemble.

In order to lay the groundwork we recall briefly that the connection between the expectation value $(\alpha|G|\alpha)$ of an operator G in the representation labeled by α is related to its matrix elements in the representation in which it is diagonal (labeled by β) through the relation

$$
\begin{aligned}
(\alpha|G|\alpha) &= \sum_\beta (\alpha|\beta)(\beta|G|\beta)(\beta|\alpha)\,, \\
&= \sum_\beta (\beta|G|\beta)\,|(\beta|\alpha)|^2 .
\end{aligned}
\tag{1}
$$

If we define in the diagonal representation

$$g_\beta \equiv (\beta|G|\beta)\,, \quad a_\beta \equiv (\beta|\alpha)\,, \tag{2}$$

then

$$G = \sum_{\beta=1}^{N} g_\beta |a_\beta|^2 , \tag{3}$$

where we have dropped the label α and let G stand for $(\alpha|G|\alpha)$ in an arbitrary nondiagonal representation. The quantities a_β are the complex direction cosines between the diagonal representation and the arbitrary representation both of dimension N.

We are interested in two sets of moments. We introduce

$$\frac{1}{N}\,\mathrm{Tr}G^k = \frac{1}{N}\sum_{\beta=1}^{N} g_\beta{}^k , \tag{4}$$

as the mean value of the kth power of the operator G in the diagonal representation. When we use G to signify an operator, it will always appear inside a trace expression; otherwise G stands for the matrix element $(\alpha|G|\alpha)$ as in (3).

Under the assumption that the representation α is at an arbitrary "angle" to the representation β, we are interested in the directional (ensemble) average of powers of the matrix element G as defined by (3), i.e.,

$$\langle G^k \rangle = \sum_{\beta,\gamma,\cdots=1}^{N} g_\beta g_\gamma \cdots \langle |a_\beta|^2 |a_\gamma|^2 \cdots \rangle , \tag{5}$$

where the dots mean that there are k factors. Because the a_β are elements of a unitary matrix, the unitary constraints plus a knowledge of $\langle |a|^{2n} \rangle$ are all that is needed to obtain the moments required in (5).

II. EVEN MOMENTS OF THE COMPLEX DIRECTION COSINE

To obtain a general expression for $\langle |a|^{2n} \rangle$ we first must know the N-dimensional "solid angle" in a unitary space. This can be developed by making a suitable parametrization of an $N\times N$ unitary matrix U which then determines the line element ds using the relation[3]

$$ds^2 = \mathrm{Tr}(dU dU^\dagger)\,. \tag{6}$$

Imagine the parameters are labeled x_μ, then each matrix element of U is a function of the x_μ, i.e., $U = U(\{x_\mu\})$. It is a fairly simple matter to count the N^2 constraints imposed by unitarity $UU^\dagger = 1$ and the single constraint imposed by $\det U = 1$, and then to subtract these from the $2N^2$ real numbers present in a complex $N\times N$ matrix to reach the conclusion that there are N^2-1 parameters x_μ. Of course, each element of dU contains, in principle, all of the differentials dx_μ. Thus, (6) can be written in the conventional form

$$ds^2 = \sum_{\mu,\nu=1}^{N^2-1} g_{\mu\nu} dx_\mu dx_\nu , \tag{7}$$

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[1] F. J. Dyson, J. Math. Phys. 3, 140 (1962).
[2] N. Rosenzweig and C. E. Porter, Phys. Rev. 123, 853 (1961). A slight notational change has been made here to distinguish the averaging procedures.
[3] We use the notation of Hua Lo-Ken, *Harmonicheskii Analiz Funktsii Mnogikh Kompleksnikh Peremennikh v Klassicheskikh Oblastyakh* (Izdatelstvo Inostrannoĭ Literatury, Moscow, 1959).

where the metric tensor $g_{\mu\nu}$ (not to be confused with g_β above) is identified by inspection after the differentiation is carried out. It is well known that the volume element $\dot{U}$ in the x_μ space is then given by

$$\dot{U}\equiv(\det g_{\mu\nu})^{1/2}dx_1dx_2\cdots dx_{N^2-1}, \tag{8}$$

where $\det g_{\mu\nu}$ implies the determinant of the $(N^2-1)\times(N^2-1)$ metric tensor. For a 2×2 unitary matrix the procedure we have outlined is straightforward, but the same procedure becomes extremely complicated when one deals with 3×3 unitary matrix although a convenient explicit parametrization having the required eight independent parameters and resembling closely a 3×3 orthogonal matrix has been written out by the first of the present authors. This approach becomes very tedious for higher dimensions.

We shall now show that the various moments $\langle|a|^{2n}\rangle$ for an N-dimensional unitary space can be obtained by going over to a $2N$-dimensional orthogonal space. Let U be an $N\times N$ unitary matrix having matrix elements

$$U_{ij}=(x_{ij}+iy_{ij})/R, \tag{9}$$

where

$$\sum_{i=1}^{N}(x_{ij}^2+y_{ij}^2)=R^2. \tag{10}$$

The corresponding $2N\times2N$ orthogonal matrix can then be written as

$$O=\begin{pmatrix} A & B\\ -B & A\end{pmatrix}, \tag{11}$$

where A and B are $N\times N$ real matrices with matrix elements

$$A_{ij}=x_{ij}/R,\quad B_{ij}=y_{ij}/R. \tag{12}$$

The orthogonality condition $O\tilde{O}=1$ on O gives

$$A\tilde{A}+B\tilde{B}=1,\quad A\tilde{B}-\tilde{A}B=0, \tag{13}$$

which are identical with the unitary condition $UU^\dagger=1$ on $U=A+iB$, i.e.,

$$(A+iB)(\tilde{A}-i\tilde{B})=1, \tag{14}$$

if real and imaginary parts are taken.

The line element for the N-dimensional unitary space can be expressed as

$$\begin{aligned} ds^2&=\mathrm{Tr}(dUdU^\dagger),\\ &=\mathrm{Tr}[(dA+idB)(d\tilde{A}-id\tilde{B})],\\ &=\mathrm{Tr}[dAd\tilde{A}+dBd\tilde{B}], \end{aligned} \tag{15}$$

while for the $2N$-dimensional orthogonal space, it is given by

$$\begin{aligned} ds^2&=\mathrm{Tr}(dOd\tilde{O}),\\ &=\mathrm{Tr}\begin{pmatrix} dA & dB\\ -dB & dA\end{pmatrix}\begin{pmatrix} d\tilde{A} & -d\tilde{B}\\ d\tilde{B} & d\tilde{A}\end{pmatrix},\\ &=2\,\mathrm{Tr}(dAd\tilde{A}+dBd\tilde{B}). \end{aligned} \tag{16}$$

Thus, the measure for the N-dimensional unitary space based on (9) is the same as the $2N$-dimensional orthogonal space based on (11).

We now write down the $2N$-dimensional spherical polar coordinates of a unit vector[4]

$$\begin{aligned} V_1&=\cos\theta,\\ V_2&=\sin\theta\cos\varphi_1,\\ &\vdots\\ V_{2N-1}&=\sin\theta\sin\varphi_1\cdots\sin\varphi_{2N-3}\cos\varphi_{2N-2},\\ V_{2N}&=\sin\theta\sin\varphi_1\cdots\sin\varphi_{2N-3}\sin\varphi_{2N-2}, \end{aligned} \tag{17}$$

in which the ranges of θ and φ_i are

$$\begin{aligned} &O<\theta<\pi,\\ &O<\varphi_1<\pi,\quad i=1,2\cdots2N-3\\ &-\pi<\varphi_{2N-2}<\pi. \end{aligned} \tag{18}$$

The $2N$-dimensional differential solid angle is given by

$$d\Omega_{2N}=\sin^{2N-2}\theta\sin^{2N-3}\varphi_1\cdots\times\sin\varphi_{2N-3}d\theta d\varphi_1\cdots d\varphi_{2N-2}. \tag{19}$$

The values of $\langle|a|^{2n}\rangle$ are then given by

$$\langle|a|^{2n}\rangle=\int\cdots\int|a|^{2n}d\Omega_{2N}\Big/\int\cdots\int d\Omega_{2N}, \tag{20}$$

where a is any one of the unit vector components. Putting $|a|^2=\cos^2\theta+\sin^2\theta\cos^2\varphi_1$, we obtain

$$\begin{aligned} \langle|a|^{2n}\rangle&=\int\cdots\int(\cos^2\theta+\sin^2\theta\cos^2\varphi_1)^n d\Omega_{2N}\Big/\int\cdots\int d\Omega_{2N},\\ &=\sum_{r=0}^{n}(-1)^r\binom{n}{r}\int_{\theta=0}^{\pi}\int_{\varphi_1=0}^{\pi}\sin^{2N+2r-2}\theta\sin^{2N+2r-3}\varphi_1 d\theta d\varphi_1\Big/\int_{\theta=0}^{\pi}\int_{\varphi_1=0}^{\pi}\sin^{2N-2}\theta\sin^{2N-3}\varphi_1 d\theta d\varphi_1,\\ &=(N-1)\sum_{r=0}^{n}(-1)^r\binom{n}{r}\frac{1}{N+r-1}, \end{aligned} \tag{21}$$

where $\binom{n}{r}$ is a binomial coefficient. The values of $\langle|a|^{2n}\rangle$ for two and three dimensions obtained from

[4] A. J. W. Sommerfeld, *Partial Differential Equations in Physics* (Academic Press Inc., New York, 1949), p. 227.

(21) are

$$\langle |a|^{2n}\rangle=\frac{1}{n+1},\qquad N=2 \tag{22}$$

$$\langle |a|^{2n}\rangle=\frac{2}{(n+1)(n+2)},\quad N=3 \tag{23}$$

which check with the values obtained by explicit parametrization of 2×2 and 3×3 unitary matrices.

III. EXPECTATION VALUE FLUCTUATIONS

In this section we shall use the results of the preceding sections to derive certain moments. The dispersion of the operator G in the diagonal representation is

$$\frac{1}{N}\,\mathrm{Tr}\left(G-\frac{1}{N}\,\mathrm{Tr}G\right)^2=\frac{N-1}{N}\sum_{i=1}^{N}g_i^2-\frac{2}{N^2}\sum_{i>j=1}^{N}g_ig_j. \tag{24}$$

Similarly, for $\langle(\delta G)^2\rangle$, we write

$$\langle(\delta G)^2\rangle=\langle G^2\rangle-\langle G\rangle^2.$$

Using (5), (21), and the unitarity constraints we get

$$\langle G\rangle=\frac{1}{N}\sum_{i=1}^{N}g_i, \tag{25}$$

$$\langle G^2\rangle=\frac{2}{N(N+1)}\sum_{i=1}^{N}g_i^2+\frac{2}{N(N+1)}\sum_{i>j=1}^{N}g_ig_j. \tag{26}$$

Substituting the values of $\langle G\rangle$ and $\langle G^2\rangle$ in the expression for $\langle(\delta G)^2\rangle$ we get

$$\langle(\delta G)^2\rangle=\frac{N-1}{N^2(N+1)}\sum_{i=1}^{N}g_i^2-\frac{2}{N^2(N+1)}\sum_{i>j=1}^{N}g_ig_j. \tag{27}$$

Comparing (24) and (27) we finally get

$$\langle(\delta G)^2\rangle=\frac{1}{N+1}\left[\frac{1}{N}\,\mathrm{Tr}\left(G-\frac{1}{N}\,\mathrm{Tr}G\right)^2\right]. \tag{28}$$

Using a similar procedure we can find that the relation between third moments turns out to be

$$\langle(\delta G)^3\rangle=\frac{2}{(N+1)(N+2)}\left[\frac{1}{N}\,\mathrm{Tr}\left(G-\frac{1}{N}\,\mathrm{Tr}G\right)^3\right]. \tag{29}$$

IV. CONCLUSIONS AND COMMENTS

The second and third moments in the orthogonal ensemble are given by[2]

$$\langle(\delta G)^2\rangle=\frac{2}{N+2}\left[\frac{1}{N}\,\mathrm{Tr}\left(G-\frac{1}{N}\,\mathrm{Tr}G\right)^2\right], \tag{30}$$

$$\langle(\delta G)^3\rangle=\frac{8}{(N+2)(N+4)}\left[\frac{1}{N}\,\mathrm{Tr}\left(G-\frac{1}{N}\,\mathrm{Tr}G\right)^3\right]. \tag{31}$$

On comparing (28) and (29) with (30) and (31), respectively, we find that for large values of N, the second and third moments in the unitary ensemble are decreased by factors of 2 and 4 compared to the corresponding moments in the orthogonal case. Therefore, the dispersion in the values of G is smaller for systems violating time-reversal invariance when compared to those which are invariant under time reversal.

The behavior found here for expectation values is quite similar to that for level widths. In the orthogonal ensemble the dispersion $\langle(\delta\Gamma)^2\rangle$ of a width Γ is related to the average width $\langle\Gamma\rangle$ according to

$$\langle(\delta\Gamma)^2\rangle=2\langle\Gamma\rangle^2, \tag{32}$$

while in the unitary ensemble (no time-reversal invariance)

$$\langle(\delta\Gamma)^2\rangle=\langle\Gamma\rangle^2. \tag{33}$$

The dispersion as given by (33) is smaller compared to the square of the average than that given by (32). Roughly speaking, bringing in an extra degree of freedom allowed by no time-reversal invariance brings on some of the tightness characteristic of the statistical central limit theorem. As the number of independent random variables is increased, the dispersion decreases for both expectation values and widths.

The results (28)–(31) also show that for large values of N the second and third moments for the orthogonal and unitary ensembles can be expressed as

$$\langle(\delta G)^2\rangle=\frac{2}{\beta N}\left[\frac{1}{N}\,\mathrm{Tr}\left(G-\frac{1}{N}\,\mathrm{Tr}G\right)^2\right], \tag{34}$$

$$\langle(\delta G)^3\rangle=\frac{8}{(\beta N)^2}\left[\frac{1}{N}\,\mathrm{Tr}\left(G-\frac{1}{N}\,\mathrm{Tr}G\right)^3\right], \tag{35}$$

while from (32) and (33) we have

$$\langle(\delta\Gamma)^2\rangle=\frac{2}{\beta}\langle\Gamma\rangle^2, \tag{36}$$

with $\beta=1$ for the orthogonal ensemble and $\beta=2$ for the unitary ensemble. It is a simple extrapolation of (34)–(36) to conjecture that the analogous results for the symplectic ensemble are obtained by setting $\beta=4$. The correctness of this conjecture has been demonstrated for (34) and (35) by Dyson.[5] In addition, he has obtained the entire expectation value distribution for the unitary ensemble.[5] A general expression for $\langle |a|^{2n}\rangle$ for arbitrary β and N has been obtained by Gunson.[6] From this result, he also can obtain the symplectic version of (34) and (35) agreeing with the conclusions of Dyson.[5] In addition, he has proven the symplectic case of (36).

[5] F. J. Dyson (private communication).
[6] J. G. Gunson (private communication).