

## Some properties of invariant random-matrix ensembles and their connection to ergodic and nonergodic Hamiltonian systems

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Standard random-matrix ensembles, for example, the well-known Gaussian ensembles, are constructed under the constraint of invariance under a canonical transformation, and have been generally developed as models for ergodic Hamiltonian systems. Herein, we consider invariant matrix ensembles that model the energy-level statistics of nonergodic systems, and contain the ergodic limit as a special case. After examining some properties of invariant matrix ensembles, we present numerical calculations of probability densities of matrix elements. We focus on the extreme case of an invariant ensemble yielding eigenvalues with Poisson statistics, i.e., level statistics of semiclassical, integrable Hamiltonians, from which we can determine essential differences between invariant ensembles modeling ergodic and nonergodic systems. The ensemble presented here is compared with a specific model Hamiltonian, whose degree of ergodicity is determined by variation of a single parameter. The model Hamiltonian is block diagonalized to an "ensemble" of small blocks for parameter values varied between the ergodic and nonergodic limits. Distributions of elements observed in the blocks are compared with those predicted by the matrix ensembles.

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### I. INTRODUCTION

The recognition that individual level assignments of nuclear spectra containing stretches of levels beginning at very large quantum numbers is a practical impossibility led to the development of the theory of spectral statistics. It was conjectured that the energy-level statistics of complex nuclear spectra could be predicted by those of an ensemble of random matrices, where each random element of any matrix is chosen from a Gaussian distribution [1]. Numerous level statistics of the Gaussian ensembles have been solved, notably the probability density of nearest-neighbor level spacings [2], which is nearly the same as that surmised by Wigner, closely matching the spacings observed in complex nuclear spectra. The same level spacings have been since observed in atomic [3] and molecular spectra [4], and the statistics of the Gaussian ensembles are now recognized as universal to spectra of ergodic Hamiltonian systems [5].

The Gaussian ensembles may be formulated by imposing two conditions on the matrix ensemble [1]: (1) that it be invariant under a canonical transformation, either orthogonal, unitary, or symplectic; and (2) that each matrix element be statistically independent from all the others. The first assumption amounts to choosing an ensemble of Hamiltonians independent of any particular representation. The second condition is one of convenience. Nevertheless, by only choosing condition (1), one may arrive at the level statistics of the Gaussian ensembles under quite general conditions. In a narrow range of energy where the local level density is constant, the level fluctuations found in the Gaussian ensembles are also found in invariant ensembles where the probability density of the matrix elements is not Gaussian [6,7]. This situation is, of course, desirable, since there is no physical basis for

supposing that the matrix elements of a Hamiltonian be independent.

Our purpose in this paper is to investigate invariant random matrix ensembles that predict energy-level statistics *different* from those of the Gaussian ensembles. Though we seek characteristics of invariant ensembles for arbitrary statistics, we focus on sequences of random levels, and also consider level statistics intermediate between random and those of the Gaussian ensembles. The reason to choose random level sequences is that these form an additional universality class, those of semiclassical, integrable Hamiltonians [8]. We seek, then, to understand differences between ensembles modeling entirely different physical systems, i.e., integrable and chaotic, or equivalently ensembles containing very different eigenvalue statistics, i.e., random and the highly correlated eigenvalues of the Gaussian ensembles. It should be noted that as opposed to ergodic Hamiltonian systems, a natural basis is known if the Hamiltonian is integrable, namely quantization of the classically invariant tori. In this basis, each member of the matrix ensemble contains random diagonal elements and all off-diagonal elements are 0. We may still ask, however, what the structure of a Hamiltonian would be without specifying the representation, and we do this in the following. In this way we also observe how representation-independent matrix element distributions change with transitions from random level sequences to those of the Gaussian ensembles, or as the level statistics change from those of integrable to those of ergodic systems.

Determination of matrix element distributions or even some of their lower moments based solely on the invariance condition and a general energy-level statistic, such as a random sequence or any other, is extremely difficult. Some general properties of invariant ensembles have been

derived, such as some correlations among matrix elements [9], and these will be summarized in the following section. To these we add the following observation for orthogonal ensembles. For  $\mathbf{H}$  a member of the orthogonal ensemble, and

$$V = 2H_{ij}, \quad D = H_{ii} - H_{jj}, \quad i \neq j, \quad (1)$$

we find  $P_V(V) = P_D(V)$ , where  $P_V$  and  $P_D$  are, respectively, the probability densities of  $V$  and  $D$ . This is easily shown for the two- and  $\infty$ -dimensional ensembles, and in the Appendix we show this relation to hold for ensembles of general dimension.

The corresponding relation for the unitary case is found by breaking up  $V$  into its real and imaginary parts. Calling the real part again  $V$  and the imaginary part  $U$ ,  $P_V(V) = P_U(V) = P_D(V)$ . As the orthogonal ensembles, corresponding to semiclassical Hamiltonians with time-reversal symmetry, apply to most problems of physical interest, our discussions and examples will largely focus on these rather than others, but generalizations to the unitary and symplectic cases are straightforward.

While we cannot express  $P_V(V)$  or, equivalently,  $P_D(D)$ , explicitly for general eigenvalue statistics and finite matrices, we obtain the densities  $P_V(V)$  numerically by exploiting the relation between matrix elements of  $\mathbf{H}$  and the statistical mechanics of its eigenvalues  $E_i$ . We may thereby apply efficient Monte Carlo procedures standardly employed in many-body statistical mechanics. We have chosen the well-known Metropolis method summarized in Sec. III, where we also give results of its application in determining  $P_V(V)$  for small-dimensional ensembles. As we shall see, for the matrix ensembles modeling nonergodic systems, matrix dimensions as small as 10 have distributions that are already quite close to Gaussian. In fact, the essential difference between invariant ensembles yielding level statistics of the Gaussian ensembles and those that do not is most easily seen in the probability density of all the matrix elements,  $P_H(\mathbf{H})$ , which contains singularities in the latter case, whereas it is smooth in the former.  $P_V(V)$ , obtained upon integrating out all matrix elements but one, can hardly be distinguished numerically among various large-dimensional invariant ensembles, differences from a Gaussian being very subtle.

We finally ask if the distributions so obtained are realized in actual Hamiltonians sharing the same eigenvalue statistics. To determine this, all representations of a semiclassical Hamiltonian that is, say, integrable would have to be considered, and this is of course not possible. Moreover, as remarked above,  $P_V(V)$  itself differs noticeably from a Gaussian only when the matrix dimensions are very small. Both of these restrictions may be avoided by block diagonalizing a Hamiltonian to an "ensemble" of very small blocks and analyzing  $P_V(V)$  over this ensemble. The effect of any one representation of  $\mathbf{H}$  will be minimized when  $\mathbf{H}$ , originally large, is block diagonalized to very small blocks. The smallness of the blocks, furthermore, allows us to examine if  $P_V(V)$  predicted in Sec. III is found in the specific case of a Hamiltonian matrix. The block-diagonalization procedure, its application to the quartic oscillator Hamiltonian, and comparisons with

theoretical  $P_V(V)$  are given in Sec. IV. In Sec. V we summarize our results.

## II. INVARIANCE CONDITION

Various consequences of imposing transformational invariance on a matrix ensemble were studied by Ullah and co-workers [9]. These led to conclusions concerning moments of the off-diagonal and diagonal matrix elements of a member of the ensemble  $\mathbf{H}$  and correlations among matrix elements, some of which we mention below. In determining these, one exploits the fact that  $P_H(\mathbf{H})$ , where the elements of  $\mathbf{H}$  are

$$H_{ij} = \sum_{\alpha} E_{\alpha} a_{\alpha i} a_{\alpha j}, \quad (2)$$

may be expressed in terms of the product of the probability density of the eigenvalues  $E_{\alpha}$  and eigenvectors  $\mathbf{a} = \{a_{\alpha j}\}$ , so that the joint density  $P_{E,\mathbf{a}}(\mathbf{E}, \mathbf{a})$  may be written  $P_E(\mathbf{E})P_{\mathbf{a}}(\mathbf{a})$ . This separability is a consequence of transformational invariance. The probability density of all the matrix elements of  $\mathbf{H}$  is found by integrating over all the  $a_{\alpha j}$ 's. One then has that  $P_H(\mathbf{H})$  is a function of the energies alone [1]

$$P_H(H_{11}, \dots, H_{dd}; \beta) = K_{\beta} \frac{P_E(E_1, E_2, \dots, E_d; \beta)}{\prod_{\substack{i,j=1 \\ i < j}}^n |E_i - E_j|^{\beta}}, \quad (3)$$

where the denominator is the Jacobi determinant,  $K_{\beta}$  is the normalization constant, and  $\beta$  represents the canonical group, and is 1, 2, or 4 for the orthogonal, unitary, or symplectic groups, respectively. The former two values are of most significance semiclassically, and will be the only ones considered explicitly in the examples that follow.  $\beta=1$  corresponds to Hamiltonians with time-reversal invariance and  $\beta=2$  to noninvariance.

To compute ensemble averages of products of individual elements of  $\mathbf{H}$ , one needs to return to Eq. (2) and, noting the independence of  $E_{\alpha}$  and  $a_{\alpha i}$ , calculate expressions such as

$$\begin{aligned} \langle H_{ij} H_{kl} \dots \rangle &= \sum_{\alpha_1, \alpha_2, \dots=1}^d \langle E_{\alpha_1} E_{\alpha_2} \dots \rangle \\ &\quad \times \langle a_{\alpha_1 i} a_{\alpha_1 j} a_{\alpha_2 k} a_{\alpha_2 l} \dots \rangle, \end{aligned} \quad (4)$$

so that what is needed in addition to averages of products of eigenvalues is averages of products of eigenvectors. The latter is obtained from the probability density of products of eigenvector components, for which Ullah obtained expressions for products of up to two eigenvectors, more being exceedingly difficult to calculate [9]. Using these he showed, for example, that all odd moments of  $P_H(H_{ij})$ ,  $i \neq j$ , are 0, so that  $P_H(H_{ij})$  is a symmetric function. From definition (1), we see that both  $P_V$  and  $P_D$

have vanishing odd moments. Another conclusion reached by Ullah is that there are no correlations between an odd power of  $H_{ij}$ ,  $i \neq j$ , and any power of any other element of  $\mathbf{H}$ .

To look more closely at the relation between  $V$  and  $D$  of Eq. (1), we turn to Eq. (3) for orthogonal ensembles,  $\beta=1$ . For  $d=2$ , we define  $S=E_2-E_1$  and set the trace to 0 since it is irrelevant to what follows. Then, since  $S^2=V^2+D^2$ ,  $P_{V,D}(V,D)$  reads as

$$P_{V,D}(V,D;\beta=1) = \frac{1}{2\pi} \frac{P_S(\sqrt{V^2+D^2})}{\sqrt{V^2+D^2}}. \quad (5)$$

$P_V(V)$  [ $P_D(D)$ ] is found by integrating Eq. (5) over  $D$  ( $V$ ), and due to the symmetry of  $V$  and  $D$  in (5), it is clear that  $P_V(V)=P_D(D)$  for  $V=D$ .

In the same way, one finds that  $P_V(V)=P_D(D)=P_U(U)$  for the  $d=2$  unitary ensembles, as mentioned in the Introduction, where  $V$  and  $U$  are, respectively, the real and imaginary parts of  $2H_{ij}$ . Then

$$P_{V,U,D}(V,U,D;\beta=2) = \frac{1}{4\pi} \frac{P_S(\sqrt{V^2+U^2+D^2})}{V^2+U^2+D^2}. \quad (6)$$

For the infinite-dimensional case, we observe that while there are  $O(d^2)$  elements in  $\mathbf{H}$ , there are at most  $O(d)$  constraints, so that Eq. (3) approaches the limit of a product of independent Gaussians as  $d \rightarrow \infty$ . Then again  $V(U)$  and  $D$  are described by the same probability density, as this is the case for the Gaussian ensembles [1].

In the Appendix, we show that  $P_V(V)=P_D(D)$ , where  $V=D$  for any  $d$ -dimensional ensemble.

### III. DISTRIBUTIONS OF MATRIX ELEMENTS

It is useful to rewrite  $P_H$  given by Equation (3) to read as

$$P_H(\mathbf{H};\beta) = K_\beta e^{-\beta W}, \quad (7a)$$

$$W = -\ln[f_E(\mathbf{E})] + \sum_{\substack{i,j \\ i < j}}^d \ln|E_i - E_j|, \quad (7b)$$

where  $f_E(\mathbf{E})=[P_E(\mathbf{E})]^{1/\beta}$ . Then,  $P_H(\mathbf{H};\beta)$  has the form of a Boltzmann distribution with potential  $W$  and inverse temperature proportional to  $\beta$ . Equation (7) is analogous to the statistical mechanics introduced by Dyson [10] for the energy-level distributions of the circular and Gaussian ensembles.

For the Gaussian ensembles, the probability density of the energies is

$$P_E(E_1, \dots, E_n; \beta) \propto \exp \left[ -\beta \sum_i (E_i - E_c)^2 \right] \times \prod_{\substack{i,j \\ i < j}} |E_i - E_j|^\beta, \quad (8)$$

where  $E_c$  is a parameter fixed for the ensemble; then  $P_H(\mathbf{H};\beta)$  is, of course, just the product of independent Gaussians. Defining  $E_c$  instead to be a variable such that  $E_c=(1/N)\sum_i E_i$ ,  $P_E$  is the probability density derived by Yukawa [11] for the case of a strongly perturbed Hamil-

tonian. The overall level density is constant rather than semicircular as in the Gaussian ensembles. Nevertheless, the local level statistics are identical in both cases. In fact, investigations have shown that by replacing the exponential in (8) with a variety of smooth functions, the level statistics of the Gaussian ensembles are obtained in flat regions of the energy density [6]. The implication is that these statistics are universal when  $\beta W$  in (7a) is a smooth function of the energies, and this has indeed been rigorously shown to be the case [7].

Now consider  $P_E$  such that the levels form a random sequence described by Poisson statistics. We constrain the levels to have a constant mean density over the whole sequence, allow them unlimited range, and so choose

$$P_E \propto e^{-\beta \Delta E_d}, \quad (9a)$$

where  $\Delta E_d$  is the energy difference between the highest and lowest eigenvalues of a matrix. The potential in (7a) is then

$$W = \Delta E_d + \sum_{\substack{i,j \\ i < j}}^d \ln|E_i - E_j|, \quad (9b)$$

which is logarithmic and pairwise *attractive*, having a "minimum" where all the energies are identical,  $E_1=E_2=\dots=E_d=E$ , corresponding to a matrix  $\mathbf{H}$  with elements  $H_{ij}=0$  and  $H_{ii}=H_{jj}$  for all  $i$  and  $j$ .

Although the invariant ensembles are defined by discrete values of  $\beta$ , it is of interest to consider the limits  $\beta=0$  and  $\beta \rightarrow \infty$ . In doing so, we take the ensemble to be defined by a single canonical group, e.g., orthogonal. Then using (7a) and (9b), we consider how the orthogonal ensemble  $P_H(\mathbf{H};\beta)$  varies with  $\beta$ . At  $\beta \rightarrow \infty$  (0 temperature),  $P_H(\mathbf{H};\infty)$  lies at the minimum of the potential, so that  $P(H_{ij};\infty)=\delta(H_{ij})$  for  $i \neq j$ , and  $P(H_{ii};\infty)=\delta(E-H_{ii})$ . In the other limit,  $\beta=0$ ,  $P_H(\mathbf{H};0)$  is independent of the energies, and the singularities in  $W$  are irrelevant so that the statistics of the Gaussian ensembles are obtained in this limit. If one further constrains the eigenvalues to lie in the range  $-1 \leq E_i \leq 1$ , the orthogonal  $P_H(\mathbf{H};0)$  is identical to the Legendre ensemble proposed by Leff [6a], who showed that the local eigenvalue statistics of the latter are the same as those of the Gaussian orthogonal ensemble. From this perspective, the parameter  $\beta$  may be thought of as a continuous variable that determines the statistical properties of a particular invariant ensemble, i.e., an ensemble selected to be invariant under one of the three canonical groups. In this way,  $\beta$  is analogous to the Brody parameter for the spacings distribution of orthogonal ensembles [13].

Having defined by Eqs. (7) and (9) an invariant ensemble that produces random level sequences, i.e., the level statistics of semiclassical, integrable Hamiltonians, we now wish to examine the distribution of matrix elements of  $\mathbf{H}$ . Besides providing a description of the transition from ensembles of matrices yielding Poisson statistics to those of the Gaussian ensembles, the formulation of  $P_H(\mathbf{H})$  in terms of a Boltzmann distribution offers a convenient framework to employ numerical methods com-

monly applied to many-body statistical mechanics problems. We will do this for general dimension  $d$ . However, for  $d=2$  we may use (5) to get an explicit expression for  $P_V(V)$  for the orthogonal ensemble, and a corresponding expression for the unitary case, and we do this first.

For 2 random levels and unit mean spacing,

$$P_S(S) = e^{-S}. \quad (10)$$

Since  $S^2 = V^2 + D^2$ , integrating (5) and (10) over  $D$  yields

$$P_V(V; \beta=1) = \frac{1}{\pi} K_0(|V|), \quad (11)$$

where  $K_0$  is a modified Bessel function. For the unitary ensemble,  $P_V(V)$  is obtained after integration of (6) and (10) over  $D$  and  $U$ .

The expressions  $P_V(V)$  for both the  $d=2$  orthogonal and unitary ensembles given by Eq. (11) and integration of (6) using (10), respectively, are plotted in Fig. 1(a). From the dependence of  $P_H(\mathbf{H}; \beta)$  on  $\beta$  for a fixed  $d$ , we expect that at higher  $\beta$ , or lower temperatures,  $P_V(V)$  will be more peaked near  $V=0$ , i.e., lie more around the potential minimum, than at lower  $\beta$ . We observe this to be the case in Fig. 1(a), where  $P_V(V)$  of the unitary en-

semble is clearly more sharply peaked around  $V=0$  than is the orthogonal expression (11), as expected from the discussion above. In both cases,  $P_V(0)$  is singular. From Eq. (11), one finds that the  $d=2$  orthogonal ensemble approaches the singularity at  $V=0$  logarithmically. The same is true for the unitary ensemble, as one finds by integrating (6) and (10) at  $V=0$ .

For  $d > 2$ , we turn to the Metropolis Monte Carlo method [12] referred to above. We seek the equilibrium distribution of matrix elements of  $\mathbf{H}$  that satisfies the equilibrium distribution (7a) with potential  $W$  given by (9) (or more generally any  $W$ ), starting with some trial distribution of  $\mathbf{H}$ . So that the initial distribution converges to equilibrium, the Metropolis method imposes the detailed balance condition [12]

$$P_{\text{eq}}(H_{ij})T(H_{ij} \rightarrow H'_{ij}) = P_{\text{eq}}(H'_{ij})T(H'_{ij} \rightarrow H_{ij}), \quad (12)$$

where  $T(H_{ij} \rightarrow H'_{ij})$  is the transition probability from  $H_{ij}$  to  $H'_{ij}$ . Defining  $\delta W = W(H'_{ij}) - W(H_{ij})$ , the transition probability  $T$  is satisfied by [12]

$$T(H_{ij} \rightarrow H'_{ij}) = \begin{cases} \exp(-\beta\delta W) & \text{if } \delta W > 0 \\ 1, & \text{otherwise.} \end{cases} \quad (13)$$

Equation (13) means that a randomly selected value of  $H'_{ij}$  is always accepted if  $\delta W \leq 0$ . It is sometimes accepted if  $\delta W > 0$ , and its probability of acceptance in this case is given by  $P_T = \exp(-\beta\delta W)$ . Selecting a random number  $r$  between 0 and 1, we accept  $H'_{ij}$  if  $P_T \geq r$  and do not otherwise, in which case we keep the old value  $H_{ij}$ . This process is repeated over and over for each element of the matrix, until convergence to equilibrium is established. In practice, we have needed to select  $O(10^6)$  random elements to obtain  $P_V(V)$  for the small- $d$  ensembles.

In Fig. 1(b) we plot  $P_V(V)$  obtained from the Metropolis method for the orthogonal ensemble with Poisson level statistics and  $d=2, 3, 4, 5$ , and 10, along with a Gaussian function.

As mentioned above, the  $d=2$  expression for  $P_V(V)$  has a logarithmic singularity at  $V=0$ , which we know from the form of Eq. (11) near  $V=0$ . In Fig. 1(b), it appears that  $P_V(0)$  is nonsingular but also nonanalytic, and we conjecture that  $P_V(V)$  is nonanalytic at  $V=0$  for general  $d$ . Our ability to describe  $P_V(V)$  in the neighborhood of  $V=0$  for general  $d$  is limited by the range of  $V$  over which the Monte Carlo results are binned, or  $dV$ . [In Fig. 1(b),  $dV$  is 0.1 in units of the standard deviation.] Thus, the fact that  $P_V(V)$  for  $d=10$  appears everywhere smooth can be attributed to numerical smoothing over the interval  $dV$ .

In addition to the smooth appearance of the  $d=10$  curve plotted in Fig. 1(b), it also looks very much like the Gaussian superimposed in the figure. Even for a matrix ensemble producing very different level statistics than that of the Gaussian ensembles, i.e., random levels with Poisson statistics, the matrix elements appear to arise from a Gaussian distribution for even relatively small-dimensional ensembles. This is deceptive, because  $dV$  is too large to observe the precise form at  $V=0$ , as discussed above. On the other hand, it is important to real-

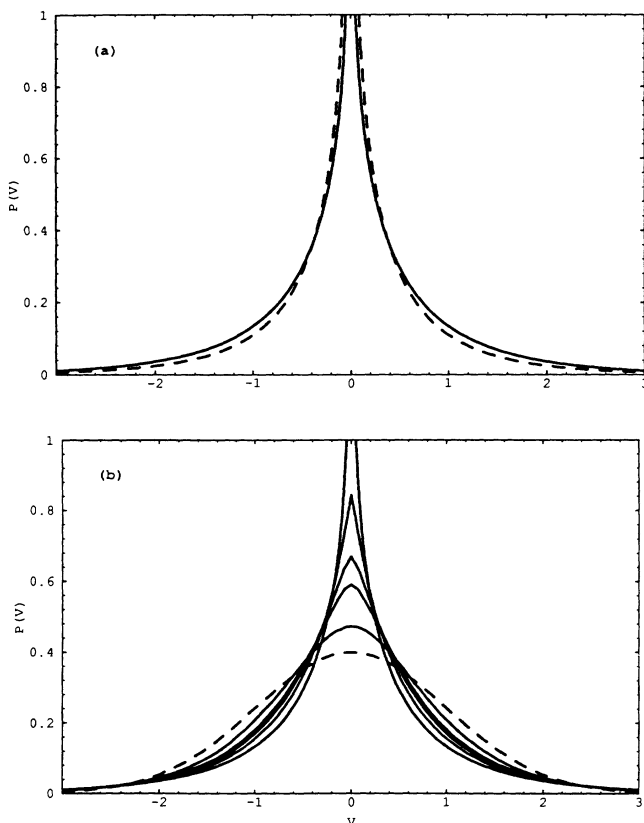


FIG. 1. (a)  $P_V(V; \beta=1)$  (solid curve) and  $P_V(V; \beta=2)$  (dashed curve) for  $d=2$  ensemble, given by Eq. (11) and integration over (6) using (10), respectively; (b)  $P_V(V; \beta=1)$  for ensemble containing eigenvalues with Poisson statistics, in units of the standard deviation. The full curves from top to bottom are the distributions for matrix dimensions 2, 3, 4, 5, and 10, respectively. The dashed curve is Gaussian.

ize, since if we try to observe any differences between matrix element distributions of Hamiltonians whose eigenvalue statistics are Poisson and those of the Gaussian ensembles, we can only do this if the Hamiltonian is transformed to small blocks. This we do in the following section.

Before turning to the block diagonalization of a model Hamiltonian, we mention that the above discussion and examples of matrix ensembles whose eigenvalues are random, can be carried over straightforwardly to any eigenvalue statistics. The probability density of the eigenvalues, and hence  $W$ , would be selected appropriately, and the above methods are, of course, still valid. As the eigenvalue statistics approach those of the Gaussian ensembles, we expect  $P_V(V)$  to look even more Gaussian for even smaller  $d$  than those just shown for the random level case. This may be illustrated by simply looking at  $d=2$ , for which the most dramatic differences between general invariant ensembles and the Gaussian ensembles can be observed. Instead of choosing  $P_S(S)=e^{-S}$  in Eq. (5), we could, for example, choose  $P_S(S)$  to be the Brody distribution [13]

$$P_S(S; \omega) = (1 + \omega) \alpha S^\omega \exp(-\alpha S^{1+\omega}), \quad (14)$$

$$\alpha = \Gamma \left[ \frac{2 + \omega}{1 + \omega} \right]^{1 + \omega}.$$

Equation (14) interpolates between level statistics that are Poisson ( $\omega=0$ ) and those of the  $d=2$  Gaussian orthogonal ensemble ( $\omega=1$ ), the latter being the Wigner distribution. Combining Eqs. (5) and (14), we find that  $P_V(0)$  is singular for  $\omega=0$ , finite but nonanalytic for  $0 < \omega < 1$ , and analytic only in the GOE limit,  $\omega=1$ . For general  $\omega$ , one finds  $P_V(0) \propto \Gamma(\omega/\omega+1)$ . Examples of intermediate level statistics using the Brody distribution will be given in the next section, together with results of the block-diagonalized quartic oscillator Hamiltonian.

#### IV. BLOCK DIAGONALIZATION

To make contact with a Hamiltonian system, we consider the relation of a model Hamiltonian to the ensemble defined above. For many physical Hamiltonians and typical bases, the structure of a semiclassical Hamiltonian is banded in the sense that elements generally become smaller the further they are from the diagonal [14]. Such representations are not typical members of the ensemble. Therefore, to compare the elements of the model Hamiltonian with those of the ensemble, we must reduce the effect of the particular representation as much as possible, as well as keep to small matrices, for which clear differences in the matrix element distributions can be observed for ensembles containing different energy-level statistics, describing different degrees of ergodicity. We accomplish both by transforming a large Hamiltonian in a given basis to block-diagonal form, and comparing the distribution of elements in the  $d$ -dimensional blocks, where  $d$  is small, to those of the  $d$ -dimensional random matrix ensemble plotted in Fig. 1(b).

The model Hamiltonian is the coupled quartic oscillator,

$$H = (p_x^2 + p_y^2 + x^4 + y^4)/2 - kx^2y^2. \quad (15)$$

For  $k=0$ , the Hamiltonian is integrable, and the energy-level statistics have been observed to be Poissonian. The minimum value of  $k$  for which this Hamiltonian is strongly chaotic has been determined numerically, and is around 0.6 [15]. For  $0 < k < 0.6$ , the classical phase space is described by chaotic regions separating regions of regular dynamics, and the energy-level statistics are intermediate between Poisson and those of the GOE [15b].

We represent  $\mathbf{H}$  in a basis of coupled harmonic oscillators and  $A_1$  symmetry. In this basis,  $\mathbf{H}$  given by (15) is banded about the diagonal, and for no value of  $k$  does it appear as a representative member of any of the matrix ensembles discussed above.

The matrix  $\mathbf{O}$  that transforms  $\mathbf{H}$  to block-diagonal form  $\mathbf{H}_{BD}$  is uniquely defined by the condition  $\|\mathbf{O} - 1\| = \text{minimum}$  [16], which means that one block-diagonalizes  $\mathbf{H}$  in such a way that it remains as close as possible to its original representation. If  $\mathbf{S}$  is the matrix of eigenvectors of  $\mathbf{H}$ , and  $\mathbf{S}_{BD}$  the matrix containing the block-diagonal part of  $\mathbf{S}$ , then

$$\mathbf{O} = \mathbf{S} \mathbf{S}_{BD}^{\alpha\dagger} (\mathbf{S}_{BD}^\alpha \mathbf{S}_{BD}^{\alpha\dagger})^{-1/2}. \quad (16)$$

A given block of  $\mathbf{H}_{BD}$  labeled by  $\alpha$  will be determined by

$$\mathbf{H}_{BD}^\alpha = \mathbf{O}^{\alpha\dagger} \mathbf{E}^\alpha \mathbf{O}^\alpha, \quad (17)$$

$$\mathbf{O}^\alpha = \mathbf{S}_{BD}^{\alpha\dagger} (\mathbf{S}_{BD}^\alpha \mathbf{S}_{BD}^{\alpha\dagger})^{-1/2},$$

where  $\mathbf{E}^\alpha$  contains the  $d$  eigenvalues of block  $\alpha$ . The blocks of the transformed  $\mathbf{H}$  are members of the ensemble which we now study and compare with the ensemble discussed in the previous sections. In determining  $P_V(V)$  of the blocks, it is important to account for variation of the level density. Thus, in the process of block diagonalization, we “unfold” the eigenvalues of  $\mathbf{H}$  so that the mean spacing is 1. The following results come from matrices of dimension 2000, and energy levels between 200 and 800.

Figure 2 shows  $P_V(V)$  for two values of  $k$  in Eq. (15).

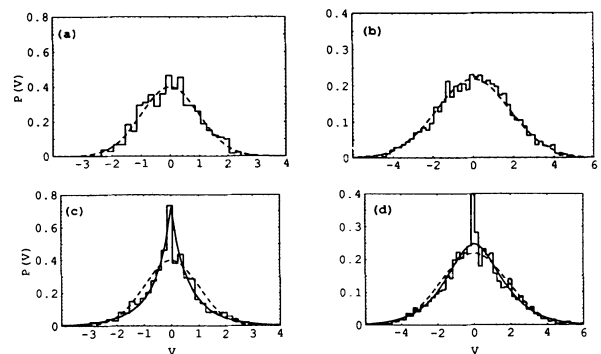


FIG. 2.  $P_V(V)$  for the  $d$ -dimensional blocks of the transformed Hamiltonian (15); (a)  $k=0.6$ ,  $d=3$ ; (b)  $k=0.6$ ,  $d=10$ ; (c)  $k=0.0$ ,  $d=3$ ; (d)  $k=0.0$ ,  $d=10$ . The dashed curves are Gaussians, theoretical forms for the data in (a) and (b). The solid curves in (c) and (d) are predictions from the ensemble containing random eigenvalues. The size of the matrix elements is fixed by the local mean level spacing, here set to unity.

$k=0.0$  and  $0.6$ , representing the integrable and ergodic limits, respectively. The level spacing distribution at  $k=0.6$  fits the Wigner distribution, and we thus expect the matrix elements to be distributed as a Gaussian, at least for small blocks. It is not obvious, however, that this expectation should be fulfilled for large blocks, since then the specific representation of  $\mathbf{H}$  appears, which in this case is very structured and nothing like the independent matrix element assumption taken for the Gaussian ensembles. We nevertheless observe in Fig. 2 that the Hamiltonian (15) expressed in a basis of coupled harmonic oscillators can be transformed to at least ten-dimensional blocks and the distribution of the matrix elements is very close to Gaussian.

For  $k=0$ , the Hamiltonian (15) is integrable and the eigenvalue statistics are Poissonian. It is for this value of  $k$ , then, that we can compare  $P_V(V)$  of the ensemble of blocks with that generated in Sec. III for various  $d$ . We do this in Figs. 2(c) and 2(d) for  $d=3$  and  $10$ , respectively. From 2(c), we observe that the resemblance of the empirical distribution to the theoretical distribution for  $d=3$  is unambiguous, and clearly different from the Gaussian, which we obtained for  $k=0.6$  [Fig. 2(a)]. This result extends that found previously for  $d=2$ , for which agreement between the empirical and theoretical distributions is also excellent [17]. For  $d>3$ , we have found empirical  $P_V(V)$  to also remain very close to the theoretical curves, with the only exception being that  $P_V(0)$  is always larger than in theory, the discrepancy growing with  $d$ . This trend is evident in Fig. 2(d), which shows  $d=10$ , where the empirical result is indeed very close to what we expect, even following the minor differences from the superimposed Gaussian. The most apparent difference from theory is the very large  $P_V(0)$ , which we would expect to be smoothed away over the bin size used in our study. That we do observe some discrepancy would, however, have to be expected, and reflects the particular basis that we chose, which is particularly suitable for describing the integrable Hamiltonian.

Finally, we consider cases between the universal regimes, i.e., level-spacing statistics that are distributed between the limits of Poisson and Gaussian ensemble statistics. As discussed at the end of Sec. III, we may define a two-dimensional ensemble straightforwardly by using a spacings distribution that interpolates between the Poisson and Wigner limits, and we have chosen the Brody distribution, which, though *ad hoc*, fits the level-spacings distribution of a variety of semiclassical spectra satisfactorily. Using Eqs. (5) and (14), and integrating over  $D$ , we have a form for  $P_V(V)$  which may be compared with that of Hamiltonian (15) block diagonalized to an ensemble of two-dimensional blocks. We have done this for  $k=0.2$  and  $0.3$ , and the empirical  $P_V(V)$  is plotted in Fig. 3. From the level-spacings distribution of the eigenvalues of  $\mathbf{H}$  at these two values of  $k$ , we find  $\omega$  in (14) to be  $0.42$  and  $0.57$  for  $k=0.2$  and  $0.3$ , respectively. Using these values of  $\omega$ , we superimpose theoretical  $P_V(V)$  in Fig. 3. The trend in  $P_V(0;\omega)$  with increasing  $\omega$ , predicted at the end of Sec. II, is clearly seen here, namely the approach from a singularity at  $\omega=0$  to always smaller values as

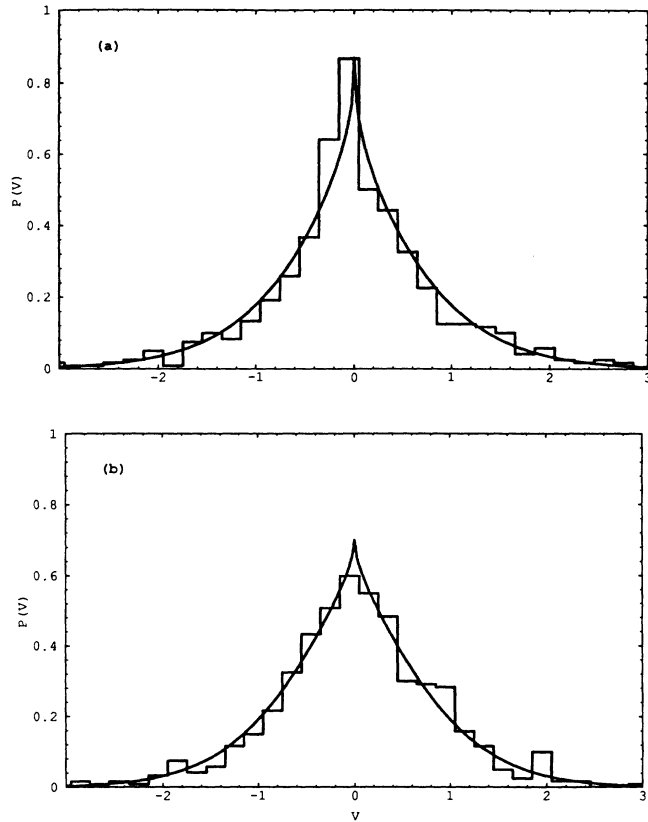


FIG. 3. Same as Fig. 2, but with (a)  $k=0.2$ ,  $d=2$ ; (b)  $k=0.3$ ,  $d=2$ . The superimposed theoretical curves are from Eqs. (5) and (14) with (a)  $\omega=0.42$  and (b)  $\omega=0.57$ , obtained by fitting Eq. (14) to the empirical level-spacings distribution of cases (a) and (b).

$\omega \rightarrow 1$ . Agreement between the theoretical curves and the data is seen to be very good in both cases.

## V. CONCLUSIONS

We have constructed random matrix ensembles that are independent of any representation, and contain eigenvalue statistics of nonergodic Hamiltonian systems. Among our aims has been to study the distribution of matrix elements of members  $\mathbf{H}$  of the ensemble, and we found we could do this by defining a single distribution  $P_V(V)$ , where  $V=2H_{ij}$  for orthogonal ensembles, and may easily be generalized to unitary as discussed above. The relation to the diagonal matrix elements comes from defining  $D=H_{ii}-H_{jj}$ , and the observation that  $P_V(V)=P_D(D)$  for  $V=D$ , shown in the Appendix.

The numerical method we use to construct  $\mathbf{H}$  and observe  $P_V(V)$  is the Metropolis Monte Carlo procedure that is standardly used in many-body statistical mechanics. We may adopt this due to the appearance of  $P_H(\mathbf{H})$  as a Boltzmann equation with potential  $W$  that determines the eigenvalue statistics of the ensemble. The “temperatures” are inversely related to the canonical

transformation group of the ensemble  $\beta$ . In selecting  $W$  such that the eigenvalues of the ensemble are random, it contains the Poisson level statistics of semiclassical, integrable Hamiltonians.

As is now well established, a sufficient criterion for obtaining eigenvalue statistics of the Gaussian ensembles from an invariant ensemble is that  $P_H(\mathbf{H})$  and the eigenvalue density be smooth. We therefore expect that an invariant ensemble containing completely random eigenvalues must be defined with a  $P_H(\mathbf{H})$  that is somewhere non-analytic, and this is clear from the definition of Eqs. (7) and (9). What is surprising to us is that the singular function  $P_H(\mathbf{H})$  yields  $P_V(V)$  that converges rapidly to a Gaussian with matrix dimension, where the essential difference from a Gaussian can be seen only very close to  $V=0$ . Figure 1 illustrates how rapid the convergence is, where we see the close resemblance to a Gaussian already at  $d=10$ . Differences would be found near  $V=0$ , where cusps observed at smaller  $d$  are numerically smoothed away at  $d=10$ .

We also explored the relation between a ‘‘typical’’ Hamiltonian system and the ensemble by representing a model Hamiltonian in block-diagonal form, and compar-

ing the distributions of the matrix elements in the blocks with those expected from the ensemble. The distributions in the blocks compare well with those of the matrix ensemble, though departing somewhat and not unexpectedly as the block dimension increases, due to the influence of the particular representation of the Hamiltonian.

An open problem arising from this study is to describe  $P_V(V)$  [ $P_D(D)$ ] in the neighborhood of  $V=0$  ( $D=0$ ). We have done this above for  $d=2$ , where we found in general a nonanalytic point at  $V=0$ , except for the Gaussian ensembles. For  $d=2$  invariant ensembles containing Poisson level statistics, this nonanalytic point is a logarithmic singularity. The numerical studies presented herein strongly suggest that  $P_V(0)$  is nonanalytic for general  $d$ , and an analytical investigation would be desirable.

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#### APPENDIX

We show here that  $P_V(V)=P_D(V)$ , where  $V$  and  $D$  are defined by Eq. (1). In terms of eigenvalues  $E_\alpha$ , and eigenvectors  $\mathbf{a}$  and  $\mathbf{b}$ , we may write  $V$  and  $D$  as

$$V=2 \sum_{\alpha} E_{\alpha} a_{\alpha} b_{\alpha} , \quad (\text{A1})$$

$$D = \sum_{\alpha} E_{\alpha} (a_{\alpha}^2 - b_{\alpha}^2) . \quad (\text{A2})$$

Then their respective probability densities  $P_V$  and  $P_D$  are

$$P_V(V) = \int \prod_{\alpha} da_{\alpha} db_{\alpha} dE_{\alpha} P_E(\dots, E_{\alpha}, \dots) \delta \left[ V - 2 \sum_{\alpha} E_{\alpha} a_{\alpha} b_{\alpha} \right] \delta(\mathbf{a} \cdot \mathbf{b}) \delta(1 - \mathbf{a} \cdot \mathbf{a}) \delta(1 - \mathbf{b} \cdot \mathbf{b}) , \quad (\text{A3})$$

$$P_D(D) = \int \prod_{\alpha} da_{\alpha} db_{\alpha} dE_{\alpha} P_E(\dots, E_{\alpha}, \dots) \delta \left[ D - E_{\alpha} (a_{\alpha}^2 - b_{\alpha}^2) \right] \delta(\mathbf{a} \cdot \mathbf{b}) \delta(1 - \mathbf{a} \cdot \mathbf{a}) \delta(1 - \mathbf{b} \cdot \mathbf{b}) , \quad (\text{A4})$$

where the last three  $\delta$  functions in (A3) and (A4) impose orthogonality of  $\mathbf{a}$  and  $\mathbf{b}$ , normalization of  $\mathbf{a}$ , and normalization of  $\mathbf{b}$ , respectively. We define vectors  $\mathbf{a}'$  and  $\mathbf{b}'$  as

$$\mathbf{a}' = \frac{1}{\sqrt{2}} (\mathbf{a} + \mathbf{b}) , \quad (\text{A5})$$

$$\mathbf{b}' = \frac{1}{\sqrt{2}} (\mathbf{a} - \mathbf{b}) , \quad (\text{A6})$$

Then

$$\prod_{\alpha} da_{\alpha} db_{\alpha} \rightarrow \prod_{\alpha} da'_{\alpha} db'_{\alpha} , \quad (\text{A7})$$

$$\delta(\mathbf{a} \cdot \mathbf{b}) \delta(1 - \mathbf{a} \cdot \mathbf{a}) \delta(1 - \mathbf{b} \cdot \mathbf{b}) \rightarrow \delta(\mathbf{a}' \cdot \mathbf{b}') \delta(1 - \mathbf{a}' \cdot \mathbf{a}') \delta(1 - \mathbf{b}' \cdot \mathbf{b}') , \quad (\text{A8})$$

since  $\mathbf{a}$  and  $\mathbf{b}$  have been simply rotated in the  $ab$  plane by  $\pi/4$ . Substituting  $2a'_{\alpha}b'_{\alpha}$  for  $(a_{\alpha}^2 - b_{\alpha}^2)$  in (A4), and using (A7) and (A8), the integral on the right-hand side becomes identical to the integral on the right-hand side of (A3), so that  $P_V(V)=P_D(V)$ .

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