

Statistical Theory of Energy Levels and Random Matrices in Physics

M. Carmeli¹

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In this paper the physical aspects of the statistical theory of the energy levels of complex physical systems and their relation to the mathematical theory of random matrices are discussed. After a preliminary introduction we summarize the symmetry properties of physical systems. Different kinds of ensembles are then discussed. This includes the Gaussian, orthogonal, and unitary ensembles. The problem of eigenvalue-eigenvector distributions of the Gaussian ensemble is then discussed, followed by a discussion on the distribution of the widths. In the appendices we discuss the symplectic group and quaternions, and the Gaussian ensemble in detail.

KEY WORDS : Random matrices; eigenvalues; multivariate analysis; distributions; energy levels; nuclear physics; statistical theory; ensembles.

1. INTRODUCTION

Within the theory of quantum mechanics⁽¹⁾ the behavior of a physical system is determined by a state function Ψ . The state function is a solution of the familiar Schrödinger equation,

$$H\Psi = E\Psi \quad (1)$$

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¹ Department of Physics, University of Negev, Beer Sheva, Israel.

where H is the Hamiltonian operator, a Hermitian operator, and E is a constant which denotes the energy levels of the system. Thus the energy levels are characteristic values (eigenvalues, or roots) of Hermitian operators. The stationary states of the system are the corresponding characteristic vectors (or eigenfunctions).

Although theoretical analyses have had impressive success^(2,3) in interpreting the detailed structure of the *low-lying* excited states of complex systems,² still, there must come a point beyond which such analyses of individual levels cannot usefully go.⁽⁴⁾ For example, observations of levels of heavy nuclei in the neutron-capture region⁽⁵⁾ give exact information on the energy levels from number N to number $N + n$, where n is an integer of the order of 100 whereas N is an integer of the order of one million. It appears improbable that energy level assignments, based on various models, can ever be pushed as far as the millionth level.

One is then led to ask whether the highly excited states may be understood from the opposite point of view, by assuming no structure for the system and that no quantum numbers other than spin and parity remain good. Such an inquiry leads to a *statistical theory of energy levels*.

Such a statistical theory is not supposed to predict the detailed sequence of energy levels in any one nucleus or atom, but is expected to describe the general appearance and the degree of irregularity of the level structure that is to occur in a complex system which is otherwise too complicated to be understood in detail.

As Dyson has pointed out,⁽⁴⁾ in ordinary statistical mechanics a comparable renunciation of exact knowledge about the system is also made. By assuming that all states of a very large ensemble are equally probable, one obtains useful information about the overall behavior of a complex system when the observation of the state of the system in all its detail is impossible. This standard type of statistical mechanics is clearly inadequate for the discussion of energy levels. What one wishes is to make statements on the fine detail of the energy level structure, and such statements cannot be made in terms of an ensemble of states. What is required is a *different* kind of statistical mechanics in which one renounces exact knowledge *not* of the state of a system but of the *nature* of the system itself. One might picture a complex nucleus as a "black box" in which a large number of particles are interacting according to unknown laws. The problem then is to define in a mathematically precise way an ensemble of systems in which all possible laws of interaction are equally probable. The idea of a statistical mechanics of nuclei based on an ensemble of systems is due to Wigner.

² The word system is used for a physical quantum system that can be described by the Schrödinger equation. A system could be, for example, a complex nucleus, as is discussed in Refs. 2 and 3, or an atomic system.

The difference between the usual statistical mechanics and the statistical theory of energy levels can also be seen, according to Wigner, as follows.⁽⁶⁾ A system in quantum mechanics can be characterized by the Hamiltonian H , which is a self-adjoint linear operator in the infinite-dimension Hilbert space of functions Ψ . If one introduces a coordinate system in the Hilbert space, the Hamiltonian operator may then be looked at as a Hermitian matrix of infinitely many dimensions. Therefore, an ensemble of systems can be considered as an ensemble of Hermitian matrices. At this stage one might consider matrices of very high dimensionality rather than infinite matrices. However, the question arises as to what ensemble of such matrices one has to consider. Herein lies the difference between the ensembles of statistical mechanics and the ensemble of the statistical theory of energy levels.

In statistical mechanics one considers a system of particles with definite masses interacting among themselves by a given law. The state of such a system can be specified, in classical mechanics, by the generalized coordinates q_i and the generalized momenta p_i of the particles, where both q_i and p_i are functions of time. The physical quantities one is then interested in are the time averages of continuous functions f of the coordinates and momenta,

$$\lim_{T \rightarrow \infty} (1/T) \int_t^{t+T} f(q_1(\tau), q_2(\tau), \dots, p_1(\tau), p_2(\tau), \dots) d\tau \quad (2)$$

Using Newton's law of motion, one can, in principle, determine the coordinates and momenta as functions of time and their initial values (see, e.g., Ref. 7). Hence the averaging process is an entirely *definite* one, and the result is a function only of the constants of motion, such as energy, but independent of other initial conditions. This result, except for rare cases, has long been proved and known by von Neumann and others.⁽⁸⁻¹²⁾

The averaging process in the theory of random processes, on the other hand, is *not* defined. One again deals with a specific system with its proper, though in many cases unknown, Hamiltonian and pretends that one deals with a multitude of systems, all with their own Hamiltonians, and averages over the properties of these systems. Such a procedure can be meaningful only if it turns out that the properties in which one is interested are the same for the vast majority of the admissible Hamiltonians. What are the admissible Hamiltonians, and what is the proper measure in the ensemble of these Hamiltonians? And suppose the ensemble of admissible Hamiltonians with a proper measure is given. Are the properties in which we are interested common for the vast majority of them?

Figures 1-3 illustrate the situation which leads to the idea of the statistical properties of the spectrum in the higher-energy region, as compared to low-energy region, where one desires to have a rather complete description

of the stationary states and as complete a listing as possible of the exact values of the energy levels.

Figure 1 gives the energy levels of the nuclei beryllium, boron, and carbon (Be^{10} , B^{10} , and C^{10}). The diagram shows the eight lowest energy levels of B^{10} and the lowest two energy levels of Be^{10} and C^{10} . It gives the position of these energy levels, their total angular momenta J , and parities T .⁽¹³⁾

Of much interest, but not shown in the diagram, are the transition probabilities between these levels. Such transition probabilities can be calculated if the characteristic functions associated with the characteristic values are known. Conversely, agreement between the observed transition probabilities and the calculated values of these quantities gives an indication of the accuracy of the calculated characteristic function.⁽¹⁴⁾

Figure 2 gives the energy levels of Hf^{180} . This nucleus has a rotational band.⁽¹⁵⁾ The angular momenta of the states shown are $J = 0, 2, 4, 6, 8$ in units of $h/2\pi$, where h is Planck's constant. The energy levels of these states are proportional to $J(J + 1)$, where J is the angular momentum quantum number.

Figure 3 gives the energy levels of U^{239} , the angular momentum quantum number of which is one-half.⁽¹⁶⁾ The diagram extends over 200 eV and its

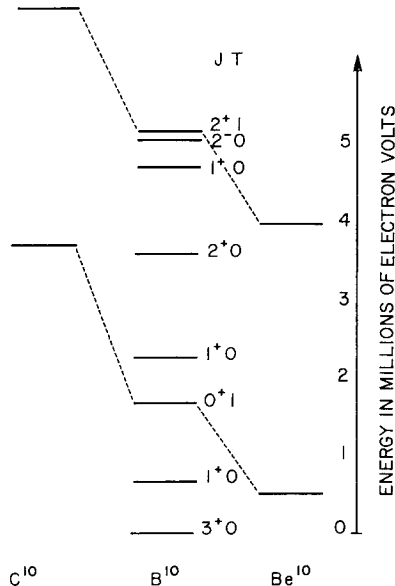


Fig. 1. Energy levels of the nuclei Be^{10} , B^{10} , and C^{10} . From Ref. 3.

CONSTANT X J(J+1)	J	ENERGY IN THOUSANDS OF ELECTRON VOLTS
1097	8	1085,3
640,5	6	641,7
305	4	309,3
91,5	2	93,3
0	0	0

Fig. 2. Energy levels of Hf¹⁸⁰. From Ref. 5.

lowest point is about 4.88 MeV over the lowest energy level. It is of little interest and is almost impossible to calculate the exact position of these energy levels. The reason one knows their position with the accuracy shown in the diagram is that the addition of a low-energy neutron to a U²³⁸ nucleus gives the U²³⁹ nucleus with an energy of about 4.88 MeV.

The last diagram gives an example of energy levels in a region where one will be interested mostly in the statistical statements such as the density of the energy levels, their average width (i.e., the square of the wave function at the nuclear boundary), etc. Furthermore, one is also interested in the probability for certain spacings, including the question of whether the levels are, on the whole, equidistant or distributed according to a certain probability law. In addition to the average width of the levels, one is interested in the

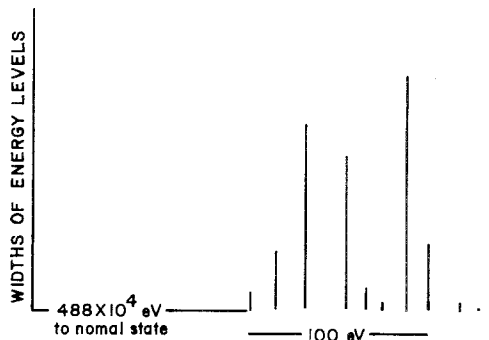


Fig. 3. Energy levels of U²³⁹. From Ref. 6.

distribution of the widths, i.e., the fraction of levels the widths of which are in unit interval at a certain width.

From the point of view of mathematics, the statistical questions are far more interesting than the question of the exact properties of the low-lying energy levels. This is so since it is likely that the statistical properties of a large class of real symmetric operators are in many respects identical. They should depend then on only a few parameters which are characteristic of the problem. For example, one may confine one's attention to the class of real symmetric operators since the energy operators are not only Hermitian but are also real. This statement is a result of the time inversion symmetry of most physical systems.³

2. PRELIMINARIES

What guidance has one in order to phrase the questions to be answered in the spectroscopy of highly excited complex systems?⁴ To start with, one recalls the energy levels comprising the spectra of a few well-known one-dimensional quantum mechanical problems:

Harmonic oscillator: $E_n \sim n + 1/2$.

Infinite square well: $E_n \sim (n + 1)^2$.

Hydrogen atom: $E_n \sim -1/(n + 1)^2$, and continuum for $E > 0$.

where $n = 0, 1, 2, \dots$. For each of the three potentials there is another constant of the motion, the parity, which acts as an additional quantum number. In the one-dimensional hydrogen atom case all energy levels, except the ground state, are doubly parity degenerate (i.e., the even solutions which are rejected by boundary condition requirements in the three-dimensional hydrogen s state are present in the one-dimensional case). Degeneracy is a statement concerning energy level spacings. Accordingly, in the case of the one-dimensional hydrogen atom the spacing between corresponding levels of even and odd parity is zero.

If one ignores the question of degeneracy associated with parity labeling and also ignores the existence of a continuum for positive energies for the one-dimensional hydrogen atom, one sees that the E_n form a countable sequence of numbers. Thus one might learn something about the positions of energy levels of highly excited states by examining the mathematics of number sequences.

³ It appears that not all physical systems have time symmetry. This was first pointed out as a result of experiments which show a violation of CP invariance in the decay $K_2^0 \rightarrow \pi^+ + \pi^-$ in 1964 by Christenson *et al.*⁽¹⁷⁾ For a recent development see Beier *et al.*⁽¹⁸⁾

⁴ The following is based on Ref. 19.

What sequences of numbers does one know in mathematics? Perhaps the best-known sequence of numbers which is not trivial is the sequence of prime numbers. It is well known that no simple formula for the n th prime number p_n exists, although there are formulas involving limiting operations.

The best-known result concerning the prime numbers is the so-called prime number theorem.^(20,21) It gives an answer to the question of how many primes $N(n)$ there are between the integers 1 and n for a large integer n . The result, for large n , is

$$N(n) = \int_0^n (dt/\log t) \tag{3}$$

In Fig. 4 this function is plotted as a function of n .⁵ The density of prime numbers $dN(n)/dn$, given by

$$dN(n)/dn = 1/\log n \tag{4}$$

is also given in this figure.

It will be noted that statistical concepts are already involved in the discussion of the prime numbers, such as the notion of the density of the primes.

⁵ This figure appears in Ref. 19. It is based on Lehmer's⁽²²⁾ tables.

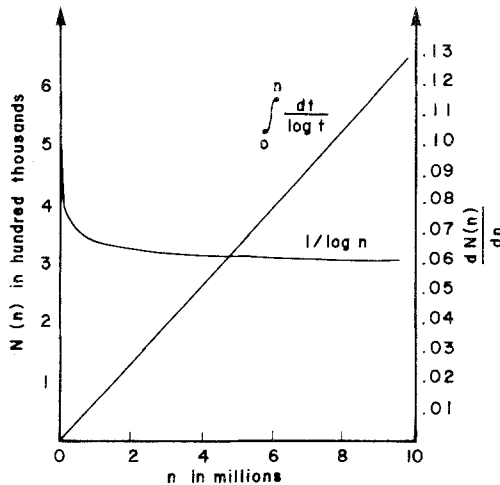


Fig. 4. Cumulative distribution $N(n)$ of prime numbers versus integers n , and the density dN/dn of the prime numbers. From Ref. 19, based on tables in Ref. 22.

This is similar to the situation one finds in quantal spectra where, given a Hamiltonian, there is nothing random about the solution of the Schrödinger equation. On the other hand, there is apparently enough complexity in the prime number sequence that the density is not without what might be considered as fluctuations about the mean density.

What then would one mean by a completely random sequence? For an experimentalist this is a rather simple question since it is the same problem as the determination of the singles, doubles, etc., counting rate for a decaying radiative source. The major property of a decaying source is not that the decay occurs at random, but that the events are ordered in time.

It is well known that the relevant decay law for the differential probability $P^k(x)$, where $x = t/\tau$ is the time measured in units of the mean life τ of the source between two counts having k counts occur between them, is the Poisson distribution

$$P^k(x) = (x^k/k!) \exp(-x) \quad (5)$$

Hence one expects the nearest-neighbor spacing distribution for an ordered sequence of random numbers to be $P^0(x) = \exp(-x)$ and the next-nearest-neighbor spacing distribution to be $P^1(x) = x \exp(-x)$, etc., where $x = S/D$ is the spacing measured in units of the mean distance D between random numbers.

Let us now return from the mathematical digression to the problem of quantal spectra. Most of quantum spectroscopy is based on the Schrödinger equation given in the introduction, where the operator (Hamiltonian) H is

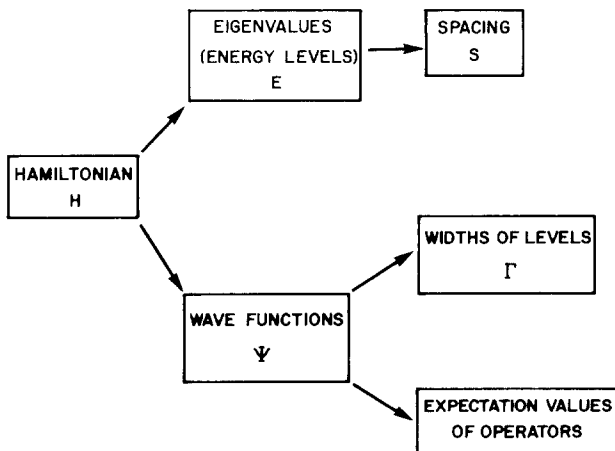


Fig. 5. Typical theoretical calculation of energy levels. From Ref. 19.

taken in the form

$$H(1, 2, \dots, A) = \sum_{i=1}^A (T_i + V_i) + \sum_{i < j=1}^A V_{ij} \quad (6)$$

for a system of A particles when one assumes that there is a two-body interaction potential. The Schrödinger equation is then solved for the eigenvalues E (which give the spacing S) and the wave functions Ψ . Once the wave functions are found one can then calculate expectation values of operators such as magnetic dipoles, electric quadrupoles, and so on. One can also calculate widths of energy levels. The situation is summarized in Fig. 5.

The case for which the discrete levels under consideration are unstable to particle emission is somewhat more complicated in practice since there is often a background amplitude that cannot be neglected. This is so since the scheme presented in Fig. 5 is typically used where the potential scattering is negligible, namely, for low excited states.

3. SYMMETRY PROPERTIES OF PHYSICAL SYSTEMS

The symmetry properties of any physical system are an expression of the Hamiltonian of the system.^(19,23) Thus, for example, if the Hamiltonian H is independent of time, then the energy of the system is conserved. Hence energy conservation is associated with invariance of the Hamiltonian under time translation. For an isolated system of particles with interactions depending only on the distances between the particles, or invariant combinations of spin and interparticle coordinate vectors, translations along the spatial axes of a chosen coordinate system then leave the Hamiltonian unchanged, thus leading to the law of conservation of total linear momentum of the system. The conservation of angular momentum can be related to rotations in an appropriate way. One can subtract from the total energy the kinetic energy associated with the total momentum. This leads to the notion of internal energy of the isolated system which is also conserved. The internal energy of the complex system is of great interest for the statistical theory of energy levels since the latter deals with spectra arising from changes in the internal state of excitation of the system. Spatial inversion transformation (improper transformation) leads, in an odd number of dimensions, to changing the sign of every coordinate q_i and momentum p_i in the Hamiltonian. If the Hamiltonian remains unchanged by this transformation (in technical language this means if the parity transformation operator commutes with the Hamiltonian, as is the case for gravitational, electromagnetic, and strong interactions), then the parity of the system is also conserved. Although the inversion transformation operator does not commute with the translation

operators, there are simultaneous eigenstates of the translation operator and the parity operator so that the energy, total linear momentum, and parity become simultaneously constants of the motion.

We will now come back to the reversal of the direction of time. A measurable physical quantity is invariant under a canonical transformation. For example, the quantity $|(\Psi, \Phi)|^2$, where the bracket describes a scalar product between the two-state functions Ψ and Φ , is invariant under the canonical transformations $\Psi \rightarrow A\Psi$, $\Phi \rightarrow A\Phi$. This means⁽²⁴⁻²⁷⁾

$$|(\Psi, \Phi)|^2 = |(A\Psi, A\Phi)|^2 \quad (7)$$

To satisfy Eq. (7), the operator A should be *unitary*, i.e., $AA^\dagger = 1$. But A could be either *linear* or *antilinear*, depending on whether it satisfies the equation

$$A(a\Psi + b\Phi) = a(A\Psi) + b(A\Phi) \quad (8a)$$

or

$$A(a\Psi + b\Phi) = \bar{a}(A\Psi) + \bar{b}(A\Phi) \quad (8b)$$

where \bar{a} and \bar{b} are the complex conjugates of a and b . The two possibilities (8a) and (8b) are uniquely compatible with the physical requirement (7).

The symmetry operators corresponding to space-time translations and spatial inversions are linear in the coordinate representation, whereas the time inversion operator is antilinear. The last result can also be inferred by considering the time-dependent Schrödinger equation,

$$H\Psi = i\hbar \partial\Psi/\partial t \quad (9)$$

If one expands the solution Ψ in terms of eigenstates Ψ_k ,

$$\Psi(t) = \sum_k C_k [\exp(-iE_k t/\hbar)] \Psi_k \quad (10)$$

the result of replacing t by $-t$ is equivalent to replacing $\exp(-iE_k t/\hbar)$ by its complex conjugate, thus showing that the operation of time inversion is related to complex conjugation, an antilinear operation. This is also seen from the operator $i\hbar \partial/\partial t$ appearing on the right-hand side of the Schrödinger equation (9), where complex conjugation means time reversal. Time reversal does not change the coordinate q but reverses the direction of the momentum p since the latter involves a time rate. Denoting the time-reversal operator by T , one then has $TqT^{-1} = q$, but $TpT^{-1} = -p$. Applying these relations to the commutation relation $[q, p] = i\hbar$ leads to $TiT^{-1} = -i$, which shows again the antilinear effect of T .

It thus follows that T is antiunitary. However, if one defines a complex conjugation operator K such that $K\Psi = \bar{\Psi}$, then $K^2 = 1$ and the combination TK is unitary. T can then be written as $T = Uk$, where U is unitary. A simple calculation then shows that $T^2 = \pm 1$.

If the particles of the system do not have spin, then the unitary operator U can be chosen in the coordinate representation to be the identity operator. If the particles have spins, however, the choice of U is determined by the total angular momentum J , which satisfies $TJT^{-1} = -J$. The operator K gives the needed behavior for the orbital part of angular momenta in the coordinate representation. For one particle with spin, one can represent T as

$$T = [\exp(\frac{1}{2}i\pi\sigma_y)]K \tag{11}$$

where σ_y is one of Pauli's spin matrices. For a system having A particles, T can be presented as

$$\begin{aligned} T &= \{\exp[\frac{1}{2}i\pi(\sigma_{1y} + \sigma_{2y} + \dots + \sigma_{Ay})]\}K \\ &= [\exp(i\pi S_y/2)]K \end{aligned} \tag{12}$$

which has the property $T^2 = 1$ for even A and $T^2 = -1$ for odd A .

One thus has the set of commuting operators shown in Table I. Can any conclusion be reached about the structure of the Hamiltonian matrix from these general invariance properties? If the Hamiltonian has none of the symmetries mentioned above, then the Hamiltonian matrix must be complex Hermitian and hence is not real in general. The appropriate canonical transformation group is therefore the unitary group which preserves the Hermitian property of the Hamiltonian under a similarity transformation. Suppose now that the Hamiltonian is time-reversal invariant. Then one faces two situations according to whether the total angular momentum of the system in units of \hbar is integral or half-integral, thus depending upon whether

Table I

Invariance	Operator
Space translation	Total linear momentum
Time translation	Total energy
Space inversion	Parity
Time inversion	Time reversal
Space rotation	Total angular momentum

$T^- = +1$ or $T^2 = -1$. The $T^2 = 1$ case is easily handled and the Hamiltonian can be made real by an appropriate choice of basis. If $T^2 = -1$, again the Hamiltonian matrix can be made real provided that it is rotationally invariant. Accordingly, the Hamiltonian matrix can be made real provided it is time-reversal invariant and either the system has integral spin or, if it has half-integral total angular momentum, the Hamiltonian is invariant under rotations. Thus one deals with real symmetric matrices and canonical transformations that correspond to a change from one basis in which the Hamiltonian is symmetric and real to another basis in which it remains the same. The aggregate of such transformations R provides a group of transformations, the orthogonal group,

$$RR^t = 1 \quad (13)$$

The situation for which the spin of the system is half-integral and the Hamiltonian is time-reversal invariant but the total angular momentum is not conserved, such as that of an atom located in a multipole external crystalline electric field, is related to the well-known Kramers degeneracy,^(28,29) where Ψ and $T\Psi$ are orthogonal. Since both Ψ and $T\Psi$ satisfy the Schrödinger equation (H is time-reversal invariant) for the same energy, there is at least a doublet degeneracy in this case. The Kramers degeneracy appears in the structure of the Hamiltonian matrix in an intrinsic way and may be seen as follows.^(4,30) Since $T^2 = -1$, one has $UKUK = -1$, or $UU = -1$. Since U is unitary, one sees that it must be skew-symmetric. Under a unitary basis transformation V , $T \rightarrow VTV^{-1}$, and hence $U \rightarrow VUV^t$. Under such a transformation the skew-symmetric unitary matrix U can be brought into a form $Z_{ij} = \delta_{i,j+1} - \delta_{i,j-1}$, i.e., a banded diagonal matrix with $+1$ in the sub-diagonal, -1 in the superdiagonal.⁽³¹⁾ Further canonical unitary transformations S are possible if they commute with the time-reversal operator $T = ZK$. Hence one requires for S

$$ZKS - SZK = 0 \quad (14a)$$

$$SZS^t = Z \quad (14b)$$

Equation (14b) defines what is known as the *symplectic* transformation.^(32,33) There is a *quaternion* structure associated with the symplectic group of transformations. To express this, one introduces a unit matrix I and three 2×2 complex matrices $\tau = -i\sigma$, where the three matrices σ are the familiar Pauli spin matrices

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (15)$$

where $i, j = 1, \dots, N$, and N is a fixed integer. One thus has $N(N + 1)/2$ matrix elements which are assumed to be independent Gaussian random variables with the joint distribution function

$$D(H_{ij}) = A \exp \left[- \left(\sum_i H_{ii}^2 + 2 \sum_{i < j} H_{ij}^2 \right) / 4a^2 \right] \quad (16)$$

where A and a are constants. Thus one assumes that each system with N quantum states occurs in the ensemble E_G with a statistical weight given by (16). The reality of the Hamiltonian ensures that the system is time-reversal invariant. It can be shown^(39,40) that Eq. (16) is a consequence of two assumptions: (1) The components H_{ij} are statistically independent and (2) the function $D(H_{ij})$ is invariant under the transformation $H \rightarrow R^{-1}HR$, where R is a *real orthogonal* matrix. Although the assumption (2) is natural in order to give equal weight to all kinds of interactions, the definition of the Gaussian ensemble E_G is nevertheless somewhat arbitrary since assumption 1 is artificial and without physical motivation. The unsatisfactory feature of the distribution function (16) is that one cannot define a uniform probability distribution on an infinite range, and hence a restriction on the magnitudes of H_{ij} has to be made since otherwise it is impossible to define an ensemble in terms of H_{ij} in which all interactions are equally probable.

The *orthogonal ensemble*,⁽⁴⁾ denoted by E_1 , is defined with a slight change from the Gaussian ensemble E_G . A system is represented in E_1 not by its Hamiltonian H but by an $N \times N$ unitary matrix S whose eigenvalues are N complex numbers $\exp(i\theta_j)$, where $j = 1, \dots, N$, distributed around the unit circle. The matrix S is a function of the Hamiltonian H so that the angles θ_j are functions of the energy levels E_j of the system, and over a small range of angles, θ_j is linear in E_j . The basic statistical hypothesis here is that the behavior of n consecutive levels of an actual system, where n is small compared with the total number of levels, is statistically equivalent to the behavior in the ensemble E_1 of n consecutive angles θ_i on the unit circle, where n is small compared with N .

Both the Gaussian ensemble and the orthogonal ensemble are restricted to $N \times N$ matrices, and are mutilations of an actual nucleus with an infinite number of energy levels. The most one can ask of such an ensemble is that it correctly reproduce level distributions over an energy range small compared with the total energy of excitation. The connection between the matrix S and the Hamiltonian is vague. The energy level distributions predicted by the Gaussian ensemble and by the orthogonal ensemble are unrealistic.

The first gives the so-called *semicircle distribution*⁽³⁷⁾

$$\begin{aligned} P(E) &= (2\pi Na^2)^{-1} (4Na^2 - E^2)^{1/2}, & E^2 < 4Na^2 \\ P(E) &= 0, & E^2 > 4Na^2 \end{aligned} \quad (17)$$

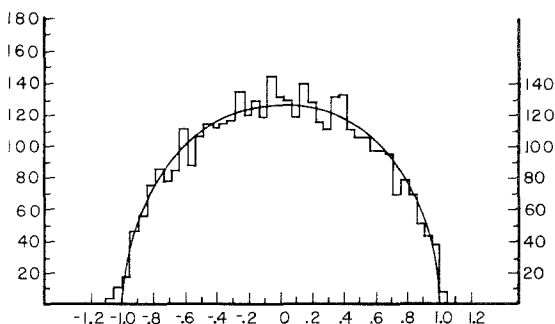


Fig. 6. The histogram of the semicircle distribution obtained by diagonalizing 197 real symmetric 20×20 matrices. From Ref. 6.

which does not resemble the level distribution of a nucleus. The distribution (17) is also very different from that of the real roots of an algebraic equation of order N . Figure 6 is a histogram of $P(E)$ obtained by diagonalizing 20×20 matrices, selected at random from a certain ensemble. As can be seen, the distribution approaches a semiellipse. In fact a semicircle is actually a misnomer since the two axes do not even have the same dimensions.⁽⁶⁾

As has been pointed out before, the distribution (17) shows no similarity to the observed distribution in spectra. The behavior at large positive E is not relevant since what is known, and what could be hoped to be reproduced by the ensemble, is the distribution in the neighborhood of the lowest energy level. The density in the neighborhood of the lowest state in nuclei, for example, is such that there are few levels per million electron volts. Around 5 meV, on the other hand, there are several levels in an interval of 100 eV. There seems to be an exponential increase with energy. The density of the levels as a function of the energy is convex from below, whereas the semicircle or semiellipse is concave. It could be surmised that the convex distribution applies only in the neighborhood of the lower range of the asymptotic formula in the region where the asymptotic formula does not hold. The density in the range of the semicircle law is proportional to $N^{1/2}$, where N is the dimension of the random matrix. If it were proportional to a lower power of N outside the ellipse, this would not show in the asymptotic law but might explain the region in which the density of levels increases fast. This region was discussed in more detail for the so-called *Wishart ensemble*,⁽⁴¹⁾ an ensemble in which the matrix elements are independent of each other and each shows a Gaussian distribution. It was found that the semicircle law is too accurate. On the average there are only about two levels outside its range. It is clear that the existence of a reasonably large region in which the second energy derivative of the density of levels is positive does not follow from the assumptions made so far.

The orthogonal ensemble gives in the large a uniform distribution around the unit circle. Although the orthogonal distribution, like the Gaussian distribution, is unphysical, it has the advantage of simplicity and absence of spurious end effects.

The precise definition of the orthogonal ensemble E_1 is as follows: A system is characterized by an $N \times N$ symmetric unitary matrix S . Since the space T_1 of all matrices S is compact, it makes sense to require that the ensemble E_1 contain all possible S with equal probability.

To give a meaning to equal probability, one requires a measure μ in the space T_1 . Since the matrices S do not form a group, the definition of μ is not easy, and is done as follows: One writes S as $U^t U$, where U is a unitary matrix. An infinitesimal neighborhood of S in T_1 is given by

$$S + dS = U^t(1 + i dM)U \quad (18)$$

where dM is a real, symmetric, infinitesimal matrix with elements dM_{ij} , and dM_{ij} , with $i \leq j$, vary independently through some small intervals of lengths $d\mu_{ij}$. The measure of this neighborhood is then defined as

$$\mu(dS) = \prod_{i < j} d\mu_{ij} \quad (19)$$

The ensemble E_1 is then defined by demanding that the probability that a system of E_1 belongs to the volume element dS is

$$P(dS) = (V_1)^{-1} \mu(dS) \quad (20)$$

where V_1 is the total volume of the space T_1 ,

$$V_1 = \int \mu(dS) \quad (21)$$

It can be shown that $\mu(dS)$ is independent of the particular U that was chosen to represent S . It also follows that for fixed S the unitary matrix U is undetermined precisely to the extent of a transformation

$$U \rightarrow RU \quad (22)$$

where R is an arbitrary real orthogonal matrix. In addition, one can show that the ensemble E_1 is uniquely defined in the space T_1 of symmetric unitary matrices by the property of being invariant under every automorphism $S \rightarrow W^t S W$ of T_1 into itself, where W is any unitary matrix. Thus one states in mathematical language the precise meaning of the vague statement "all systems occur in E_1 with equal probability."

The automorphism $S \rightarrow W^t S W$ is not a mere change in the representation of states. It is a physical alteration of the system S into a different

system. One may visualize S as representing an unknown system enclosed in a "black box," and S is the transformation matrix of the system from some initial state ψ_i to a final state ψ_f . The transformation $S \rightarrow W^t S W$ then means that one subjects the initial state to some further interaction W , and the final state to the same interaction W^t in a time-symmetric way. If we are totally ignorant of the interactions occurring inside the black box, the additional interaction W cannot increase or decrease our ignorance, and if all systems S were equally probable at the beginning, the application of W must not change that. Invariance of the ensemble E_1 under the transformation $S \rightarrow W^t S W$ is a mathematical idealization of the hypothetical state of total ignorance.

It remains only to justify, on physical grounds, the choice of the basic space T_1 of symmetric unitary matrices. Alternative choices are discussed in Appendix A. The choice of T_1 has the same motivation as the choice of real symmetric matrices for the Gaussian ensemble E_G . Symmetric unitary matrices are physically appropriate under two alternative conditions: (1) the systems are invariant under time inversion and space rotations, or (2) the systems are invariant under time inversion and contain an even number of half-integer spin particles. The symmetry of the S matrix for systems satisfying condition (1) has been proven in a particularly simple case.⁽⁴²⁾ In the neutron capture resonances case, for example, condition (1) always holds and the ensemble E_1 is the one to use.

5. UNITARY ENSEMBLE

In Section 4 we discussed the Gaussian and orthogonal ensembles, and in Appendix A we discuss the symplectic ensembles. We now briefly discuss systems without time-reversal symmetry, a unitary ensemble.⁽⁴⁾

The unitary ensemble, denoted by E_2 , is a simple one. From the physical point of view such a system is easily created, for example, by putting an ordinary atom or nucleus into an externally generated magnetic field, provided the splitting of the levels by the magnetic field is of the same order of magnitude as the average level spacing in the absence of the field. The magnetic interaction must in fact be so strong that it completely mixes up the level structure which would exist in the zero field. This situation does not occur in nuclear physics, but it could occur in atomic or molecular physics.

The Hamiltonian of a system without invariance under time reversal is usually an arbitrary Hermitian matrix which is not restricted to the symmetric or self-dual. The system is represented by an $N \times N$ unitary matrix S belonging to the space T_2 of all unitary matrices. Since the space T_2 is the unitary group $U(N)$, it is a simple matter to define a uniform ensemble E_2 in T_2 , and an invariant group measure in $U(N)$ can easily be established.

The ensemble E_2 is then defined as follows: A neighborhood of S in T_2 is given by

$$S + dS = U(1 + i dH)V \tag{23}$$

where U and V are two unitary matrices such that $S = UV$, dH is an infinitesimal Hermitian matrix with elements $dH_{ij} = dH_{ij}^1 + i dH_{ij}^2$, and dH_{ij}^1 and dH_{ij}^2 vary independently through small intervals of lengths $d\mu_{ij}^1$ and $d\mu_{ij}^2$, respectively. The invariant group measure $\mu(dS)$ is defined by

$$\mu(dS) = \prod_{i,j} d\mu_{ij}^1 d\mu_{ij}^2 \tag{24}$$

independently of the choice of the two matrices U and V . The ensembles E_2 give each neighborhood dS the statistical weight

$$P(dS) = (V_2)^{-1} \mu(dS) \tag{25}$$

where V_2 is the volume of the space T_2 . The unitary ensemble E_2 is uniquely defined in the space T_2 of unitary matrices by the property of being invariant under every automorphism $S \rightarrow USW$ of T_2 into itself, where U and W are two matrices of the space T_2 .

6. EIGENVALUE-EIGENVECTOR DISTRIBUTIONS OF THE GAUSSIAN ENSEMBLE

The detailed calculation of the measure and the matrix element distribution for the Hamiltonian submatrix H corresponding to one set of symmetry labels (like spin J and parity P) discussed in previous sections leads to (see Appendix B)

$$\begin{aligned} d\mu(H_\beta) &= 2^{\beta N(N-1)/4} \left[\prod_{\mu=1}^N dH_{\mu\mu} \right] \left[\prod_{\mu < \nu=1}^N \prod_{k=0}^{\beta-1} dH_{k\mu\nu} \right] \\ &\simeq \left[\prod_{\lambda < \mu=1}^N |E_\lambda - E_\mu|^\beta \right] d\mu(H_D) \times \begin{cases} d\mu(R) \\ d\mu(U) \\ d\mu(S) \end{cases} \end{aligned} \tag{26}$$

for the measure, and to

$$\begin{aligned} P(H, \beta) &= \frac{\exp\{-[\text{Tr}(H - E_0 I)^2]/4a^2\}}{(4\pi a^2)^{[N + \beta N(N-1)/2]}} \tag{27} \\ \int P(H; \beta) d\mu(H_\beta) &= 1 \end{aligned}$$

for the matrix element distribution, where $\beta = 1$ corresponds to the orthogonal, $\beta = 2$ to the unitary, and $\beta = 4$ to the symplectic cases. These formulas, however, are not directly useful to obtaining numerical results for comparing

with energy level spacings, widths, and expectation values. From these equations, however, one can obtain the eigenvalue distributions $P(E_1, \dots, E_N; \beta)$ and the eigenvector distributions $P(R)$, $P(U)$, or $P(S)$ according to the symmetry of the problem. Since the distribution function $P(H)$ is invariant and the Jacobian [Appendix B, Eq. (B.12)] factors in the eigenvalues and the measures, it follows that the eigenvectors are statistically *independent* of the eigenvalues in the Gaussian ensembles. Hence there is no statistical correlation between the eigenvalue spacings and the widths or expectation values.⁷ One has for the eigenvalue distributions

$$P(E; \beta) \simeq \exp\left[-\frac{1}{4a^2} \sum_{\lambda=1}^N (E_\lambda - E_0)^2\right] \left[\prod_{\lambda < \mu=1}^N |E_\lambda - E_\mu|^\beta \right] \quad (28)$$

whereas the eigenvector distributions $P(R)$, $P(U)$, and $P(S)$ are constants proportional to the inverse of the total integrals of the measures $d\mu(R)$, $d\mu(U)$, and $d\mu(S)$, respectively. Hence the eigenvectors form a set of random, mutually perpendicular vectors, and therefore one can obtain the single-eigenvalue distribution $P(E; \beta)$ corresponding to the level density in some sense, the spacing distributions $P_N^k(x; \beta)$, where $x = S/D$ and S is the spacing while D is the mean spacing between levels. A complete unified treatment for the spacing distributions and the single-eigenvalue distribution is not available.

Example. The Gaussian ensembles of 2×2 matrices. From Eq. (28) one obtains

$$P(E_1, E_2; \beta) = C_\beta |E_1 - E_2|^\beta \times \exp\{-[(E_1 - E_0)^2 + (E_2 - E_0)^2]/4a^2\} \quad (29)$$

where C_β is a normalization factor given by $C_\beta = 1/(2a)^{2+\beta} 2^{\beta/2} \Gamma[(1 + \beta)/2] \times \Gamma(1/2)$. The mean spacing is given by

$$D = a2^{3/2} \frac{\Gamma[1 + (\beta/2)]}{\Gamma[(1 + \beta)/2]} \quad (30)$$

and the nearest-neighbor spacing distributions are given by

$$\begin{aligned} P_2^0(x; 1) &= \frac{\pi}{2} x \exp\left(-\frac{\pi}{4} x^2\right) && \text{(orthogonal)} \\ P_2^0(x; 2) &= \frac{32}{\pi^2} x^2 \exp\left(-\frac{4}{\pi} x^2\right) && \text{(unitary)} \\ P_2^0(x; 4) &= \frac{2^{18}}{3^6 \pi^3} x^4 \exp\left(-\frac{64}{9\pi} x^2\right) && \text{(symplectic)} \end{aligned} \quad (31)$$

Here $x = S/D$, where S is the spacing and D is given by Eq. (30).

⁷ Some data suggest a small correlation, however. See Ref. 43.

In general, the characteristic values of a real symmetric matrix, or a complex Hermitian matrix, “repel” each other.⁽⁴⁴⁾ This means that if the matrix elements depend on a number of continuous parameters, then the dimension of the domain in the space of the parameters for which the matrix has a double root is, in general, lower by two than the dimension of the parameter space itself.

To see this, we go back to the case of 2×2 matrices discussed above.⁽¹⁴⁾ Let the symmetric matrix be given by

$$\begin{bmatrix} a & b \\ b & c \end{bmatrix} \quad (32)$$

Then the roots (characteristic values) of this matrix are given by the solution of the quadratic equation

$$E^2 - (a + c)E + (ac - b^2) = 0$$

Hence they are

$$E = \frac{1}{2}(a + c) \pm \frac{1}{2}[(a - c)^2 + 4b^2]^{1/2} \quad (33)$$

As can easily be seen, the two roots are equal if $a = c$ and $b = 0$. Now the space of parameters of the matrix (32) is three dimensional. In this space, whose coordinates are given by a , b , and c , the equations $a = c$ and $b = 0$ represent a straight line in the $b = 0$ plane, which has one dimension, of course. It follows from this property of matrices that the probability for a spacing S (interval between adjacent roots) is proportional to S itself if S is very small compared with the average spacing D .

The property of a “repulsion” of energy levels (characteristic values, or roots of the matrix) can also be seen from Eqs. (31), which shows how the three ensembles are reflected in the nearest-neighbor spacing distribution. For small $x = S/D$ the exponential parts of Eq. (31) approach one and hence the distribution functions vary as x^β for the three cases. This is in contrast to an ordered sequence of random numbers following the Poisson distributions $P^0(x) = \exp(-x)$ [see Eq. (5) in Section 2], which approaches a constant as x goes to zero. Hence, there is a repulsion of energy levels associated with an absence of small spacings (namely absence of degeneracy).⁽⁴⁵⁾

The behavior of Eqs. (31) for large spacings is also interesting in the two-dimensional case. The result, when $x \rightarrow \infty$, is given by

$$\ln P_2^0(x; \beta) \rightarrow \text{const} - \left[\frac{\Gamma(1 + \beta/2)}{\Gamma[(1 + \beta)/2]} \right]^2 x^2 + \beta \ln x \quad (34)$$

In the case of large dimension where $N \rightarrow \infty$, Eq. (34) has to be modified by the addition of a linear term.⁽⁴⁶⁾ But Eqs. (31) do not differ numerically very much from the infinite-dimensional results.⁽⁴⁷⁾

It is interesting to note that the first of Eqs. (31) is identical with a conjecture made by Wigner in 1957 for the spacing distribution.⁽⁴⁸⁾ The formula was supposed to apply to a series of levels having the same values of all identifiable quantum numbers, such as angular momentum and parity. It is very well supported by experimental data and by numerical tests with random matrices of high order. However, it is known to be false. The correct distribution function was obtained later by Mehta and Gaudin,^(47,49,50) who computed it numerically. They found that Wigner's distribution function is not identical with the one they derived but is surprisingly close to it, the difference being less than 0.0162 over the whole range of $x = S/D$. Hence for practical purposes Wigner's formula is justified. Within experimental uncertainties, changing the dimension N in the Gaussian ensemble does not affect significantly the form of the predicted nearest-neighbor spacing distribution. In fact almost every other approach to the nearest-neighbor spacing distribution yielded results indistinguishable experimentally from the first of Eqs. (31).

The *distribution of the λ th eigenvalue* is defined by (for the two-dimensional case)

$$P_2(E; \beta, \lambda) = 2! C_{2\beta} \int_{-\infty}^{\infty} dE_1 \int_{E_1}^{\infty} dE_2 |E_1 - E_2|^\beta \times \exp[-(E_1^2 + E_2^2)/4a^2] \delta(E - E_\lambda) \tag{35}$$

Here $\lambda = 1, 2$. In N dimensions there are N distributions $P_N(E; \beta, \lambda)$. The *single-eigenvalue distribution* is defined as

$$P_N(E; \beta) = N^{-1} \sum_{\lambda=1}^N P_N(E; \beta, \lambda)$$

and can therefore be written in the two-dimensional case as

$$P_2(E; \beta) = C_{2\beta} \int_{-\infty}^{\infty} dE_1 \int_{-\infty}^{\infty} dE_2 |E_1 - E_2|^\beta \times \exp[-(E_1^2 + E_2^2)/4a^2] \delta(E_1 - E) \tag{36}$$

The detailed calculation of this function for the three cases (orthogonal, unitary, and symplectic) gives

$$\begin{aligned} P_2(\epsilon; 1) &= (2\pi)^{-1/2} \exp(-2\epsilon^2) + 2^{-1/2}\epsilon[\exp(-\epsilon^2)] \Phi(\epsilon) \\ P_2(\epsilon; 2) &= \pi^{-1/2}[\exp(-\epsilon^2)](1 + 2\epsilon^2) \\ P_2(\epsilon; 4) &= (12)^{-1}\pi^{-1/2}[\exp(-\epsilon^2)](3 + 12\epsilon^2 + 4\epsilon^4) \end{aligned} \tag{37}$$

where $\epsilon = E/2a$, and $\Phi(z)$ is an error function,

$$\Phi(z) = (2/\sqrt{\pi}) \int_0^z \exp(-t^2) dt$$

The *level density* is then given by $\rho_N(E; \beta) = NP_N(E; \beta)$, where $P_N(E; \beta)$ is the single-eigenvalue distribution defined above, and one has $\rho_N \rightarrow 1/D$ in the limit when $N \rightarrow \infty$, where D is given by Eq. (30). However, one finds in the case of two dimensions at $E = 0$ that $1/\rho_2(0; \beta)$ is equal to $(2\pi)^{1/2}a$, $\pi^{1/2}a$, and $4\pi^{1/2}a$ for $\beta = 1, 2$, and 4 respectively, whereas D is given by $(2\pi)^{1/2}a$, $4(2/\pi)^{1/2}a$, and $16(2/\pi)^{1/2}a$ for the same cases.

We now discuss in some detail the concepts of the mean level density and the nearest-neighbor spacing.⁽¹⁹⁾ For the Gaussian ensemble one can develop the asymptotic semicircle law of Wigner (see Section IV, and Refs. 36, 38, and 41),

$$P_N(E; \beta) \xrightarrow{N \rightarrow \infty} \frac{G}{\pi a(\beta N)^{1/2}} \left(1 - \frac{E^2}{4a^2\beta N}\right)^{1/2} \quad (38)$$

valid for $E \leq 2a(\beta N)^{1/2}$. Hence $\rho_N(E; \beta) = NP_N(E; \beta)$ is given by $\rho_N(0; \beta) \rightarrow_{N \rightarrow \infty} (1/\pi a)(N/\beta)^{1/2}$ for the case of $E = 0$. In addition to the nearest-neighbor spacing distributions $P_N^0(x; \beta)$, the higher-order spacing distributions $P_N^k(x; \beta)$ (see above) are of interest for comparison with experimental results. The case for which N goes to infinity is again of great interest. This has been worked out by Dyson for the circular ensemble.^(51,52) A complete Monte Carlo calculation of quantities using the Gaussian orthogonal ensemble with a sample of 10,000 10×10 matrices was carried out by Porter,⁽⁵³⁾ who obtained all spacing distributions up to $k = 8$ and showed that the rate of change of these distributions with dimension is small over the range of major probability. Dyson and Mehta⁽⁵⁴⁾ have developed efficient statistics, one of which is sensitive to long-range order properties of a sequence of levels, where the concept of selecting a set of N levels in sequence out of sequence of N levels in the circular orthogonal ensemble was developed to meet the experimental results.

Finally some remarks should be made on the unitary and symplectic ensembles.⁽¹⁹⁾ In the case of the circular unitary ensemble⁽⁴⁾ a sequence of energy levels can be obtained from the circular orthogonal ensemble by superposing two energy level sequences having the same mean spacing.⁽⁵⁵⁾ A sequence of energy levels in the circular symplectic ensemble can also be generated from a sequence of levels in the circular orthogonal ensemble by selecting alternate levels.⁽⁵⁶⁾ It is conjectured that similar relationships hold in the Gaussian ensembles in the infinite-dimensional case, in which the orthogonal ensemble underlies the unitary and symplectic ensembles. Next-nearest-neighbor spacing distributions have been obtained for the Gaussian orthogonal and unitary ensembles in three dimensions, showing no appreciable difference in the range of major probability from results in very large dimension.^(57,58) Use of generalized ensembles based on the classical polynomials affects the eigenvalue distribution (hence the level density). For ex-

ample, the nearest-neighbor spacing distribution obtained in the unitary ensemble based on the Legendre polynomials is identical to that of the circular unitary ensemble in the infinite-dimensional case.^(59,60) In the unitary ensemble the spacing distributions are implied by a certain kernel function.⁽⁶¹⁾ The situation when only energy level positions are known but not the other associated symmetry quantum numbers (like spin and parity) was discussed.^(40,61-64) The Brownian motion model for the eigenvalue distribution, and spacing distributions, were also discussed.⁽⁶⁵⁻⁶⁷⁾

7. DISTRIBUTION OF THE WIDTHS

We now discuss the fluctuation properties of the *widths* of energy levels, that is, of the square of the wave function at the nuclear or atom surface, and the expectation values. Although a detailed theoretical argument is yet lacking, Scott,⁽⁶⁸⁾ and Porter and Thomas,⁽⁶⁹⁾ found, on the basis of experimental results by Hughes and Harvey,^(70,71) that the probability that the value of the wave function is between γ and $\gamma + d\gamma$ is

$$(2\pi\bar{\gamma}^2)^{-1/2} \exp(-\gamma^2/2\bar{\gamma}^2) d\gamma \quad (39)$$

Here $\bar{\gamma}^2$ denotes the average value of γ^2 . Equation (39) essentially shows that the matrix elements in complex spectra produce a Gaussian distribution, and represents a generally accepted rule, the so-called Porter-Thomas distribution. It is also well confirmed experimentally.

The calculation of the statistics of the matrix elements, in general, involves two self-adjoint operators, the Hamiltonian H defining the coordinate system, and another operator M representing the physical quantity such as the dipole moment, whose matrix elements one wishes to find.⁸ Let us assume that the two operators H and M are both real. This means there is a coordinate system in which all permissible operators, representing the physical quantity one is interested in, have real matrix elements. If one chooses the coordinates in such a way that the states represented by them are time-inversion invariant, then the matrix elements of the Hamiltonian become real. If the physical quantity one is interested in is time-inversion invariant, then the matrix elements of its operator will also be real.

Most interesting physical quantities do have the property of time-inversion invariance, i.e., retaining their signs when the directions of the velocities are reversed, or the opposite property of reversing their signs if the directions of velocities are reversed. The operators representing these

⁸ The following is based on Ref. 7.

physical quantities, such as the magnetic moment, that reverse their signs when the velocities are reversed are Hermitian and purely imaginary, hence skew-symmetric.

The calculation of the distribution function of the matrix elements of time-reversal-invariant operators can be modified and applied to antiinvariant operators. Therefore the same distribution function is expected for the matrix elements of the antiinvariant operators as for real, time-inversion-invariant operators.

It is also assumed that the density of the characteristic values of the physical quantity is an even function of the characteristic value. This condition is fulfilled for the antiinvariant operators, but also all known time-inversion-invariant transition operators satisfy this condition.

Let, then, use be made of a coordinate system whose axes are the characteristic functions of the operator M (and not of the Hamiltonian H) and let the characteristic values be denoted by μ . The matrix element can then be given by $m = \sum \mu_i x_i y_i$, where x_i and y_i are the coordinates of the states between which the matrix element is taken. Furthermore, x_i , y_i , and m are real. The problem is then to calculate the distribution of m for the Hamiltonians of the ensemble chosen. If one assumes that this is rotationally invariant in the Hilbert space, then one can calculate the distribution of the above expression for m when the vectors x and y are each normalized to unitary but remain perpendicular to each other, $\sum x_i^2 = \sum y_i^2 = 1$, $\sum x_i y_i = 0$. This calculation can be carried out in detail, leading to the fact that the distribution is Gaussian:

$$(2\pi\bar{\mu}^2)^{-1/2} \exp(-m^2/2\bar{\mu}^2) \quad (40)$$

Introducing the transition rate $\Gamma = m^2$, one then obtains from Eq. (40) the distribution

$$(2\pi\bar{\mu}^2\Gamma)^{-1/2} \exp(-\Gamma/2\bar{\mu}^2) \quad (41)$$

Equation (41) is the familiar Porter–Thomas distribution mentioned at the beginning of this section. It is confirmed experimentally in the case of neutron emission and various moments in atomic physics.⁽⁷²⁾

For more on the expectation value problem, the reader is referred to Refs. 73 and 74.

It is worthwhile to comment on the assumptions that led to the distribution formula (41). It has been shown⁽⁷⁵⁾ that it is plausible that the replacement of Hilbert space by a space of high dimensionality is justified here more than in previous cases discussed. The assumption that the matrices considered were real is also important. An ensemble of complex Hermitian matrices would lead to a transition probability Γ (proportional to the absolute square

of the matrix element), $(\bar{\mu}^2)^{-1} \exp(-\Gamma/2\bar{\mu}^2)$, which is different from Eq. (41). As Wigner has pointed out, this is significant. There are experiments which show that the actual Hamiltonian is not strictly time-inversion invariant but has a small antiinvariant part. This part would manifest itself in the region where the levels are close to each other. Hence, an experimental check on the Porter–Thomas distribution would give an indication on the magnitude of the non-time-inversion-invariant part of the Hamiltonian. The effect here is similar to what would occur in the level-spacing distribution; the non-time-inversion-invariant part of the Hamiltonian would manifest itself in this case in an added repulsion of the levels.

8. CONCLUDING REMARKS

We have seen how the statistical theory of energy levels is related to the theory of random matrices. The theory is applicable to a variety of subjects (see, e.g., Ref. 76): theoretical aspects of resonance reaction theories, statistics of resonance parameters such as level spacings, neutron fission radiative and reaction widths, level densities, fluctuations in cross sections, strength functions and their relation to the optical model, intermediate structure in particle- and photon-induced reactions, and statistical aspects of the decay of the compound nucleus. However, as Wigner⁽⁷⁷⁾ has pointed out recently, the subject is not precisely defined as compared to the theory of statistical mechanics. The latter subject is clearly defined since it deals with time-averaged properties which depend only on the energy and are independent of the other initial conditions, as the quasiergodic theorem asserts. On the other hand, in the theory of statistical properties of nuclei one considers situations in which one is not interested in as detailed a picture of the nucleus as one is generally interested in physics but tries to find properties and rules which are reasonably simple and general, shared by most nuclei under appropriate conditions.

The role of the Hamiltonian in both statistical mechanics theory and in the statistical theory of energy levels is very important and worth a few remarks.⁽⁷⁷⁾ It is well known that some of the very interesting laws of statistical mechanics can be derived from the simple assumption that the equations of motion can be derived from a Hamiltonian through the usual variational principle. For example, the entropy theorem and the equipartition theorem belong in this category (see, e.g., Ref. 78). Also, much of other work in the theory of statistical mechanics is based on the explicit knowledge of the Hamiltonian itself (which is known in most practical cases). There are, however, no known theorems which are as fundamental as the entropy theorem or the equipartition theorem. In fact, as is well known, one does not even know the nuclear Hamiltonian. Moreover, some relevant properties of the

Hamiltonian are complicated, even though its explicit form is not known. Of course, the Hamiltonian in the statistical theory of energy levels is an operator, and hence a matrix, defined in a certain Hilbert space.

The most natural set of properties to be made use of are those shared by self-adjoint matrices in Hilbert space. This then leads to the concept of ensembles of self-adjoint, or real symmetric, matrices in Hilbert space, which is a definition of the measure for such matrices in Hilbert space. The concept of "vast majority of all self-adjoint matrices" or "practically all self-adjoint matrices" is then mathematically defined.

A particular case of distribution, which is of much interest for both physicists and mathematicians, is that of the Wishart distribution.⁹ If one demands that the measure be invariant with respect to unitary transformations, the measure is then an arbitrary function of the invariants of the matrix, multiplied by the differentials of the independent components of the matrix elements. If, further, one demands that the probabilities of the independent components of the matrix elements be independent of each other, one then obtains, essentially, the Wishart distribution, and the ensemble obtained is such that the number of matrices within unit interval of the independent components of the matrix elements M_{ik} is proportional to $\exp(\alpha \sum M_{ii} - \beta \sum |M_{ik}|^2)$, where α and β are arbitrary constants. However,⁽⁷⁷⁾ practically none of the matrices of this distribution have characteristics similar to those observed for actual Hamiltonians. In particular, the density of the characteristic values of most matrices as a function of energy (the semicircle law) has, in the neighborhood of the lower bound, a negative second derivative,⁽⁴¹⁾ whereas the measured density has a positive second derivative with respect to the energy. Hence one should be careful to draw other consequences that are obtained from the Wishart model.

To overcome this difficulty, one might use the independent particle model.⁽⁷⁹⁻⁸²⁾ The result obtained by these recent studies is that the density of the levels as a function of the energy is a Gaussian, rather than the semicircle of the Wishart and related ensembles, and at its lowest range its second derivative is positive. Another result^(80,82) is that the distance of the second and further neighbors is subject to much larger fluctuations than in the Wishart ensemble case. However, the independent particle model has its own restricted validity.⁽⁷⁷⁾

Another model that might replace the Wishart ensemble is that in which the matrix elements are viewed as particles in Brownian motion.⁽⁶⁶⁾ It then follows that the characteristic values can also be viewed as Brownian particles.

A third model is based on an ensemble of matrices of the form $H =$

⁹ There seems to be a difference on the use of terminology "Wishart distribution" between physicists and statisticians. See comment by Krishnaiah, in Ref. 76, p. 20.

$m^\dagger m + m^t m$, where m is again an arbitrary complex matrix. This model seems to promise the important factor of mathematical simplicity.^{(77),10}

A fourth model, which is based on the information theory treatment of the random Hamiltonians, is given by Balian.⁽⁸³⁾

Before we end this section we mention once again that one respect in which all the matrix models differ from physics is that they all deal with finite matrices, whereas physics deals with infinite matrices. Thus one must always, in interpreting the results of the matrix model, be careful not to use those results which specifically have to deal with the finiteness of the matrix.

Finally, to conclude our discussion, we point out that our review does not include the tremendous volume of work done on the mathematical aspects of the theory of random matrices, and the reader is referred to the literature.⁽⁸⁴⁻⁸⁸⁾

APPENDIX A. SYMPLECTIC GROUP AND QUATERNIONS⁽⁴⁾

A set of matrices B form an N -dimensional symplectic group, denoted by $Sp(N)$, if B is a $2N \times 2N$ unitary matrix and satisfies the relation [see Eq. (14b)]⁽³³⁾

$$Z = BZB^t \tag{A.1}$$

(The matrix Z was defined in the text and is given in footnote 6.) It is well known⁽³²⁾ that the algebra of the symplectic group can be expressed most naturally in terms of quaternions. We here give a brief discussion of quaternions.

Introducing the standard quaternion notation for 2×2 matrices

$$\tau^1 = \begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix}, \quad \tau^2 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad \tau^3 = \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix} \tag{A.2}$$

satisfying the multiplication table

$$(\tau^1)^2 = (\tau^2)^2 = (\tau^3)^2 = -1 \tag{A.3}$$

$$\{\tau^i, \tau^j\} = \epsilon^{ijk} \tau_k \tag{A.4}$$

where $\{\tau^i, \tau^k\}$ denotes an anticommutator $\tau^i \tau^k + \tau^k \tau^i$ and ϵ^{ijk} is the skew-symmetric tensor such that $\epsilon^{123} = 1$. All $2N \times N$ matrices will be considered as cut into N^2 blocks of 2×2 , and each 2×2 block is regarded as a quaternion. Hence a $2N \times 2N$ matrix with complex elements becomes an

¹⁰ Professor Wigner has kindly informed me (private communication) that his proposal to use $m^\dagger m + m^t m$, with m a complex Wishartian ensemble member, has proved to be invalid; there is a finite gap in the distribution of the roots at zero and it is at least unlikely that there is an energy region with a positive second derivative of the level density following this gap.

$N \times N$ matrix with complex quaternion elements. For example, the matrix Z (see footnote 6) can now be written as

$$Z = \tau^2 I \quad (\text{A.5})$$

where I is the $N \times N$ unit matrix. It is interesting to note that the matrix rules for multiplication are not changed by this transcription.

A quaternion q is called *real* if it has the form

$$q = q^0 + (\mathbf{q} \cdot \boldsymbol{\tau}) \quad (\text{A.6})$$

and the coefficients $q^0, q^1, q^2,$ and q^3 are real numbers. Hence a real quaternion is not a real 2×2 matrix. The *conjugate* quaternion q^* to the complex quaternion q is defined by

$$q^* = q^0 - (\mathbf{q} \cdot \boldsymbol{\tau}) \quad (\text{A.7})$$

Note that the conjugate quaternion q^* is *different* from the *complex conjugate* quaternion \bar{q} defined by

$$\bar{q} = \bar{q}^0 + (\bar{\mathbf{q}} \cdot \boldsymbol{\tau}) \quad (\text{A.8})$$

A quaternion q satisfying $\bar{q} = q$ is real. A quaternion q with $q^* = q$ is a *scalar*. The *Hermitian conjugate* quaternion q^\dagger is defined by applying both types of conjugation together,

$$q^\dagger = \bar{q}^* = \bar{q}^0 - (\bar{\mathbf{q}} \cdot \boldsymbol{\tau}) \quad (\text{A.9})$$

Consider now a general $2N \times 2N$ matrix A which one writes as an $N \times N$ matrix Q with quaternion elements q_{ij} , with $i, j = 1, 2, \dots, N$. The standard matrix operations on A then reflect themselves on Q as follows:

Transposition

$$(Q^\dagger)_{ij} = -\tau^2 q_{ji}^* \tau^2 \quad (\text{A.10})$$

Hermitian conjugation

$$(Q^\dagger)_{ij} = q_{ji}^\dagger \quad (\text{A.11})$$

Time reversal

$$(Q^R)_{ij} = q_{ji}^* \quad (\text{A.12})$$

The usefulness of the quaternion algebra is a result of the simplicity of Eqs. (A.11) and (A.12). Using Eqs. (A.11) and (A.12), one sees that the condition

$$Q^R = Q^\dagger \quad (\text{A.13})$$

is necessary and sufficient for the elements of Q to be real quaternions. When Eq. (A.13) is satisfied one calls Q *quaternion real*.

A unitary matrix B satisfying Eq. (A.1) is automatically quaternion real, and satisfies the conditions

$$B^R = B^\dagger = B^{-1} \tag{A.14}$$

which can be considered as defining the symplectic group. Matrices S representing physical systems are not quaternion real. They are unitary and self-dual, i.e.,

$$S^R = S, \quad S^\dagger = S^{-1} \tag{A.15}$$

The theorem of quaternion algebra states:

Theorem 1. Let H be any Hermitian, quaternion-real, $N \times N$ matrix. Then there exists a symplectic matrix B such that

$$H = B^{-1}DB \tag{A.16}$$

where D is diagonal, real, and scalar. The statement that D is scalar means that it consists of N blocks of the form

$$\begin{bmatrix} D_j & 0 \\ 0 & D_j \end{bmatrix} \tag{A.17}$$

Hence the eigenvalues of H consist of N equal pairs.

The Hamiltonian of any system that is invariant under time reversal and has odd spin satisfies the condition of the theorem stated above. The energy levels of such a system, as was pointed out in the text, must be doubly degenerate. This is the Kramers degeneracy^(28,29) and the above theorem shows how it appears naturally in the quaternion language.

An extension of the above theorem states that if S_1 and S_2 are two commuting, Hermitian, quaternion-real matrices, then there exists a symplectic matrix B such that

$$S_1 = B^{-1}D_1B, \quad S_2 = B^{-1}D_2B \tag{A.18}$$

where D_1 and D_2 are diagonal, real, and scalar. From this extension one can prove:

Theorem 2. Let S be any unitary, self-dual, $N \times N$ quaternion matrix. Then there exists a symplectic matrix B such that

$$S = B^{-1}EB \tag{A.19}$$

where E is diagonal and scalar. The diagonal elements of E are N complex numbers $\exp(i\theta_k)$ on the unit circle, each being repeated twice.

To prove the theorem, one writes

$$S = S_1 + S_2 \tag{A.20}$$

where S_1 and S_2 are quaternion real. Since the operation of time reversal applied to a matrix does not involve complex conjugation, when S is self-dual each of S_1 and S_2 must be separately self-dual. Hence S_1 and S_2 are also Hermitian. Moreover, since S is unitary,

$$S^\dagger S = (S_1 - iS_2)(S_1 + iS_2) = 1 \tag{A.21}$$

Separating the quaternion-real and -imaginary parts of Eq. (A.21), one finds

$$S_1^2 + S_2^2 = 1, \quad S_1 S_2 - S_2 S_1 = 0 \tag{A.22}$$

Hence S_1 and S_2 commute, and therefore the extension of Theorem 1 applies. If B is chosen to satisfy Eq. (A.18), then Eq. (A.19) will hold with

$$E = D_1 + iD_2 \tag{A.23}$$

being diagonal and scalar. Let d_{k_c} and d_{k_c}' be the corresponding eigenvalues of D_1 and D_2 . Equation (A.22) then gives

$$(d_{k_c})^2 + (d_{k_c}')^2 = 1 \tag{A.24}$$

This shows that d_{k_c} and d_{k_c}' can be taken as

$$d_{k_c} = \cos \theta_{k_c}, \quad d_{k_c}' = \sin \theta_{k_c} \tag{A.25}$$

and therefore the diagonal elements of E become

$$e_k = d_{k_c} + i d_{k_c}' = \exp(i\theta_{k_c}) \tag{A.26}$$

each occurring twice.

The analog of Theorem 2 for the even-spin case is:

Theorem 3. Let S be any unitary, symmetric, $N \times N$ matrix. Then there exists a real orthogonal matrix R such that

$$S = R^{-1}ER \tag{A.27}$$

where E is diagonal. The diagonal elements of E are N complex numbers $\exp(i\theta_{k_c})$ on the unit circle.

The proof of this theorem is the same as that for Theorem 2 if one replaces self-dual for symmetric, quaternion-real for real, and symplectic for orthogonal.

Return now to the odd-spin case and define the *symplectic ensemble* E_4 , the odd-spin analog of the orthogonal ensemble E_1 (see text). One then works in the space T_4 of unitary self-dual quaternion matrices. We now define an *invariant measure* in T_4 in spite of the fact that the matrices of T_4 do not form a group. First one notices that every matrix S in T_4 can be written in the form

$$S = U^R U \tag{A.28}$$

where U is unitary. Given S , the unitary matrix U has a freedom of

$$U \rightarrow BU \tag{A.29}$$

where B is an arbitrary symplectic matrix. An infinitesimal neighborhood of S in T_4 is given by

$$S + dS = U^R[1 + i dM]U \tag{A.30}$$

where dM is a quaternion-real, self-dual, infinitesimal matrix with elements

$$dM_{ij} = dM_{ij}^0 + (dM_{ij} \cdot \tau) \tag{A.31}$$

where the real coefficients dM_{ij} satisfy

$$dM_{ij}^0 = dM_{ji}^0, \quad dM_{ij}^\alpha = -dM_{ji}^\alpha, \quad \alpha = 1, 2, 3 \tag{A.32}$$

One has $N(2N - 1)$ independent real variables dM_{ij}^α , which vary through some small intervals of length $d\mu_{ij}^\alpha$. The neighborhood of S so defined therefore has the measure

$$\mu(dS) = \prod_{\alpha, i, j} d\mu_{ij}^\alpha \tag{A.33}$$

The symplectic ensemble E_4 is therefore defined like E_1 (see text), with the statistical weight of the neighborhood dS in E_4 given by

$$P(dS) = (V_4)^{-1} \mu(dS) \tag{A.34}$$

where V_4 is the total volume of the space T_4 .

Finally one has:

Theorem 4. The symplectic ensemble E_4 is uniquely defined, in the space T_4 of self-dual, unitary quaternion matrices, by the property of being invariant under every automorphism $S \rightarrow W^R S W$ of T_4 into itself, where W is a unitary matrix.

This theorem shows that the symplectic ensemble uniquely represents the notion of uniform a priori probability in the space T_4 .

APPENDIX B. GAUSSIAN ENSEMBLE⁽¹⁹⁾

In Section 4 we discussed the Gaussian and orthogonal ensembles. We here give some more details. The Gaussian ensembles^(35-40, 48) have the unifying feature that eigenvector and eigenvalue distributions are produced directly from a single set of hypotheses concerning the Hamiltonian of the system which usually reflects the actual dynamics. This means that data on *level widths*, *expectation values*, and *level spacings* can be used to test the same ensemble.

Let us examine the orthogonal case in which the Hamiltonian can be

made a real symmetric matrix. As a model, one considers a real symmetric matrix of dimension N to represent the infinite submatrix of the Hamiltonian H associated with some symmetry property. Hence the Hamiltonian will include $N(N + 1)/2$ real parameters. To associate a measure (volume) with the matrix H , one introduces a metric in the parameter space defined by

$$ds^2 = \text{Tr}(dH dH^\dagger) \quad (\text{B.1})$$

where dH represents a matrix whose elements are infinitesimal increments of the elements of the matrix H . Comparing (B.1) with the standard form of line element

$$ds^2 = \sum g_{\mu\nu} dx^\mu dx^\nu \quad (\text{B.2})$$

one finds that the metric $g_{\mu\nu}$ is diagonal with N of the elements equal to one and the remaining $N(N - 1)/2$ elements equal to $\sqrt{2}$. A measure can then be defined as

$$d\mu(H) = 2^{N(N-1)/4} dH_{11} dH_{22} \cdots dH_{NN} dH_{12} \cdots dH_{N-1,N} \quad (\text{B.3})$$

in analogy to the volume element in a Riemannian space

$$dV = (\det g)^{1/2} dx_1 dx_2 \cdots dx_M \quad (\text{B.4})$$

where M is the dimension of the space, $M = N(N + 1)/2$. The quantities $dH_{11}, \dots, dH_{N-1,N}$ are the elements of the matrix dH .

With the matrix H one can associate a distribution function

$$P(H) = P(H_{11}, H_{22}, \dots, H_{NN}, H_{12}, \dots, H_{N-1,N}) \quad (\text{B.5})$$

such that the differential probability dP that H_{11} is in dH_{11} at H_{11} , etc., is

$$dP = P(H) d\mu(H) \quad (\text{B.6})$$

Since the matrix H is Hermitian, and Hermitian matrices do not form a group, one encounters a difficulty in defining a measure in terms of H . However, H is related to a diagonal matrix H_D containing the eigenvalues of H by the orthogonal transformation R ,

$$H = RH_D R^{-1} = RH_D R^t \quad (\text{B.7})$$

The last equation is actually the Schrödinger equation written in matrix form, where R contains the eigenvectors usually written as ψ and H_D contains the eigenvalues. One can thus associate the volume element (B.3) with R and H_D , where, as is well known, the matrices R do provide a group. Using (B.7), one can then write

$$dH = R dH_D R^t + [dR R^t, H] \quad (\text{B.8})$$

Hence the $N(N + 1)/2$ variables of H are transformed into the N eigenvalues

in H_D and $N(N - 1)/2$ angles of rotation in the matrix R . One can then insert for dH of Eq. (B.1) its value given in (B.8) in terms of the eigenvalues in H_D and the angles of R . The measure $d\mu(H_D)$ associated with H_D is given by

$$d\mu(H_D) = dE_1 dE_2 \cdots dE_N \tag{B.9}$$

In order to find the measure of \hat{R} , one writes¹¹ Eq. (B.7) in terms of matrix elements,

$$H_{\mu\nu} = \sum_{\alpha=1}^N E_{\alpha} R_{\mu\alpha} R_{\nu\alpha} \tag{B.10}$$

Equation (B.10) defines a transformation from the eigenvalue and eigenvector variables to the Hamiltonian matrix element variables. Hence one can write the measure (B.3) as

$$\begin{aligned} d\mu(H) &= 2^{N(N-1)/4} dH_{11} \cdots dH_{NN} \\ &= 2^{N(N-1)/4} J dE_1 \cdots dE_N d\alpha_1 \cdots d\alpha_{N(N-1)/2} \end{aligned} \tag{B.11}$$

where $\alpha_1, \dots, \alpha_{N(N-1)/2}$ are the $N(N - 1)/2$ parameters of the orthogonal matrix R . In Eq. (B.11) the term J stands for the Jacobian of the transformation (B.10) and is given by the determinant

$$J = \begin{vmatrix} \partial H_{11}/\partial E_1 & \cdots & \partial H_{11}/\partial E_N & \partial H_{11}/\partial \alpha_1 & \cdots & \partial H_{11}/\partial \alpha_{N(N-1)/2} \\ \vdots & & & & & \\ \partial H_{NN}/\partial E_1 & & \cdots & & & \partial H_{NN}/\partial \alpha_{N(N-1)/2} \end{vmatrix} \tag{B.12}$$

It can be shown that J is a polynomial of degree $N(N - 1)/2$ in the eigenvalues. Since the eigenvectors are not unique, if one pair of eigenvalues are equal it follows that the transformation inverse to (B.10) is singular and therefore J vanishes. Hence J is proportional to

$$\prod_{\lambda < \mu = 1}^N |E_{\lambda} - E_{\mu}| \tag{B.13}$$

Thus J can be written as

$$J = h(\alpha_1, \dots, \alpha_{N(N-1)/2}) \prod_{\lambda, \mu} |E_{\lambda} - E_{\mu}| \tag{B.14}$$

Since the measure of the n -dimensional orthogonal group can be written as

$$d\mu(R) = h(\alpha_1, \dots, \alpha_{N(N-1)/2}) \cdots d\alpha_{N(N-1)/2} \tag{B.15}$$

we see that

$$d\mu(H) = d\mu(H_D) d\mu(R) \prod_{\lambda < \mu = 1}^N |E_{\lambda} - E_{\mu}| \tag{B.16}$$

¹¹ This approach is somewhat different from that of Hua.⁽⁶⁹⁾ For measure of the group R in three dimensions see Naimark.⁽⁶⁰⁾

How should the function $P(H)$, appearing in Eq. (B.6), be specified? One knows that it depends only on the eigenvalues and not on the eigenvectors. One requires that $P(H)$ be independent in the matrix elements. Moreover, if one does not know the Hamiltonian H , then one also does not know in what representation H will be diagonal and therefore one does not know R , thus choosing it at random. Hence it follows that $P(H)$ should be independent of R , namely, $P(H)$ is an invariant function of H . It follows that the requirements of invariance and independence are necessary and sufficient conditions to determine the form of $P(H)$, where, mathematically, invariance means

$$dP/d\alpha = 0 \quad (\text{B.17})$$

and independence means

$$P(H) = f_{11}(H_{11}) \cdots f_{NN}(H_{NN}) \cdots f_{N-1,N}(H_{N-1,N}) \quad (\text{B.18})$$

A detailed calculation, using Eqs. (B.17) and (B.18), shows that

$$f_{\mu\mu} = \frac{\exp[-(H_{\mu\mu} - E_0)^2/4a^2]}{(4\pi a^2)^{1/2}} \quad (\text{B.19})$$

$$f_{\mu\nu} = \frac{\exp(-H_{\mu\nu}^2/2a^2)}{(2\pi a^2)^{1/2}} \quad \mu < \nu$$

with the normalization condition

$$\int_{-\infty}^{\infty} f_{\mu\nu}(H_{\mu\nu}) dH_{\mu\nu} = 1 \quad (\text{B.20})$$

In these equations a and E_0 are constants. Finally, the expression for the function $P(H)$ becomes

$$P(H) = \frac{\exp\{-[\text{Tr}(H - E_0 I)]^2/4a^2\}}{(4\pi a^2)^{N(N+1)/4}} \quad (\text{B.21})$$

normalized such that

$$\int P(H) d\mu(H) = 1 \quad (\text{B.22})$$

This is the situation for the orthogonal ensemble.

The corresponding formulas in the unitary ensemble are

$$d\mu(H) = d\mu(H_D) d\mu(U) \prod_{\lambda < \mu = 1}^N (E_\lambda - E_\mu)^2 \quad (\text{B.23})$$

where H_D and U are related to H by

$$H = UH_D U^\dagger \quad (\text{B.24})$$

and

$$P(H) = \frac{\exp\{-[\text{Tr}(H - E_0 I)^2]/4a^2\}}{(4\pi a^2)^{N^2/2}} \tag{B.25}$$

In the symplectic case one obtains

$$d\mu(H) = d\mu(H_D) d\mu(S) \prod_{\lambda < \mu} (E_\lambda - E_\mu)^4 \tag{B.26}$$

where H_D and S are related to H by

$$H = SH_D S^+ \tag{B.27}$$

and S is symplectic (see Appendix A), and

$$P(H) = \frac{\exp\{-[\text{Tr}(H - E_0 I)^2]/4a^2\}}{(4\pi a^2)^{(2N^2 - N)/2}} \tag{B.28}$$

These results of the Gaussian ensembles can be summarized by writing

$$\begin{aligned} d\mu(H_\beta) &= 2^{\beta N(N-1)/4} \left[\prod_{\mu=1}^N dH_{\mu\mu} \right] \left[\prod_{\mu < \nu=1}^N \prod_{k=0}^{\beta-1} dH_{k\mu\nu} \right] \\ &\simeq \left[\prod_{\lambda < \mu=1} |E_\lambda - E_\mu|^\beta \right] d\mu(H_D) \times \begin{cases} d\mu(R) \\ d\mu(U) \\ d\mu(S) \end{cases} \end{aligned} \tag{B.29}$$

and

$$\begin{aligned} P(H; \beta) &= \frac{\exp\{-[\text{Tr}(H - E_0 I)^2]/4a^2\}}{(4\pi a^2)^{[N + \beta N(N-1)/2]/2}} \tag{B.30} \\ \int P(H; \beta) d\mu(H_\beta) &= 1 \end{aligned}$$

Here $\beta = 1$ corresponds to the orthogonal, $B = 2$ to the unitary, and $\beta = 4$ to the symplectic ensemble.

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