ANALYSIS OF DISTANT-NEIGHBOUR SPACING DISTRIBUTIONS FOR k-BODY INTERACTION ENSEMBLES*

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ABSTRACT: The widths of the distant-neighbour spacing distributions for the eigenvalues of k-body Hamiltonians acting in finite-dimensional m-particle spaces are considered. The relationship between the spacing widths, as calculated by using a single spacing unit for the entire ensemble, and by using separate units for each matrix (which has been of consequence in studying whether energy-level fluctuations can yield information about many-body components in the interaction), is calculated explicitly. A related question about the validity of an elementary ergodic theorem is settled.

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Level spacing distributions for many-particle systems have been conventionally described[1] via a Gaussian orthogonal ensemble of matrices (GOE). Recently however[2], particle structure has been explicitly taken into account by using operator ensembles of two-body Hamiltonians (TBRE). One then asks, for example, whether analysis of high-order-spacing distributions can distinguish between two-body interactions and the multi-body interactions which are in fact implied by the GOE, this question being of obvious physical interest[3,4]. In the absence of analytic results for the new ensembles, Monte-Carlo calculations have been made, these in parallel with calculations for GOE ensembles of the same matrix dimensionality. Certain questions have arisen about the method of analysis which we wish to clear up in this note.

In one method of analysis one spacing (or a few spacings) of the order in question, say p (nearest neighbours correspond to $p = 0$), is taken from the immediate neighbourhood of the centre of each matrix; the average of these spacings ($= (p + 1)\,\overline{D}$) defines the ensemble-averaged nearest-neighbour spacing $\overline{D}$, which, to within finite-matrix and sample-size effects, should be independent of p. Each spacing S is then measured in terms of $\overline{D}$ and the spacing distribution (that of $S/\overline{D}$) then constructed.

In the second method, which treats the results of each matrix as one would treat a set of experimental data, one chooses a run of spacings from the central region of each matrix, calculates with these a D for that matrix and uses that to reduce the spacings; collecting the reduced spacings from each matrix one constructs the distribution, in this case of S/D. Since (for each method) the centroids are at $(p + 1)$ and since, for $p > 3$ say, the distributions are close to Gaussian, the width of the distribution is the only significant quantity.

To within the errors mentioned above these two methods give in practical cases the same results for GOE. The two sets of TBRE results agree for very small spacings but diverge rapidly as the spacing order increases[3,4], the ensemble-D spacing ($\hat{\sigma}(p)$) being larger than that given by the second method ($\sigma(p)$) by a factor which reaches 2–3 for $p \sim 10$ in the cases considered.

In contrast to the first method, the second gives TBRE values which are found[4] to be stable under variation of the matrix dimensionality, as one would demand of a satisfactory analysis if the finite-size effects could be ignored. It is not surprising also that these results are in agreement with those derived by considering single large shell-model matrices. They are very close also to those from GOE, but of course that is a significant outcome rather than an *a priori* requirement. The first method which assigns a real significance to the ensemble itself has however its own claim to consideration,

based on an elementary ergodic property[5] which would assert that, to within finite-size effects, the two methods should give the same results. We ask therefore whether this expectation is in fact correct, which is a matter of formal interest, and if so, why the analyses which have been carried out with this method run into a surprisingly large finite-size effect, a matter of more practical interest.

It has already been recognized that a finite-size effect arises in the Monte Carlo calculations from matrix-to-matrix fluctuations in the spectrum span, which results, *ceteris paribus*, in a fluctuation in the mean level spacing D which supplies the natural energy unit. We thus get an apparent increase in the ensemble variance of the nearest-neighbour spacing D. Similarly the variance of the p'th-order spacing, which involves an addition of $(p+1)$ nearest neighbours, grows by an apparent factor which increases with p. We shall calculate this effect as a function of the parameters of the system.

Before proceeding, we remark that the second method involves a separate finite-size effect arising from the curvature in the density, which gives a secular change in D over the range of the spectrum considered. This is of secondary importance unless we wish to cover a large fraction of the spectrum, and even in that case may be essentially eliminated by a spectrum unfolding[4]; so we ignore it. We may also in the first method, use a run of levels from each spectrum instead of the one or two levels called for above.

We start now by decomposing the matrix ensemble into "fixed-strength" subensembles[6] characterized by values of λ where, for a given matrix,

$$\lambda^2 = d_m^{-1} \operatorname{Tr}(H^2) = d_m^{-1} \sum_{i=1}^{d_m} E_i^2 \equiv \langle H^2 \rangle^m \qquad (1)$$

Here the number of particles is m, d_m is the matrix dimensionality and the E_i are the eigenvalues. λ is then the spectrum width, a measure of the extent or "strength" of the matrix, and all matrices of the same λ form the λ-subensemble. Let us now make the assumption, whose validity we consider ahead, that all the subensembles are identical except for their scale and their measure $h(\lambda)$, ($h(\lambda)\,d\lambda$ being the relative probability of finding a matrix in the $(\lambda, \lambda + d\lambda)$ interval). It follows from this that $\mathfrak{D}(\lambda)$, the subensemble-averaged spacing unit (derived as above by considering a subset of levels from each λ-matrix), is proportional to λ, so that we may classify the subensembles instead by $\mathfrak{D}$ with subensemble probability measure $g(\mathfrak{D})$. Then the centroid and width (square root of the second central moment) of $g(\mathfrak{D})$ which we write as $\overline{\mathfrak{D}}, \Sigma$ are related to $\overline{\lambda}, \Sigma_\lambda$, the same quantities for $h(\lambda)$ by $\Sigma/\overline{\mathfrak{D}} = \Sigma_\lambda/\overline{\lambda}$. $(p+1)\overline{\mathfrak{D}}$ is of course the ensemble-averaged value of S, and thus $\overline{\mathfrak{D}} = \overline{D} = \overline{S}/(p+1)$, while $\overline{\lambda}$ is the average spectrum width and the

Σ's are the RMS deviations of these quantities.

If the S values are distributed according to $\mathcal{P}_S(x)$ we have then

$$\mathcal{P}_S(x) = \int g(\mathfrak{D})\, P_S^{(\mathfrak{D})}(x)\, d\mathfrak{D} = \int g(\mathfrak{D})\, \mathfrak{D}^{-1}\, P_{S/\mathfrak{D}}^{(\mathfrak{D})}(x/\mathfrak{D})\, d\mathfrak{D} \ , \qquad (2)$$

where the last form follows by a scale change. $P_{S/\mathfrak{D}}^{(\mathfrak{D})}(y)$, defined for the $\mathfrak{D}$-subensemble, is, by our assumption, the same function for all subensembles and by its definition is the spacing distribution as given by the second method; its second moment is then $\{\sigma^2(p) + (p+1)^2\}$. The ensemble-averaged value of S^2 is now

$$\overline{S^2} = \int g(\mathfrak{D})\, \mathfrak{D}^{-1}\, d\mathfrak{D} \int P_{S/\mathfrak{D}}^{(\mathfrak{D})}(x/\mathfrak{D})\, x^2 dx = \int g(\mathfrak{D})\, \mathfrak{D}^2\, d\mathfrak{D} \int P_{S/\mathfrak{D}}^{(\mathfrak{D})}(y)\, y^2\, dy$$

$$= \{\Sigma^2 + \overline{\mathfrak{D}}^2\}\{\sigma^2(p) + (p+1)^2\} \ , \qquad (3)$$

and since $\hat{\sigma}^2(p) = \overline{D}^{-2}\{\overline{S^2} - \overline{S}^2\}$ we have

$$\hat{\sigma}^2(p) = \sigma^2(p) + \{\sigma^2(p) + (p+1)^2\}\, \Sigma^2/\overline{D}^2$$

$$= \sigma^2(p) + \{\sigma^2(p) + (p+1)^2\}\, \Sigma_\lambda^2/\overline{\lambda}^2 \ , \qquad (4)$$

which, in somewhat different notation, has already been given[4] (without derivation) and used in discussing the difference between the two methods of analysis. We must now verify that our basic assumption about the subensemble structure is correct, and we must calculate $\Sigma_\lambda^2/\overline{\lambda}^2$.

The Monte-Carlo calculations have dealt with two-body interactions as encountered in conventional spectroscopy, namely those which preserve angular momentum (and isospin wherever that is relevant) acting in a space defined by a set of spherical orbits. Let us drop these restrictions, which lead to great complications in a formal analysis but which appear to be irrelevant for our present purpose*; at the same time let us extend to k-body

* There is good evidence, though as yet little or no theoretical understanding for it, that the fixed-J spaces display the same energy-level fluctuations as the simpler ones.

interactions. We consider then, a system defined by four quantities (N, m, k, v), a Gaussian orthogonal ensemble of k-body interactions acting in a d_m-dimensional vector space, formed by distributing m particles over N single-particle states $\left(d_m = \binom{N}{m}\right)$. The individual matrix elements $W_{\alpha,\beta}$, where α,β are k-particle states, are taken real and with a Gaussian distribution centered about zero with variance v^2 for off-diagonal and $2v^2$ for diagonal. We shall see that in the large-N limit this operator ensemble shares with the GOE, to which it becomes equivalent in $m = k$ spaces, the important property of invariance under orthogonal transformations. In general $m \geqslant k$ spaces we may speak of the "embedded GOE" or EGOE for short.

For the GOE, i.e. $k = m$, it is easy to see that the ensemble structure is as we have assumed; the probability of finding any preassigned $H(k)$ in the ensemble depends only on the k-particle trace of $H^2(k)$ and this, to within a dimensionality factor $\binom{N}{k}$ is simply the k-particle spectrum variance, the square of the spectrum width. Thus the fixed-strength sub-ensembles, those in which λ is fixed, differ from each other only in their measure (which is looked after by $g(\mathbb{N})$) and in their scale, just as we have assumed. We see that this separation of scale and spectrum-shape effects has come about because of an isotropy in the matrix-element space (invariance under orthogonal transformations), every k-particle matrix element entering into λ^2 with equal weight, due allowance being made for the difference between diagonal and off-diagonal ones.

This isotropy does not strictly apply when we proceed to the m-particle EGOE; for while $\lambda^2(m)$ is of course quadratic in the k-particle $W_{\alpha\beta}$, it is not a multiple of $\lambda^2(k)$. This comes about because there are different classes of k-particle matrix elements, the members of a class behaving uniformly but in a manner which depends on the class, when we proceed from k to m particles. The classes derive from the $U(N)$ decomposition of $H(k)$ which transforms according to a sum of $(k+1)$ irreducible representations whose column structures are $[N-\nu, \nu]$ with dimensionalities

$$d(\nu) = \frac{(N - 2\nu + 1)}{(N + 1)} \binom{N+1}{\nu}^2 \; ; \; \sum_{\nu} d(\nu) = \binom{N}{k}^2 \; , \qquad (5)$$

where $\nu = 0, 1, 2 \ldots k$. For large N, $d(\nu) \sim (\nu!)^{-2} N^{2\nu}$, so that the highest symmetry, $\nu = k$, dominates in the k-particle space (it is in fact this dominance which enables one to ignore diagonal matrix elements and to make similar approximations in the asymptotic GOE). The explicit decomposition for a specified k-body H is given by[7]

$$H(k) = \sum_{\nu=0}^{k} H^{\nu}(k) = \sum_{\nu=0}^{k} \binom{n-\nu}{k-\nu} \mathcal{H}(\nu) \quad , \tag{6}$$

where n is the number operator and $\mathcal{H}(\nu)$, a ν-body irreducible operator, vanishes in states with less than ν particles or holes, and is invariant to within a sign under hole $\leftrightarrows$ particle transformations. Since the trace operation is $U(N)$ scalar, $\lambda^2(m)$ also decomposes by ν (no cross terms appearing); thus[7],

$$\lambda^2(m) = \sum_{\nu=1}^{k} \lambda^2(m{:}\nu) = \sum_{\nu=1}^{k} \binom{m-\nu}{k-\nu}^2 \binom{m}{\nu}\binom{N-m}{\nu}\binom{N-\nu}{\nu}^{-1} < \mathcal{H}^2(\nu) >^{\nu}$$

$$= \sum_{\nu=1}^{k} \binom{m-\nu}{k-\nu}^2 \binom{m}{\nu}\binom{k}{\nu}^{-1}\binom{N-m}{\nu}\binom{N-k}{\nu}^{-1} \lambda^2(k{:}\nu) \quad . \tag{7}$$

In the second step we have used the fact that the m-particle average expectation value of an operator of maximum particle rank u ($= 2\nu$ for $\mathcal{H}^2(\nu)$) is a polynomial of order u in m; $\binom{m}{\nu}\binom{N-m}{\nu}\binom{N-\nu}{\nu}^{-1}$ is such a polynomial and satisfies the defining conditions of reducing to unity when $m = \nu$ and vanishing when $m < \nu$ and when $(N - m) < \nu$. In the third step we have eliminated $< \mathcal{H}^2(\nu) >^{\nu}$ by using the $m = k$ result; we observe now that the fixed-ν widths do "propagate" from k-particles to m but with ν-dependent coefficients so that the exact matrix-element isotropy is lost.

To average this result over the k-body GOE we note that, because of the isotropy in the k-particle space

$$\overline{\lambda^2(k{:}\nu)} = \overline{\lambda^2(k)}\; d(\nu)/\sum_{\nu} d(\nu) = \overline{\lambda^2(k)}\; \frac{(N - 2\nu + 1)}{(N+1)} \binom{N+1}{\nu}^2 \binom{N}{k}^{-2}$$

$$\xrightarrow{\text{large } N} (k!/\nu!)^2\; N^{-2(k-\nu)} \cdot \overline{\lambda^2(k)} \quad , \tag{8}$$

and thus in the large-N limit (m, k fixed) $\nu = k$ is dominant in the k-particle space. Since moreover the propagation coefficient of (7) which connects $\lambda^2(m)$ with $\lambda^2(k{:}\nu)$ is in the same limit independent of N, $\nu = k$ is dominant for m

particles as well. From (7, 8) we find

$$\overline{\lambda^2(m:\nu-1)} \,/\, \overline{\lambda^2(m:\nu)} = \frac{m-\nu+1}{(k-\nu+1)} \frac{\nu^2}{N^2} \xrightarrow{\nu=k} (m-k+1)\frac{k^2}{N^2} \quad , \tag{9}$$

so that for large enough N we may take $\nu = k$ and then (see (11) ahead)

$$\overline{\lambda^2(m)} \to \binom{m}{k} \overline{\lambda^2(k)} = d_k \binom{m}{k} v^2 \quad , \tag{10}$$

and thus for N large we do have isotropy in the m-particle space. It is hard to say just how large N should be for a given fluctuation measure, because no information is available about energy-level fluctuations for H's of fixed unitary symmetry, and thus we cannot predict the effect of admixtures of symmetries $\nu < k$. But reducing ν is equivalent to reducing the particle rank in a sense defined by (6) and, since fluctuations are believed insensitive to rank, we would expect that even for quite small N, say for $N \geqslant 10$, the subensemble structures should be essentially identical and equation (4) applicable. From the proportionality of the two quadratic traces it follows, moreover, that the probability measure for the m-particle trace is also invariant under orthogonal transformations, so that in the large-N limit the EGOE becomes an orthogonal ensemble (which, however, is presumably not Gaussian and whose matrix elements are not statistically independent).

There remains now the explicit evaluation of $\Sigma_\lambda^2/\overline{\lambda}^2$ needed in (4), which we carry out in the large-N limit. For a given $H(k)$ with defining matrix elements $W_{\alpha\beta}$ we have now

$$\lambda^2(m) = d_k^{-1}\binom{m}{k} \sum_{\alpha,\beta} (W_{\alpha\beta})^2 \to 2\, d_k^{-1}\binom{m}{k} \sum_{\alpha<\beta} (W_{\alpha\beta})^2 \quad , \tag{11}$$

and thus is distributed over the ensemble as the sum of squares of $\frac{1}{2} d_k^2$ independent Gaussian random variables (centroid = 0, RMS deviation $= \{2 d_k^{-1}\binom{m}{k} v^2\}^{1/2}$. This distribution[8] is $\chi^2(\frac{1}{2} d_k^2)$ and for large d_k becomes Gaussian[8] $(d_k\binom{m}{k} v^2,\ 2\binom{m}{k} v^2)$; since $d_k \gg 1$ we have from this that $\overline{\lambda} = \{d_k \binom{m}{k} v^2\}^{1/2}$, $\Sigma_\lambda = \{d_k^{-1}\binom{m}{k} v^2\}^{1/2}$, and $\Sigma_\lambda/\overline{\lambda} = d_k^{-1}$, a result which is entirely to be expected since d_k is the number of degrees of freedom (independent matrix elements).

We would predict for the GOE ($m = k$), taking $v = 1$, that $\overline{\lambda} = d^{1/2}$, $\Sigma\lambda = d^{-1/2}$ where d now is the matrix dimensionality; for $d = 294$ this gives $\overline{\lambda} = 17.15 \pm 0.058$ which compares with the Monte-Carlo values[4] 17.17 ± 0.057. The TBRE Monte-Carlo calculations which have been made, are however, not strictly EGOE because of the (J, T) conservation, and thus *a priori* calculation of d_k is not possible, nor in fact is it obvious how accurate in this case is the concept of a single d_k. From the observed results for the 294-dimensional matrices[4] ($N = 32$, $m = 6$, $k = 2$, $\overline{\lambda} = 7.8 \pm 1.0$) we have very roughly d_k (effective) $\sim 5 - 10$, so that the effective dimensionality is greatly reduced and the fluctuations greatly increased because of the symmetry restrictions, a result which is not surprising at all. Eq. (4) is found to be still valid even for these more complex ensembles, and one may have confidence in its prediction that the ensemble-D method of calculating spacing widths, will show deviations due to spectrum-span fluctuations as soon as the spacing order becomes comparable with the effective dimensionality d_k. We remark also that if one renormalizes the matrices, all to have the same spectrum width, then the two methods of analysis should become equivalent. This is found to be true[4] not only for spacing widths but also for other long-range fluctuation measures, as the analysis would indicate.

Returning now to the EGOE and the question of "internal ergodicity" we stress that, for fixed N and k, the relevant fluctuations, and hence the deviation between $\hat{\sigma}(p)$ and $\sigma(p)$, cannot be reduced by increasing the particle number even though this does result in larger matrices; for the number of degrees of freedom, d_k, is independent of particle number. On the other hand, if for fixed (m, k) we increase N, the fluctuations decrease rapidly and, for any preassigned spacing order, we can always take N large enough so that ergodicity is restored.

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RESUMEN

Se discuten las anchuras de las distribuciones de espaciamientos entre vecinos lejanos para un hamiltoniano estocástico de k cuerpos. Se obtiene la relación entre las anchuras calculadas al usar un sólo espaciamiento promedio para todo el ensemble, y las calculadas al usar un espaciamiento promedio para cada matriz. Esta relación ha sido importante para resolver el problema siguiente: ¿Pueden las fluctuaciones en el espectro de energías de un sistema dar información sobre la existencia de fuerzas de muchos cuerpos? Se aclaran también algunos puntos sobre la validez de un teorema ergódico elemental.