Random matrix ensembles for semi-separable systems

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Abstract. – Many models for chaotic systems consist of joining two integrable systems with incompatible constants of motion. The quantum counterparts of such models have a propagator which factorizes into two integrable parts. Each part can be diagonalized. The two eigenvector bases are related by an orthogonal (or unitary) transformation. We construct a random matrix ensemble that mimics this situation and consists of a product of a diagonal, an orthogonal, another diagonal and the transposed orthogonal matrix. The diagonal phases are chosen at random and the orthogonal matrix from Haar's measure. We derive asymptotic results (dimension $N \to \infty$) using Wick contractions. A new approximation for the group integration yields the next order in $1/N$. We obtain a finite correction to the circular orthogonal ensemble, important in the long-range part of spectral correlations.

It is usually assumed that the spectral fluctuation properties of classically chaotic systems coincide with those of the corresponding canonical ensemble of random matrix theory ("quantum chaos conjecture"). There is abundant numerical evidence for the conjecture. In addition, several approaches have aimed at an analytical proof for the conjecture, see Section 5.9 of the review [1]. Naturally, these approaches have addressed generic systems. However, many of the commonly studied chaotic systems have a very particular form: They can be divided into two parts each of which is integrable, albeit in different coordinates. Such systems have been called semi-separable [2]. Typical cases are: The quarter stadium, kicked systems such as the kicked rotor, chaotic Jung scattering maps for integrable Hamiltonians [3], or Lombardi's approximation for Rydberg molecules [4]. The spectral fluctuations of such semi-separable systems have been found to be essentially consistent with the quantum chaos conjecture. In view of the special nature of these systems, that finding is somewhat surprising. In the present letter, we construct two random matrix models (one for the unitary and one for the orthogonal case) for semi-separable systems which we can solve analytically. The models take account of very specific features of semi-separable systems which are not reproduced by the circular ensembles of random matrix theory. With the help of these models, we show why semi-separable systems nearly follow the predictions of standard random matrix theory, and we predict quantitatively

the deviations that are typically expected for such systems. In order to perform the ensemble averages, we develop a novel technique of approximate integration over the orthogonal or the unitary group in the limit of large matrix dimension.

Semi-separable systems are computationally relatively simple: One uses a surface of section that separates the two integrable parts. For kicked rotors one gets an intertwining of gauge transformation and Fourier transformation if (time) sections are taken before and after each kick. For scattering maps one obtains transport with the full and the free Hamiltonian if the cut is placed in the asymptotic region. In the case of time-independent systems with two degrees of freedom, one can often choose a Poincaré section such that both parts become integrable scattering systems when the other part is replaced by a scattering channel. The quantum Poincaré map (QPM) is then the product of two Jung scattering maps [5,6]. The latter can be unitarised [2]. In particular cases such as the quantum defect theory of the Rydberg molecule, the division may relate to a variable such as angular momentum that has a discrete quantum number, leading to a unitary QPM [7]. For surfaces of section, the relevant ensembles to implement the quantum chaos conjecture are the circular orthogonal and the circular unitary ensemble (COE and CUE).

Typically, the time evolution operator or the QPM of a semi-separable time-reversal invariant system consists of a sequence of four operations: The orthogonal transformation O which takes us from the basis where one part of the propagator is diagonal to the one where the other part of the propagator is diagonal, followed by a diagonal phase matrix $D_1 = \mathrm{diag}\{e^{2i\eta_n}\}$, this followed by the inverse transformation matrix O^T and this followed by another diagonal phase matrix $D_2 = \mathrm{diag}\{e^{2i\xi_n}\}$. For the propagator T' this yields the $N \times N$ matrix $T' = D_2 O^T D_1 O$. The time evolution operator can equivalently be written as

$$T = D_2^{-1/2} T' D_2^{1/2} = D_2^{1/2} O^T D_1 O D_2^{1/2} \ . \tag{1}$$

If time-reversal invariance is broken in either of the two sub-systems, the orthogonal matrix O, and its inverse O^T, have to be replaced by a unitary matrices U, and $U^\dagger = U^{-1}$. The ensembles are then generated by assuming that the phases in D_1 and D_2 are independent random variables, *i.e.*, that they obey Poissonian statistics, and that O and U are members of ensembles defined by the Haar measure for the orthogonal and unitary matrices, respectively. We denote the resulting two ensembles for T by DODO and DUDU, respectively. Note that such and similar composed ensembles of random matrices have been studied numerically in ref. [8].

We determine the spectral properties of DODO and DUDU by first computing the spectral form factors $K(m) = \langle |\mathrm{tr} T^m|^2 \rangle$ for both cases. From $K(m)$ we can calculate any 2-point statistics. For example, the number variance $\Sigma^2(L; N)$ is given by

$$\Sigma^2(L; N) = \frac{2}{\pi^2} \sum_{m=1}^{\infty} \frac{1}{m^2} \sin^2 \left(\frac{m\pi L}{N} \right) K(m) \ . \tag{2}$$

Here L is the length of the spectrum over which the variance is calculated. To leading order in $1/N$, the asymptotic result for DODO is given by

$$\Sigma^2_{\mathrm{DODO}}(L; N) = \Sigma^2_{\mathrm{COE}}(L; N) + \frac{2}{\pi^2} \sin^2(\pi L/N) + \mathcal{O}(1/N) \ , \tag{3}$$

and similarly for DUDU.

In order to compute $K(m)$, we must calculate averages of powers of T. For the quadratic term, we have

$$\langle T_{kl} T_{pq}^* \rangle_{\mathrm{DODO}} = \langle e^{i(\eta_k + \eta_l - \eta_p - \eta_q)} \rangle_\eta \sum_{a,b} \langle e^{2i(\xi_a - \xi_b)} \rangle_\xi \langle O_{ka} O_{la} O_{pb} O_{qb} \rangle_O \ . \tag{4}$$

The averages $\langle\,\rangle_\eta$ and $\langle\,\rangle_\xi$ are trivial and yield $\langle e^{i\eta_k - i\eta_l}\rangle_\eta = \delta_{k,l}$ and correspondingly for $\langle\,\rangle_\xi$. This gives $\langle T_{kl}T_{pq}^*\rangle_{\mathrm{DODO}} = \Delta(kl,pq)\sum_a \langle O_{ka}O_{la}O_{pa}O_{qa}\rangle_{\mathrm{O}}$. The factor $\Delta(kl,pq)$ equals unity if the pairs of indices kl and pq coincide (so that either $k = p$ and $l = q$ or $k = q$ and $l = p$) and vanishes otherwise. The difficulty lies in calculating the average $\langle\,\rangle_{\mathrm{O}}$ over the orthogonal group $\mathcal{O}(N)$. This is done approximately. We begin with the terms of leading order in $1/N$. We assume the matrix elements to be independent variables, and we replace the group integration by a Gaussian average $\langle\,\rangle_{\mathrm{G}}$ over the space of real $N \times N$ matrices,

$$\langle f(O)\rangle_{\mathrm{G}} = \left(\frac{N}{2\pi}\right)^{N^2/2} \int \prod_{k,l=1}^N \mathrm{d}O_{kl}\, f(O)\exp\left[-\frac{1}{2N}\operatorname{tr}(O^T O)\right]\ . \tag{5}$$

For the variances, this yields the correct expression $\langle O_{ij}O_{kl}\rangle_{\mathrm{G}} = \frac{1}{N}\delta_{ik}\delta_{jl}$. In this approximation, averages of monomials of matrix elements of O can be calculated by standard Wick contraction rules for Gaussian averages. Because of the symmetry of the matrix T, the only two non-equivalent non-vanishing quadratic moments of T are

$$\langle T_{11}T_{11}^*\rangle_{\mathrm{DODO}} \approx 3/N, \qquad \langle T_{12}T_{12}^*\rangle_{\mathrm{DODO}} \approx 1/N\ . \tag{6}$$

Comparing this to the result for COE we find that only the diagonal term differs to leading order: The COE result is $2/N$. For $K(1)$, this yields $K(1) = 3$ which leads directly to eq. (3). Higher moments of T are not affected by the difference because when compared to non-diagonal contractions, the contribution of diagonal contractions is suppressed by a factor $1/N$.

In order to obtain the subleading terms in $1/N$, we must improve our approximate group integration. We note that the Gaussian measure in eq. (5) yields orthogonality of the matrix O_{mn} only for quadratic terms, $\langle (O^T O)_{kl}\rangle_{\mathrm{G}} = \delta_{k,l}$. For higher polynomials in O_{mn}, corrections in the first subleading order occur. For example,

$$\langle (O^T O)_{k_1 l_1}(O^T O)_{k_2 l_2}\cdots(O^T O)_{k_m l_m}\rangle_{\mathrm{G}} = \delta_{k_1 l_1}\delta_{k_2 l_2}\cdots\delta_{k_m l_m} + \mathcal{O}\left(1/N\right), \qquad m \geq 2\ . \tag{7}$$

We observe that as $N \to \infty$, our approximate integration in eq. (5) is increasingly restricted to the neighborhood of the group manifold. To obtain the desired improvement, we introduce an extra weight factor $w(O)$ which is chosen such that the orthogonality relations (7) become *exact* for larger values of m, or the error terms $\mathcal{O}\left(1/N\right)$ are replaced by terms $\mathcal{O}\left(1/N^2\right)$, or both. We define the new "average" $\langle\,\rangle_{\mathrm{w}}$,

$$\langle f(O)\rangle_{\mathrm{w}} = \langle f(O)w(O)\rangle_{\mathrm{G}}\ . \tag{8}$$

To be useful, the weight function $w(O)$ has to be of low order in the matrix elements of O and should have a limited number of free parameters to adjust. We use the ansatz

$$w(O) = A + B\operatorname{tr}(O^T O) + C\operatorname{tr}(O^T O O^T O) + D[\operatorname{tr}(O^T O)]^2\ . \tag{9}$$

This expression is of fourth order in O and contains all essentially different terms up to this order. The use of traces of powers of $O^T O$ guarantees the symmetry under interchange of indices. Moreover, it causes $w(O)$ to be invariant under left and/or right multiplications with an *arbitrary orthogonal matrix* O',

$$w(O) = w(OO') = w(O'O), \qquad O' \in \mathrm{O}(N)\ . \tag{10}$$

We note that O is not a member of the orthogonal group. The invariance property (10) is desirable because it guarantees that the measure on the group manifold remains unchanged

except for a constant, and that areas close to this manifold are not affected drastically because they will be mapped onto other areas near the manifold. We determine the free parameters A, B, C, D by imposing the correct orthogonality properties for terms in $O^T O$ of order 0 (normalization), 1, and 2,

$$\langle 1 \rangle_{\rm w} = 1 \, , \tag{11}$$

$$\langle (O^T O)_{ij} \rangle_{\rm w} = \delta_{i,j} \, , \tag{12}$$

$$\langle (O^T O)_{i,j} (O^T O)_{k,l} \rangle_{\rm w} = \delta_{i,j} \delta_{k,l} \, . \tag{13}$$

Using the approximate integration, we find for the left-hand side of eq. (13) the form $f_3(A, B, C, D, N)\delta_{i,j}\delta_{k,l} + f_4(A, B, C, D, N)(\delta_{i,k}\delta_{j,l} + \delta_{i,l}\delta_{j,k})$. This yields $f_3(A, B, C, D, N) = 1$ and $f_4(A, B, C, D, N) = 0$. Together with eqs. (11), (12) one finds four linear equations for the four unknowns A, B, C, D. These were solved using Mathematica 4. We obtain ([1])

$$A = 1 - \frac{N^2}{4} \, , \qquad B = \frac{N}{2} \, , \qquad C = -\frac{N^3}{4(N^2 + N - 2)} \, , \qquad D = \frac{N^2}{4(N^2 + N - 2)} \, . \tag{14}$$

The negative signs in A and C imply that $w(O)$ is not positive definite and, thus, is not a proper measure. Yet the constant on the group manifold is positive, namely $1 + N^2/4$. Therefore, on the part of the integration area near this manifold where the Gaussian factor is not small, the weight $w(O)$ is also positive. This fact reflects the invariance condition (10).

In addition, we get the bonus that with the new integration (8) replacing the Gaussian integration (5) the correction terms on the right-hand side of eq. (7) for $m \geq 3$ are $\mathcal{O}\left(\frac{1}{N^2}\right)$. We have checked this statement explicitly for $m = 3, 4, 5$, and we conjecture that it holds for *arbitrary* $m \geq 3$. We have also checked that averages $\langle \rangle_{\rm w}$ over monomials containing the components $O_{i\alpha}$ of a single vector (fixed α) up to the 10th power are correct to subleading order $\mathcal{O}(\frac{1}{N^2})$. We also applied our procedure up to products of three indentities $(O^T O)_{ij}$ in the postulated relations (11)-(13) with a unique solution for the 6th-order polynomial ansatz for $w(O)$. For $m \geq 4$, no improvement over the 4th-order case (9), (14) was found in the approximate orthogonality relations eq. (7) (again within $\mathcal{O}(\frac{1}{N^2})$) for terms of power higher than 6; only the latter became exact.

We calculate the form factor for DODO by averaging over all the Poissonian phases, and by replacing the group integral by $\langle \rangle_{\rm w}$. For $m = 1, 2$, this yields

$$K_{\rm DODO}(1) = \sum_{k,p} \langle O_{kp}^4 \rangle_{\rm w} = \frac{3N}{N+2} \, , \tag{15}$$

$$K_{\rm DODO}(2) = 4 \sum_{k_1,k_2,p_1,p_2} \langle O_{k_1 p_1}^2 O_{k_2 p_1}^2 O_{k_2 p_2}^2 O_{k_1 p_2}^2 \rangle_{\rm w} - 4 \sum_{k,p_1,p_2} \langle O_{kp_1}^4 O_{kp_2}^4 \rangle_{\rm w} + \sum_{k,p} \langle O_{kp}^8 \rangle_{\rm w} \tag{16}$$

$$= 4 - \frac{4}{N} + \mathcal{O}\left(N^{-2}\right) \, . \tag{17}$$

The first moment is exact as the averages involved are of the type to which the weight factor was adjusted. For the second moment we stipulate that $\langle \rangle_{\rm w}$ correctly reproduces to subleading order, not only the averaged expressions mentioned above, but also the first term on the r.h.s. of eq. (17).

([1])The routines for averaging of symbolic sums of monomials of matrix elements over orthogonal and unitary groups using the approach described here can be obtained from one of the authors by e-mail request on `prosen@fiz.uni-lj.si`.
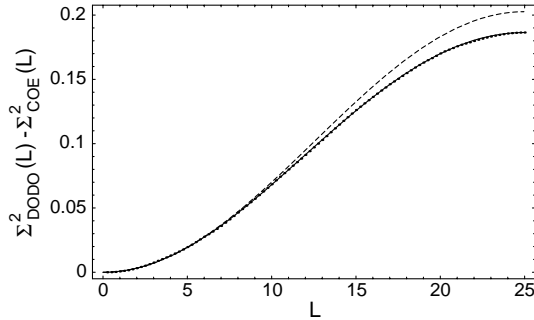
Fig. 1 – Deviation of the number variance of DODO ($N = 50$) from COE ($N = 50$) as determined by numerical Monte Carlo simulation (points), compared to the theoretical prediction with $1/N$ correction (18) (solid curve) and without $1/N$ correction ($N = \infty$) (dashed curve).

We determine the number variance from eq. (2), terminating the sum after the second moment. We expect the result to give a good account of the long-range correlations. We can calculate the COE result for finite N in the same approximation either in the conventional way or using similar techniques, see below. For the difference we obtain

$$\Sigma^2_{\text{DODO}}(L; N) - \Sigma^2_{\text{COE}}(L; N) \approx \frac{2}{\pi^2} \left\{ \left(1 - \frac{4}{N} \right) \sin^2 \left(\frac{\pi L}{N} \right) + \frac{1}{N} \sin^2 \left(\frac{2\pi L}{N} \right) \right\} . \qquad (18)$$

To lowest order in $1/N$, this formula agrees with eq. (3) and is exact, because only the first moment of T has a correction of order zero in $1/N$. We expect that the terms of next order in $1/N$ yield a good representation of the long-range behavior in L of the number variance. Finite-size effects for the short-range behavior are difficult to predict, except that we expect them to be small on general grounds, at least as long as the range L is short compared to the matrix dimension N.

We used numerical calculations to test our results and to look for finite-size corrections at short distances in the spectrum. Figure 1 shows the difference of the number variances for DODO and COE for three cases: In the limit $N \to \infty$, for $N = 50$ (in both cases, DODO results were obtained from eq. (18)), and the numerical result for $N = 50$. We find excellent agreement (even at short distances) confirming our intuitive argument. Since the number variance is at short distances not very sensitive to the changes considered in this paper, we show in fig. 2 the difference between the integrated nearest-neighbour spacing distributions $I(S) = \int_0^S \mathrm{d}s P(s)$ for DODO and COE for $N = 25$, 50, and 100. For purposes of reference, we have also included a comparison with the Wigner surmise. This shows how small the correction really is, which for $N = 100$ disappears in the statistical noise of 2×10^6 spacings. We mentioned that the ensemble we use has been studied numerically before [8]. The authors only looked at fairly short spectral ranges. This is why they failed to observe the zero-order deviation and the N-dependence.

For the unitary case, the approximate group integration can be developed in full analogy to the orthogonal case. For the weight function $w_c(U)$ (where U is a complex N-dimensional matrix) we use the ansatz $w_c(U) = A_c + B_c \operatorname{tr}(U^\dagger U) + C_c \operatorname{tr}(U^\dagger U U^\dagger U) + D_c [\operatorname{tr}(U^\dagger U)]^2$ and find

$$A_c = 1 - \frac{N^2}{2} , \qquad B_c = N , \qquad C_c = -\frac{N^3}{2(N^2 - 1)} , \qquad D_c = \frac{N^2}{2(N^2 - 1)} . \qquad (19)$$

Again, the integral of any monomial $\langle f(U) \rangle_U$ is aproximated up to the first *two* (leading and
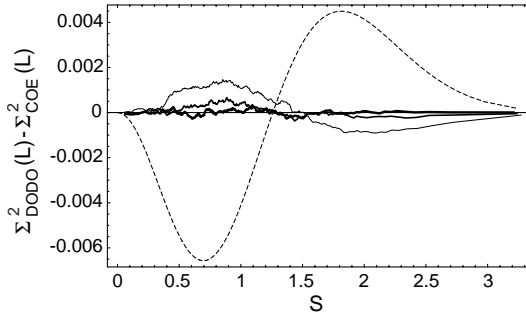
Fig. 2 – Deviation of the integrated level spacing distribution of DODO(N) from COE(N), $I_{\mathrm{DODO}(N)}(S) - I_{\mathrm{COE}(N)}(S)$, as determined by numerical simulations for $N = 25, 50, 100$ (thin, medium and thick curve, respectively). The deviation of the Wigner surmise from COE(∞) is shown by the dashed curve.

subleading) orders in $1/N$ by applying complex pairwise contraction rules to the polynomial $f(U)w_c(U)$. The results for the first two moments for DUDU are

$$K_{\mathrm{DUDU}}(1) = \frac{2N}{N+1} , \qquad K_{\mathrm{DUDU}}(2) = 2 - \frac{4}{N} + \mathcal{O}\left(\frac{1}{N^2}\right) . \qquad (20)$$

We have similarly calculated the leading and subleading terms for the COE and the CUE. The relevant matrices are represented as $U^T U$ and U, respectively. The results coincide with the leading terms of the $1/N$ expansion of the exact expressions.

Figure 1 shows that the DODO spectrum is less stiff than that of the COE. A corresponding statement applies to DUDU *vs.* CUE. The differences are caused by the Poissonian statistics of the phases η_k and ξ_a. To see this, we replace either of the two diagonal matrices D_1 and D_2 in eq. (1) by another diagonal matrix containing the eigenvalues of the COE (or of the CUE). It is straightforward to show that the resulting ensemble is identical to the COE (the CUE, respectively). In the opposite limit, we keep D_2 (Poissonian) and replace D_1 by diag$\{\exp[i\alpha n]\}$ (picket fence model). We denote the associated first moment by $K_{\mathrm{DODO}}^{\mathrm{p.f.}}(1)$. Averaging over ξ_n, summing over the n's, and calculating the averages of the O's with the help of the technique described above, we find

$$K_{\mathrm{DODO}}^{\mathrm{p.f.}}(1) = \sum_{m=1}^{N} \sum_{n=1}^{N} \exp[i\alpha(m-n)] \sum_{l=1}^{N} \langle O_{lm}^2 O_{ln}^2 \rangle_{\mathrm{O}} = \frac{2N}{N+2} + \frac{\sin^2(N\alpha/2)}{(N+2)\sin^2(\alpha/2)} . \qquad (21)$$

As we deal with a fourth-order monomial, this is an exact result. Equation (21) yields an interpolation for the long-range level statistics from the Poissonian value $K(1) = N$ (this applies in the limit of a degenerate spectrum where $\alpha = 0$) to the COE value $K_{\mathrm{COE}}(1) = 2N/(N+2)$ (with error $\mathcal{O}(1/N)$) when α becomes bigger than $2\pi/N$. This result suggests that DODO or DUDU provide a worst-case scenario for possible deviations from the canonical random matrix predictions of COE or CUE.

In summary, we have introduced random matrix ensembles for semi-separable systems. These allow us to understand why semi-separable systems follow the quantum chaos conjecture very closely, and to predict quantitatively the deviations. On scales L which are of the order of 10% of the spectral range N or less, the spectral fluctuations for each ensemble are very similar to those of the corresponding circular ensemble. Beyond this range, the deviations

reach values of up to 0.2 or so. On a relative scale, these deviations are small (we recall the logarithmic increase of Σ^2). On an absolute scale, they are not. Furthermore, they show a well-understood dependence on N.

In addition, we developed a promising novel way to perform the group integrals approximately in the limit of large matrix dimension N. Without excessive effort, this method improves the traditional Wick pair contraction technique and allows for the calculation of corrections in subleading order. It would be of interest to attain a deeper understanding of this procedure from a group-theoretical point of view.

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