

# Statistical Theory of the Energy Levels of Complex Systems. I

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New kinds of statistical ensemble are defined, representing a mathematical idealization of the notion of "all physical systems with equal probability." Three such ensembles are studied in detail, based mathematically upon the orthogonal, unitary, and symplectic groups. The orthogonal ensemble is relevant in most practical circumstances, the unitary ensemble applies only when time-reversal invariance is violated, and the symplectic ensemble applies only to odd-spin systems without rotational symmetry. The probability-distributions for the energy levels are calculated in the three cases. Repulsion between neighboring levels is strongest in the symplectic ensemble and weakest in the orthogonal ensemble. An exact mathematical correspondence is found between these eigenvalue distributions and the statistical mechanics of a one-dimensional classical Coulomb gas at three different temperatures. An unproved conjecture is put forward, expressing the thermodynamic variables of the Coulomb gas in closed analytic form as functions of temperature. By means of general group-theoretical arguments, the conjecture is proved for the three temperatures which are directly relevant to the eigenvalue distribution problem. The electrostatic analog is exploited in order to deduce precise statements concerning the entropy, or degree of irregularity, of the eigenvalue distributions. Comparison of the theory with experimental data will be made in a subsequent paper.

## I. INTRODUCTION

RECENT theoretical analyses<sup>1</sup> have had impressive success in interpreting the detailed structure of the low-lying excited states of complex nuclei. Still, there must come a point beyond which such analyses of individual levels cannot usefully go. For example, observations of levels of heavy nuclei in the neutron-capture region<sup>2</sup> give precise information concerning a stretch of levels from number  $N$  to number  $(N+n)$ , where  $n$  is an integer of the order of 100 while  $N$  is of the order of  $10^6$ . It is improbable that level assignments based on shell structure and collective or individual-particle quantum numbers can ever be pushed as far as the millionth level. It is therefore reasonable to inquire whether the highly excited states may be understood from the diametrically opposite point of view, assuming as a working hypothesis that all shell structure is washed out and that no quantum numbers other than spin and parity remain good. The result of such an inquiry will be a statistical theory of energy levels. The statistical theory will not predict the detailed sequence of levels in any one nucleus, but it will describe the general appearance and the degree of irregularity of the level structure that is expected to occur in any nucleus which is too complicated to be understood in detail.

In ordinary statistical mechanics a comparable renunciation of exact knowledge is made. By assuming all states of a very large ensemble to be equally probable, one obtains useful information about the over-all behavior of a complex system, when the observation of the state of the system in all its detail is impossible. This type of statistical mechanics is clearly inadequate for the discussion of nuclear energy levels. We wish to

make statements about the fine detail of the level structure, and such statements cannot be made in terms of an ensemble of states. What is here required is a new kind of statistical mechanics, in which we renounce exact knowledge not of the state of a system but of the nature of the system itself. We 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.<sup>3</sup> Wigner's program has been energetically pursued by Porter and Rosenzweig,<sup>4</sup> by Gaudin and Mehta,<sup>5</sup> and by others.<sup>6</sup> The results of this work are encouraging, but progress has been held back by the extreme difficulty of calculating the ensemble averages in Wigner's model. The difficulties seem to be of a purely mathematical nature, and they are as severe as those which arise in more orthodox statistical analyses of many-body systems with strong interactions. Only during the last year have Gaudin and Mehta<sup>5</sup> shown, by a beautiful exercise of analytical skill, that these difficulties are not insuperable. The way now lies open to develop the new statistical mechanics on a broad front and to use it for quantitative interpretation of experiments.

The present series of papers will explore the new statistical mechanics in its various ramifications. This, the first paper of the series, is mainly mathematical in content. Its purpose is to introduce a new type of

<sup>3</sup> E. P. Wigner, *Ann. Math.* **53**, 36 (1951); **62**, 548 (1955); **65**, 203 (1957); **67**, 325 (1958).

<sup>4</sup> C. E. Porter and N. Rosenzweig, *Suomalaisen Tiedeakat. Toimituksia, AVI*, No. 44 (1960), and *Phys. Rev.* **120**, 1698 (1960).

<sup>5</sup> M. L. Mehta, *Nuclear Phys.* **18**, 395 (1960); M. L. Mehta and M. Gaudin, *ibid.* **18**, 420 (1960); M. Gaudin, *ibid.* **25**, 447 (1961).

<sup>6</sup> R. G. Thomas and C. E. Porter, *Phys. Rev.* **104**, 483 (1956); I. I. Gurevich and M. I. Pevsner, *Nuclear Phys.* **2**, 575 (1957).

<sup>1</sup> See, for example, L. S. Kisslinger and R. A. Sorensen, *Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd.* **32**, No. 9 (1960); M. Baranger, *Phys. Rev.* **120**, 957 (1960).

<sup>2</sup> J. L. Rosen, J. S. Desjardins, J. Rainwater, and W. W. Havens, Jr., *Phys. Rev.* **118**, 687 (1960); **120**, 2214 (1960).

ensemble, different from those studied by Wigner and Mehta, and in this way to translate the whole subject into the language of abstract group theory. Powerful group-theoretical methods can then be applied to obtain results which would otherwise require heavy calculation. The new ensembles, while mathematically more elegant than Wigner's, are based on the same physical assumptions and imply the same consequences wherever a comparison has been made.

The question, whether either Wigner's ensembles or ours correspond well to the actual behavior of a heavy nucleus, can be answered only by experiment. In ordinary statistical mechanics, there is a rather strong logical expectation (though no rigorous mathematical proof) that an ensemble average will correctly describe the behavior of one particular system which is under observation. The expectation is strong, because the system "might be" in a huge variety of states, and very few of these states will deviate much from a properly chosen ensemble average. In the new statistical mechanics we have an ensemble of systems, and this ensemble is supposed to describe the behavior of a unique object, for example the nucleus  $U_{239}$ . The logical presumption that  $U_{239}$  is really a good sample of the ensemble cannot be compelling. It will not be a disaster if it turns out that  $U_{239}$  in fact deviates quite strongly from the ensemble average. On the contrary, deviations from the ensemble average will reveal important physical information concerning the extent to which hidden quantum numbers (shell structure or other unknown integrals of the motion) may persist into the domain of neutron capture resonances.

## II. GAUSSIAN ENSEMBLE AND ORTHOGONAL ENSEMBLE

The Gaussian ensemble  $E_G$ , the most convenient in practice of the class of ensembles introduced by Wigner,<sup>3</sup> may be defined as follows. A system is characterized by a Hamiltonian which is a real symmetric matrix  $H_{ij}$ ,  $i, j = 1, \dots, N$ . The integer  $N$  is fixed, and the  $H_{ij}$  for  $i \leq j$  are  $\frac{1}{2}(N^2 + N)$  independent Gaussian random variables with the joint distribution function

$$D(H_{ij}) = A \exp\left[-\left(\sum_i H_{ii}^2 + 2 \sum_{i < j} H_{ij}^2\right)/4a^2\right]. \quad (1)$$

Here  $A$  and  $a$  are constants. The meaning of (1) is that each system having  $N$  quantum states occurs in the ensemble  $E_G$  with the statistical weight  $D(H_{ij})$ . The Hamiltonian is taken real rather than merely Hermitian in order to restrict attention to systems invariant under time reversal.

It was shown by Porter and Rosenzweig<sup>4</sup> that the special form of Eq. (1) is implied by two apparently more general requirements: (i) the various components  $H_{ij}$  to be statistically independent, and (ii) the function  $D(H_{ij})$  to be invariant under all transformations

$H \rightarrow R^{-1}HR$ , where  $R$  is a real orthogonal matrix. The requirement (ii) is a natural one in any ensemble that attempts to give equal weight to all kinds of interactions. However, requirement (i) is artificial and without clear physical motivation. To picture the  $H_{ij}$  as resulting from some "random process" of a conventional kind does not seem reasonable. Therefore the definition of  $E_G$  remains somewhat arbitrary.

The basic reason for the unsatisfactory features of Eq. (1) is that one cannot define a uniform probability distribution on an infinite range. Thus some arbitrary restriction of the magnitudes of the  $H_{ij}$  is inevitable. It is impossible to define an ensemble in terms of the  $H_{ij}$  in which all interactions are equally probable.

By a rather slight formal change we can define a new ensemble  $E_1$ , which is free from the arbitrary features of  $E_G$  and which also turns out to be mathematically easier to handle. The ensemble  $E_1$  will be called "the orthogonal ensemble" because its structure is closely connected with that of the  $N$ -dimensional orthogonal group. A system is represented in  $E_1$  not by its Hamiltonian  $H$  but by an  $(N \times N)$  unitary matrix  $S$ . The eigenvalues of  $S$  are  $N$  complex numbers  $[\exp(i\theta_j)]$ ,  $j = 1, \dots, N$ , distributed around the unit circle. The precise connection between  $S$  and  $H$  need not be specified. We assume only that  $S$  is a function of  $H$ , so that the angles  $\theta_j$  are a function of the energy levels  $\epsilon_j$  of the system. Over a small range of angles, the relation between  $\theta_j$  and  $\epsilon_j$  will be approximately linear. Our basic statistical hypothesis is then the following: *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  $\theta_j$  on the unit circle, where  $n$  is small compared with  $N$ .*

It may be helpful for the reader to imagine a definite relation between  $S$  and  $H$ , for example,

$$S = \exp[-iH\tau], \quad S = [1 - i\tau H]/[1 + i\tau H]. \quad (2)$$

However, such a definite relation will never correspond to reality except over a limited range of energy. Both the Gaussian ensemble and the orthogonal ensemble which we shall shortly define are restricted to  $(N \times N)$  matrices. Both ensembles are gross mutilations of an actual nucleus, which has an infinite number of energy levels. The most one can ask of any such ensemble is that it correctly reproduces level distributions over an energy range small compared with the total energy of excitation. The relation between  $S$  and the "true Hamiltonian" is bound to be wrong, considered in the large. It is therefore better to leave the connection between  $S$  and  $H$  vague. The connection between the ensemble  $E_1$  and physical reality is then *only* the connection which we have stated above as the basic statistical hypothesis.

The over-all distributions of energy levels predicted by the Gaussian ensemble and by the orthogonal

ensemble are both unrealistic. The Gaussian ensemble gives for the distribution in the large the famous<sup>7</sup> "semi-circle distribution"

$$p(\epsilon) = [2\pi Na^2]^{-1} [4Na^2 - \epsilon^2]^{\frac{1}{2}}, \quad \epsilon^2 < 4Na^2, \quad (3)$$

$$p(\epsilon) = 0, \quad \epsilon^2 > 4Na^2,$$

which is totally unlike the level distribution of a nucleus. The orthogonal ensemble gives for the distribution in the large a uniform distribution around the unit circle. Both distributions are unphysical, but the orthogonal distribution has the advantage of simplicity and absence of spurious end effects.

After these preliminary remarks, we now state the precise definition of the orthogonal ensemble  $E_1$ . A system is characterized by a symmetric unitary matrix  $S$  having  $N$  rows and columns. Since the space  $T_1$  of all  $S$  is compact, it makes sense to require that the ensemble  $E_1$  contain all possible  $S$  with equal probability. However, to give a meaning to equal probability, we require a measure  $\mu$  in the space  $T_1$ . Since the  $S$  do not form a group, the definition of  $\mu$  is not entirely trivial. We choose the following definition. Every  $S$  can be represented in the form

$$S = U^T U, \quad (4)$$

where  $U$  is a unitary matrix,  $U^T$  its transposed matrix. An infinitesimal neighborhood of  $S$  in  $T_1$  is given by

$$S + dS = U^T [1 + idM] U, \quad (5)$$

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

$$\mu(dS) = \prod_{i \leq j} d\mu_{ij}. \quad (6)$$

The ensemble  $E_1$  is defined by the statement: *The probability that a system of  $E_1$  belongs to the volume-element  $dS$  is*

$$P(dS) = (V_1)^{-1} \mu(dS), \quad (7)$$

where

$$V_1 = \int \mu(dS) \quad (8)$$

is the total volume of the space  $T_1$ .

To make this definition unique, it remains to be proved that  $\mu(dS)$  is independent of the particular  $U$  which was chosen in Eq. (4). Suppose then

$$S = U^T U = V^T V, \quad (9)$$

where both  $U$  and  $V$  are unitary. The operator

$$R = VU^{-1} \quad (10)$$

is unitary, and also satisfies

$$R^T R = (U^T)^{-1} V^T V U^{-1} = (U^T)^{-1} U^T U U^{-1} = 1. \quad (11)$$

Therefore,  $R$  is real and orthogonal. Let

$$\mu'(dS) = \prod_{i \leq j} d\mu'_{ij} \quad (12)$$

be the measure derived from  $V$  as  $\mu(dS)$  was derived from  $U$ . We have

$$S + dS = V^T [1 + idM'] V \quad (13)$$

with

$$dM' = R dM R^{-1}. \quad (14)$$

To prove  $\mu(dS) = \mu'(dS)$ , we need to show that the Jacobian

$$J = \det |\partial dM'_{ij} / \partial dM_{kl}| \quad (15)$$

has absolute value unity, when  $dM, dM'$  are real symmetric matrices related by Eq. (14). To prove  $|J| = 1$  in general, it is sufficient to consider only two special forms of  $R$ , (i)  $R$  is a reflection

$$R_{ij} = \eta_j \delta_{ij}, \quad \eta_j = \pm 1, \quad (16)$$

and (ii)  $R$  is an infinitesimal rotation

$$R_{ij} = \delta_{ij} + a_{ij}, \quad a_{ij} = -a_{ji}. \quad (17)$$

In case (i) the result  $|J| = 1$  is trivial. In case (ii) we have to first order in the  $a_{ij}$ :

$$(\partial dM'_{ij} / \partial dM_{kl}) = \delta_{ik} \delta_{jl} + \delta_{ik} a_{jl} + a_{ik} \delta_{jl} + (i \rightleftharpoons j), \quad (18)$$

$$J = 1 + 2 \operatorname{spur}(a_{ij}) = 1. \quad (19)$$

This proves that the measure  $d\mu(S)$  is unique. Incidentally, we have established that for fixed  $S$  the unitary matrix  $U$  in Eq. (4) is undetermined precisely to the extent of a transformation

$$U \rightarrow RU, \quad (20)$$

where  $R$  is an arbitrary real orthogonal matrix.

The motivation for the choice of the ensemble  $E_1$  will become clearer in view of the following theorem.

*Theorem 1. The orthogonal ensemble  $E_1$  is uniquely defined, in the space  $T_1$  of symmetric unitary matrices, by the property of being invariant under every automorphism*

$$S \rightarrow W^T S W \quad (21)$$

of  $T_1$  into itself, where  $W$  is any unitary matrix.

Theorem 1 comprises two statements, (i) that  $E_1$  is invariant under the automorphisms (21), and (ii) that no other ensemble is invariant. To prove (i), we suppose that a neighborhood  $S + dS$  of  $S$  is transformed into a neighborhood  $S' + dS'$  of  $S'$  by the automorphism (21). Equations (4) and (5) then hold, and therefore

$$S' = V^T V, \quad V = UW, \quad (22)$$

<sup>7</sup> E. P. Wigner, *Ann. Math.* **65**, 203 (1957).

$$S' + dS' = V^T(1 + idM)V. \quad (23)$$

The measures  $\mu(dS)$  and  $\mu(dS')$  are then identical by definition. This proof of (i) becomes trivial because we made a convenient choice of the unitary operator  $V$  associated with  $S'$  by Eq. (22); it was shown before that the value of  $\mu(dS')$  is independent of the choice of  $V$ . To prove (ii), let  $E_1'$  be any ensemble invariant under Eq. (21). The probability distribution of  $E_1'$  will define a certain measure  $\mu'(dS)$  of neighborhoods in  $T_1$ . The ratio

$$\varphi(S) = \mu'(dS)/\mu(dS) \quad (24)$$

is a function of  $S$  defined on  $T_1$  and invariant under Eq. (21). But Eq. (4) shows that every  $S$  may be transformed into the identity operator by Eq. (21). Therefore  $\varphi(S) = \varphi(I) = \text{constant}$ , and  $E_1'$  is identical with  $E_1$ .

Theorem 1 states in mathematical language the precise meaning of the vague statement "all systems occur in  $E_1$  with equal probability." The point here is that the automorphism (21) is not a mere change in the representation of states; it is a physical alteration of the system  $S$  into a different system. Intuitively speaking, we may visualize  $S$  as representing an unknown system enclosed in a "black box,"  $S$  being the transformation matrix of the system from some initial state  $\varphi$  to some final state  $\psi$ . The transformation  $S \rightarrow W^T S W$  then means that we subject the initial state to some further interaction  $W$ , and the final state to the same interaction  $W^T$  in a time-symmetric manner. If we are totally ignorant of the interactions occurring inside the black box, the additional interaction  $W$  cannot increase or decrease our ignorance. If all systems  $S$  were equally probable to start with, the application of  $W$  must leave them equally probable. Invariance of the ensemble  $E_1$  under the transformations (21) is a reasonable 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. Here, alternative choices are possible, and will be discussed in the next section. The choice of  $T_1$  has the same motivation as Wigner's choice of real symmetric matrices for his ensemble  $E_G$ . Symmetric unitary matrices are physically appropriate under two alternative conditions, (i) if the systems are invariant under time inversion and under space rotations, or (ii) if 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 (i) has been proved in a particularly simple way by Coester.<sup>8</sup> In applying the theory to neutron capture resonances, conditions (i) will always hold, and so the ensemble  $E_1$  is the one to use.

### III. TIME-REVERSAL SYMMETRY. SYMPLECTIC ENSEMBLE

To find out whether the orthogonal ensemble is a reasonable one to use under all circumstances, a more careful analysis must be made of the consequences of time-reversal invariance. It will turn out that under some (perhaps not very realistic) circumstances a quite different ensemble should be used. The new ensemble will be called symplectic, because it bears the same relation to the symplectic group as  $E_1$  bears to the orthogonal group.

We begin by recapitulating the basic notions of time-reversal invariance.<sup>9</sup> The operation of time reversal applied to a state  $\psi$  is defined by

$$T\psi = K\psi^e, \quad (25)$$

where  $\psi^e$  is the complex conjugate of  $\psi$ , and  $K$  is a constant unitary matrix. The operation of time reversal applied to a matrix  $A$  is defined by

$$A^R = KA^TK^{-1}. \quad (26)$$

$A$  is called self-dual if  $A^R = A$ . A physical system is invariant under time reversal if the Hamiltonian is self-dual, i.e., if

$$H^R = H. \quad (27)$$

When Eq. (27) is satisfied, any unitary matrix  $S$  which is a function of  $H$ , for example the  $S$  given by Eq. (2), will also be self-dual,

$$S^R = S. \quad (28)$$

When the representation of states is transformed by a unitary transformation  $\psi \rightarrow U\psi$ , the  $K$  matrix transforms according to

$$K \rightarrow UKU^T. \quad (29)$$

So far the operation of time reversal has been purely formal, and the matrix  $K$  is quite arbitrary. Physical definiteness is given to the operation by requiring

$$J^R = -J, \quad (30)$$

where  $J$  is any component of the total angular momentum operator. It is not assumed that angular momentum is necessarily conserved. However, it is always true that the system has either integer spin or half-odd-integer spin. That is to say, the eigenvalues of components of  $J$  are either all integers or all half-odd integers, and the two possibilities do not mix. For brevity we call these two possibilities the even-spin case and the odd-spin case, respectively. The consequence of Eq. (30) is that in the even-spin case

$$T^2 = KK^e = 1, \quad (31)$$

and  $K$  is a symmetric unitary matrix, while in the odd-

<sup>8</sup> F. Coester, Phys. Rev. **89**, 619 (1953).

<sup>9</sup> E. P. Wigner, *Group Theory and its Application to the Quantum Mechanics of Atomic Spectra* (English translated edition, Academic Press, Inc., New York, 1959), Chap. 26.

spin case

$$T^2 = KK^c = -1, \tag{32}$$

and  $K$  is antisymmetric and unitary. Strictly speaking, Eqs. (31) and (32) need hold only for systems not possessing super-selection rules.<sup>10</sup> It will be assumed that this condition is satisfied by all the systems which we discuss.

Suppose now that the even-spin case holds and Eq. (31) is valid. Then a unitary operator  $U$  exists such that

$$K = UU^T. \tag{33}$$

By Eq. (29), the transformation  $\psi \rightarrow U^{-1}\psi$  performed on the states  $\psi$  brings  $K$  to unity. Thus in the even-spin case the representation of states can always be chosen so that

$$K = 1. \tag{34}$$

After one such representation is found, further transformations  $\psi \rightarrow R\psi$  are allowed only with  $R$  a real orthogonal matrix, so that Eq. (34) remains valid. The consequence of Eq. (34) is that self-dual matrices are symmetric. In the even-spin case, every system invariant under time reversal will be associated, if the representation of states is suitably chosen, with a symmetric unitary matrix  $S$ . For even-spin systems with time-reversal invariance, the orthogonal ensemble  $E_1$  is always appropriate.

Suppose next that we are dealing with a system invariant under space rotations. The spin may now be either even or odd. The matrix  $S$  representing the system commutes with every component of  $J$ . If we use the standard representation of the  $J$  matrices with  $J_1$  and  $J_3$  real and  $J_2$  imaginary, the conditions (30) may be satisfied by the usual choice

$$K = \exp[i\pi J_2] \tag{35}$$

for  $K$ . With this choice of  $K$ ,  $S$  and  $K$  commute and  $S^R$  reduces to  $S^T$ . Thus a rotation-invariant system is represented by a symmetric unitary  $S$ . The ensemble  $E_1$  is in this case again appropriate.

In the case of rotational symmetry, the matrices  $S$  do not couple together states of different total angular momentum. A separate ensemble  $E_1$  must be introduced for each value of  $J$ . Levels belonging to different  $J$  values belong to different ensembles and are statistically uncorrelated. A similar remark applies if there are other conserved quantities in the problem, for example parity or isotopic spin. In such cases the known integrals of the motion must first be eliminated, and the ensemble  $E_1$  applied separately to each of the resulting uncorrelated series of levels.

For the remainder of this section we shall discuss the situation to which the ensemble  $E_1$  does not apply, a

system having odd spin, invariance under time reversal, but no rotational symmetry. In this case Eq. (32) holds,  $K$  cannot be made diagonal by any transformation of the form (29), and there is no integral of the motion by means of which the double-valuedness of the time-reversal operation can be trivially eliminated.

Every antisymmetric unitary operator can be reduced by a transformation (29) to the standard form

$$Z = \begin{pmatrix} 0 & -1 & 0 & 0 & \cdot & \cdot & \cdot \\ 1 & 0 & 0 & 0 & & & \\ 0 & 0 & 0 & -1 & & & \\ 0 & 0 & 1 & 0 & & & \\ \cdot & & & & \cdot & & \\ \cdot & & & & & \cdot & \\ \cdot & & & & & & \cdot \end{pmatrix}, \tag{36}$$

consisting of  $(2 \times 2)$  blocks

$$\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

along the leading diagonal, all other elements of  $Z$  being zero. We suppose the representation of states chosen so that  $K$  is reduced to this form. The number of rows and columns of all matrices must now be even, and it is convenient to denote this number by  $2N$  instead of by  $N$ . After one representation of states is chosen for which  $K = Z$ , further transformations  $\psi \rightarrow B\psi$  are allowed only with  $B$  a unitary  $(2N \times 2N)$  matrix for which

$$Z = BZB^T. \tag{37}$$

Such matrices  $B$  form precisely the  $N$ -dimensional symplectic group,<sup>11</sup> usually denoted by  $Sp(N)$ .

It is well known<sup>12</sup> that the algebra of the symplectic group can be expressed most naturally in terms of quaternions. We therefore introduce the standard quaternion notation for  $(2 \times 2)$  matrices

$$\tau^1 = \begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix}, \quad \tau^2 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad \tau^3 = \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix}, \tag{38}$$

with the multiplication table

$$(\tau^1)^2 = (\tau^2)^2 = (\tau^3)^2 = -1, \tag{39}$$

$$\tau^1\tau^2 = -\tau^2\tau^1 = \tau^3, \quad \tau^2\tau^3 = -\tau^3\tau^2 = \tau^1, \tag{40}$$

$$\tau^3\tau^1 = -\tau^1\tau^3 = \tau^2.$$

Note that here and always  $i$  will be the ordinary imaginary unit, not a quaternion unit. All the  $(2N \times 2N)$  matrices will be considered as cut into  $N^2$  blocks of  $(2 \times 2)$ , and each  $(2 \times 2)$  block regarded as a quaternion.

<sup>11</sup> H. Weyl, *The Classical Groups* (Princeton University Press, Princeton, New Jersey, 1946), 2nd Ed., Chap. 6.

<sup>12</sup> C. Chevalley, *Theory of Lie Groups* (Princeton University Press, Princeton, New Jersey, 1946), pp. 18-24. J. Dieudonné, *Ergeb. d. Math.* **5**, (1955).

<sup>10</sup> G. C. Wick, A. S. Wightman, and E. P. Wigner, *Phys. Rev.* **88**, 101 (1952).

In general a  $(2N \times 2N)$  matrix with complex elements becomes an  $(N \times N)$  matrix with complex quaternion elements. In particular, the matrix  $Z$  is now

$$Z = \tau_2 I, \tag{41}$$

where  $I$  is the  $(N \times N)$  unit matrix. It is easy to verify that the rules of matrix multiplication are not changed by this transcription.

We call a quaternion "real" if it is of the form

$$q = q^0 + (q \cdot \tau), \tag{42}$$

with real coefficients  $q^0, q^1, q^2, q^3$ . Thus a real quaternion does not correspond to a  $(2 \times 2)$  matrix with real elements. Any complex quaternion  $q$  has a "conjugate quaternion"

$$\bar{q} = q^0 - (q \cdot \tau), \tag{43}$$

which is distinct from its "complex conjugate,"

$$q^c = q^{0c} + (q^c \cdot \tau). \tag{44}$$

A quaternion with  $q = q^c$  is real; one with  $q = \bar{q}$  is a scalar. Applying both types of conjugation together, we obtain the "Hermitian conjugate"

$$q^+ = \bar{q}^c = q^{0c} - (q^c \cdot \tau). \tag{45}$$

Now consider a general  $(2N \times 2N)$  matrix  $A$  which is to be written as an  $(N \times N)$  matrix  $Q$  with quaternion elements  $q_{ij}; i, j = 1, \dots, N$ . The standard matrix operations on  $A$  then reflect themselves on  $Q$  in the following way: Transposition,

$$(Q^T)_{ij} = -\tau^2 \bar{q}_{ji} \tau^2, \tag{46}$$

Hermitian conjugation,

$$(Q^+)_{ij} = q_{ji}^+, \tag{47}$$

Time reversal,

$$(Q^R)_{ij} = \bar{q}_{ji}. \tag{48}$$

The usefulness of the quaternion algebra is a consequence of the simplicity of the relations (47) and (48). In particular it is noteworthy that the time-reversal operator  $K$  does not appear explicitly in Eq. (48) as it did in Eq. (26). By Eqs. (47) and (48), the condition

$$Q^R = Q^+ \tag{49}$$

is necessary and sufficient for the elements of  $Q$  to be real quaternions. When Eq. (49) holds we call  $Q$  "quaternion real."

A unitary matrix  $B$  satisfying Eq. (37) is automatically quaternion real. In fact it satisfies the conditions

$$B^R = B^+ = B^{-1}, \tag{50}$$

which define the symplectic group. The matrices  $S$  representing physical systems are not quaternion real. They are unitary and self-dual, that is

$$S^R = S, \quad S^+ = S^{-1}. \tag{51}$$

We now require a theorem of quaternion algebra.<sup>13</sup>

*Theorem 2. Let  $H$  be any Hermitian quaternion-real  $(N \times N)$  matrix. Then there exists a symplectic matrix  $B$  such that*

$$H = B^{-1} D B, \tag{52}$$

where  $D$  is diagonal, real, and scalar.

The fact that  $D$  is scalar means that it consists of  $N$  blocks of the form

$$\begin{bmatrix} D_j & 0 \\ 0 & D_j \end{bmatrix}.$$

Thus the eigenvalues of  $H$  consist of  $N$  equal pairs. The Hamiltonian of any system which is invariant under time reversal and has odd spin satisfies the conditions of Theorem 2. All energy levels of such a system must be doubly degenerate. This is the Kramers degeneracy,<sup>14</sup> and Theorem 2 shows how it appears naturally in the quaternion language.

An immediate extension of Theorem 2 states that if  $S_1$  and  $S_2$  are two commuting Hermitian quaternion-real matrices, there exists a symplectic matrix  $B$  such that

$$S_1 = B^{-1} D_1 B, \quad S_2 = B^{-1} D_2 B, \tag{53}$$

with  $D_1$  and  $D_2$  both diagonal, real, and scalar. From this extension we can deduce

*Theorem 3. Let  $S$  be any unitary self-dual  $(N \times N)$  quaternion matrix. Then there exists a symplectic matrix  $B$  such that*

$$S = B^{-1} E B, \tag{54}$$

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

To prove Theorem 3, we write

$$S = S_1 + i S_2, \tag{55}$$

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

$$S^+ S = (S_1 - i S_2)(S_1 + i S_2) = 1. \tag{56}$$

Separating quaternion real and quaternion imaginary parts in Eq. (56), we find

$$S_1^2 + S_2^2 = 1, \quad S_1 S_2 - S_2 S_1 = 0. \tag{57}$$

The  $S_1$  and  $S_2$  commute, and the extension of Theorem 2

<sup>13</sup> This theorem is presumably well known to the experts, but we are unable to find a reference to it in the mathematical literature. A nonrigorous "physicist's proof" of it is given in Appendix A of this paper.

<sup>14</sup> H. A. Kramers, Proc. Acad. Sci. Amsterdam 33, 959 (1930).

applies. Let then  $B$  be chosen to satisfy Eq. (53). Equation (54) will hold, with

$$E = D_1 + iD_2$$

diagonal and scalar. If  $d_j, d'_j$  are corresponding eigenvalues of  $D_1$  and  $D_2$ , Eq. (57) gives

$$d_j^2 + (d'_j)^2 = 1. \tag{58}$$

Hence we may write

$$d_j = \cos\theta_j, \quad d'_j = \sin\theta_j, \tag{59}$$

and the diagonal elements of  $E$  become

$$e_j = d_j + id'_j = \exp(i\theta_j), \tag{60}$$

each repeated twice.

It is convenient to state at this point the analog of Theorem 3 for the even-spin case. This is

*Theorem 4. Let  $S$  be any unitary symmetric ( $N \times N$ ) matrix. Then there exists a real orthogonal matrix  $R$  such that*

$$S = R^{-1}ER, \tag{61}$$

where  $E$  is diagonal. The diagonal elements of  $E$  are  $N$  complex numbers  $[\exp(i\theta_j)]$  on the unit circle.

The proof of Theorem 4 is word for word the same as that of Theorem 3, only substituting "symmetric" for "self-dual," "real" for "quaternion real," "orthogonal" for "symplectic." This parallelism between the odd-spin and even-spin cases will always be maintained.

Now we return to the odd-spin case and define the symplectic ensemble  $E_4$ , the odd-spin analog of the orthogonal ensemble  $E_1$ . We work in the space  $T_4$  of unitary self-dual quaternion matrices. The problem is again to define an invariant measure in  $T_4$ , in spite of the fact that the matrices of  $T_4$  do not form a group.

Every matrix  $S$  in  $T_4$  can be written in the form

$$S = URU, \tag{62}$$

with  $U$  unitary. To see that this is possible, observe that in the old prequaternion notations ( $SZ$ ) is an anti-symmetric unitary matrix and can be reduced to the canonical form

$$SZ = VZV^T \tag{63}$$

with  $V$  unitary; substituting  $(UZ)^T$  for  $V$  then gives Eq. (62). For given  $S$ , the unitary matrix  $U$  in Eq. (62) is undetermined precisely to the extent of a transformation

$$U \rightarrow BU, \tag{64}$$

where  $B$  is an arbitrary symplectic matrix; the proof of this statement is word for word the same as that of Eq. (20). An infinitesimal neighborhood of  $S$  in  $T_4$  is given by

$$S + dS = U^R[1 + idM]U, \tag{65}$$

where  $dM$  is a quaternion-real self-dual infinitesimal

matrix with elements

$$dM_{ij} = dM_{ij}^0 + (dM_{ij} \cdot \tau). \tag{66}$$

The real coefficients  $dM_{ij}^\alpha$  satisfy

$$dM_{ij}^0 = dM_{ji}^0, \quad dM_{ij}^\alpha = -dM_{ji}^\alpha \quad \text{for } \alpha = 1, 2, 3. \tag{67}$$

There are  $(2N^2 - N)$  independent real variables  $dM_{ij}^\alpha$ , and they are supposed to vary through some small intervals of lengths  $d\mu_{ij}^\alpha$ . The neighborhood of  $S$  thus defined has the measure

$$\mu(dS) = \prod_{\alpha, i, j} d\mu_{ij}^\alpha. \tag{68}$$

In terms of this measure, the symplectic ensemble  $E_4$  is defined exactly like  $E_1$ . The statistical weight of the neighborhood  $dS$  in  $E_4$  is

$$P(dS) = (V_4)^{-1} \mu(dS), \tag{69}$$

where  $V_4$  is the total volume of the space  $T_4$ .

We can now repeat almost without change the arguments of Sec. II. We must first prove that the measure  $\mu(dS)$  is independent of the choice of  $U$  in Eq. (62). This involves showing that the Jacobian

$$J = \det |\partial dM_{ij}^\alpha / \partial dM_{kl}^\beta| \tag{70}$$

has absolute value unity, where

$$dM' = BdMB^{-1} \tag{71}$$

and  $B$  is symplectic. As before, it is enough to consider the case

$$B = I + A, \tag{72}$$

where  $A$  is infinitesimal, quaternion real, and anti-self-dual. Let the quaternion coefficients of  $A$  be  $a_{ij}^\alpha$ , with  $\alpha = 0, 1, 2, 3$ . The diagonal elements of the matrix  $(\partial dM_{ij}^\alpha / \partial dM_{kl}^\beta)$  can only involve the coefficients  $a_{ij}^0$ , and these occur just like the  $a_{ij}$  in Eq. (18). The conclusion that  $J = 1$  to first order in  $A$  follows as before.

The analog of Theorem 1 is

*Theorem 5. 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*

$$S \rightarrow W^R S W \tag{73}$$

of  $T_4$  into itself, where  $W$  is any unitary matrix.

Theorem 5 can be proved by following word for word the proof of Theorem 1. Theorem 5 shows that the symplectic ensemble uniquely represents the notion of "uniform a priori probability" in the space  $T_4$ .

#### IV. SYSTEMS WITHOUT TIME-REVERSAL SYMMETRY. UNITARY ENSEMBLE

For completeness we briefly discuss a much simpler ensemble, the unitary ensemble  $E_2$ , which would apply to systems without invariance under time reversal.

Such systems are in principle easily created, for example by putting an ordinary atom or nucleus into an externally generated magnetic field. However, for the unitary ensemble to be applicable, the splitting of the levels by the magnetic field must be at least as large 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 zero field. Such a state of affairs could never occur in nuclear physics; in atomic or molecular physics a practical application of the unitary ensemble may perhaps be possible.

A system without invariance under time reversal has a Hamiltonian which may be an arbitrary Hermitian matrix, not restricted to be symmetric or self-dual. We represent the system by an  $(N \times N)$  unitary matrix  $S$  belonging to the space  $T_2$  of all unitary matrices. It is now a trivial matter to define a uniform ensemble  $E_2$  in  $T_2$ , because the space  $T_2$  is simply the unitary group  $U(N)$ , and an invariant group measure in  $U(N)$  is already provided.<sup>15</sup>

The formal definition of  $E_2$  is as follows. A neighborhood of  $S$  in  $T_2$  is given by

$$S + dS = U(1 + idH)V, \tag{74}$$

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

$$\mu(dS) = \prod_{i,j} d\mu_{ij}^1 d\mu_{ij}^2, \tag{75}$$

and is independent of the choice of  $U$  and  $V$ . The ensemble  $E_2$  gives to each neighborhood  $dS$  the statistical weight

$$P(dS) = (V_2)^{-1} \mu(dS), \tag{76}$$

where  $V_2$  is the volume of the space  $T_2$ .

The invariance property of  $E_2$  analogous to Theorems 1 and 5 is stated in

*Theorem 6. 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*

$$S \rightarrow USW \tag{77}$$

of  $T_2$  into itself, where  $U, W$  are any two matrices of  $T_2$ .

This theorem merely expresses the fact that  $\mu(dS)$  is the invariant group-measure on  $U(N)$ .

### V. CALCULATION OF THE JOINT EIGENVALUE DISTRIBUTIONS

The joint distribution of the eigenvalues  $(\epsilon_1, \dots, \epsilon_N)$  of the Hamiltonian in the Gaussian ensemble was

derived by Porter and Rosenzweig.<sup>4</sup> Their result is the following

*Theorem 7. In the Gaussian ensemble defined by Eq. (1), the probability for finding an eigenvalue in each of the intervals  $[\epsilon_j, \epsilon_j + d\epsilon_j]$ ,  $j = 1, \dots, N$ , is given by  $P_N(\epsilon_1, \dots, \epsilon_N) d\epsilon_1 \dots d\epsilon_N$ , where*

$$P_N(\epsilon_1, \dots, \epsilon_N) = K_N \left\{ \prod_{i < j} |\epsilon_i - \epsilon_j| \right\} \exp\left(-\sum_j \epsilon_j^2 / 4a^2\right), \tag{78}$$

and  $K_N$  is a constant.

Following the same method of proof, we shall obtain the corresponding formulas for the joint distribution function of the eigenvalues  $[\exp(i\theta_j)]$  in the orthogonal, unitary and symplectic ensembles.

*Theorem 8. In the ensemble  $E_\beta$ , the probability for finding eigenvalues  $[\exp(i\varphi_j)]$  of  $S$  with an angle  $\varphi_j$  in each of the intervals  $[\theta_j, \theta_j + d\theta_j]$ ,  $j = 1, \dots, N$ , is given by  $Q_{N\beta}(\theta_1, \dots, \theta_N) d\theta_1 \dots d\theta_N$ , where*

$$Q_{N\beta}(\theta_1, \dots, \theta_N) = C_{N\beta} \prod_{i < j} |e^{i\theta_i} - e^{i\theta_j}|^\beta. \tag{79}$$

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

This theorem explains the choice of the notation  $E_\beta$  and  $T_\beta$  for the three ensembles and their corresponding spaces.

The unitary case ( $\beta = 2$ ) of Theorem 8 is a well-known result in the theory of the unitary group.<sup>16</sup> It will be enough for us to prove the theorem in detail for  $\beta = 1$  and to indicate the necessary modifications in the proof for  $\beta = 2, 4$ .

Let  $\beta = 1$ . By Theorem 4, every  $S$  in  $T_1$  may be diagonalized into the form

$$S = R^{-1}ER, \tag{80}$$

with  $R$  orthogonal. We wish now to express the measure  $\mu(dS)$  in terms of measures  $\mu(dE), \mu(dR)$  defined on the matrices  $E, R$  separately. Small neighborhoods of  $E$  and  $R$  are given by

$$dE = iEd\theta, \tag{81}$$

$$dR = dA.R. \tag{82}$$

Here  $d\theta$  means the diagonal matrix with elements  $[d\theta_1, \dots, d\theta_N]$ , and  $dA$  is a real antisymmetric infinitesimal matrix with elements  $dA_{ij}$ . We define

$$\mu(dE) = \prod_j d\theta_j, \tag{83}$$

$$\mu(dR) = \prod_{i < j} dA_{ij}, \tag{84}$$

the latter being the invariant group measure in the orthogonal group  $O(N)$ .

The measure  $\mu(dS)$  is defined by Eq. (6), where  $dM$  is

<sup>15</sup> H. Weyl, reference 11, p. 188.

<sup>16</sup> H. Weyl, reference 11, p. 197, Theorem 7.4C.



given by Eq. (5) and  $U$  is any unitary matrix satisfying Eq. (4). The relation between  $dM$ ,  $d\theta$ , and  $dA$  is given by Eqs. (5), (80), (81), and (82) and is

$$iRU^T dMUR^{-1} = iEd\theta + EdA - dAE. \tag{85}$$

Since  $E$  is a diagonal unitary matrix it has a square root  $F$  with elements  $[\exp(\frac{1}{2}i\theta_j)]$ . There is an ambiguity of a factor  $\pm 1$  in each element of  $F$ ; it does not matter how these signs are chosen. A convenient choice for  $U$  satisfying Eq. (4) is then

$$U = FR, \tag{86}$$

by virtue of Eq. (80). With this choice of  $U$ , Eq. (85) reduces to

$$dM = d\theta - i[FdAF^{-1} - F^{-1}dAF]. \tag{87}$$

The last equation is a separate equation for each component  $dM_{ij}$ , namely,

$$dM_{jj} = d\theta_j, \tag{88}$$

$$dM_{ij} = 2 \sin[\frac{1}{2}(\theta_i - \theta_j)] dA_{ij}, \quad i \neq j. \tag{89}$$

Assembling the definitions (6), (83), and (84), we deduce from Eqs. (88) and (89)

$$\begin{aligned} \mu(dS) &= \left\{ \prod_{i < j} |2 \sin \frac{1}{2}(\theta_i - \theta_j)| \right\} \mu(dE) \mu(dR) \\ &= \left\{ \prod_{i < j} |e^{i\theta_i} - e^{i\theta_j}| \right\} \mu(dE) \mu(dR). \end{aligned} \tag{90}$$

If now the angles  $[\theta_1, \dots, \theta_N]$  are held fixed, and Eq. (90) is integrated with respect to  $dR$  over the whole orthogonal group  $O(N)$ , the result is Eq. (79) with  $\beta = 1$ . Theorem 1 is thus proved in the orthogonal case.

Next let  $\beta = 2$ . In this case  $R$  in Eq. (80) is unitary, and  $dA$  in Eq. (82) is anti-Hermitian, while  $dM$  is Hermitian. The equations (87) and (88) hold as before, but now Eq. (89) holds separately for the real and imaginary parts of each nondiagonal  $dM_{ij}$ , these being independent variables. The diagonal elements  $dA_{jj}$  are pure imaginary and do not appear in Eq. (89). Their absence reflects the fact that  $S$  is unchanged by the substitution

$$R \rightarrow GR \tag{91}$$

in Eq. (80), if  $G$  is any diagonal unitary matrix. The relation between measures analogous to Eq. (90) then becomes

$$\mu(dS) \mu(dG) = \left\{ \prod_{i < j} |e^{i\theta_i} - e^{i\theta_j}|^2 \right\} \mu(dE) \mu(dR). \tag{92}$$

Here  $\mu(dS)$  and  $\mu(dR)$  are invariant measures on  $U(N)$ ,  $\mu(dE)$  is defined by Eq. (83), and

$$\mu(dG) = \prod_j d\eta_j, \tag{93}$$

where  $G$  is the diagonal matrix with elements  $[\exp(i\eta_j)]$ . The step from Eq. (92) to the theorem goes as before.

Lastly let  $\beta = 4$ . In this case, by Theorem 3, Eq. (80)

holds with  $R$  symplectic. A neighborhood of  $R$  in the symplectic group  $Sp(N)$  is given by Eq. (82), where  $dA$  is now an anti-Hermitian quaternion-real infinitesimal matrix. The components of  $dA$  are  $dA_{ij}^\alpha$ , which are independent real variables, antisymmetric in  $(i, j)$  for  $\alpha = 0$ , symmetric in  $(i, j)$  for  $\alpha = 1, 2, 3$ . The total number of the  $dA_{ij}^\alpha$  is  $(2N^2 + N)$ . The invariant measure on the symplectic group is

$$\mu(dR) = \prod_{i, j, \alpha} dA_{ij}^\alpha. \tag{94}$$

The measure  $\mu(dS)$  is given by Eq. (68), with  $dM$  given by Eqs. (62) and (65). The matrix  $dM$  is Hermitian and quaternion real, and has  $(2N^2 - N)$  independent components according to Eq. (67). The algebra leading up to Eq. (87) goes exactly as before. Equation (88) still holds, the diagonal elements  $dM_{jj}$  being real scalar quaternions with only one independent component. Also Eq. (89) holds, for the nondiagonal elements, separately in each of the four quaternion components  $\alpha = 0, 1, 2, 3$ .

There are now  $3N$  diagonal components  $dA_{jj}^\alpha$ ,  $\alpha = 1, 2, 3$ , which do not appear in Eq. (89). Their absence reflects the fact that  $S$  is unchanged by the substitution (91) in Eq. (80), where  $G$  may now be an arbitrary diagonal matrix whose elements are real unimodular quaternions. Let  $g_j$  be the diagonal elements of  $G$ , satisfying

$$\bar{g}_j g_j = 1. \tag{95}$$

A neighborhood of  $G$  is defined by writing

$$dg_j = (d\eta_j) g_j, \tag{96}$$

where  $d\eta_j$  is a pure vector quaternion, quaternion real and anti-Hermitian. There are  $3N$  independent components  $d\eta_j^\alpha$ , and a measure in the space of  $G$  is defined by writing

$$\mu(dG) = \prod_{\alpha, j} d\eta_j^\alpha. \tag{97}$$

A comparison of Eq. (82) with Eq. (96) gives

$$d\eta_j^\alpha = dA_{jj}^\alpha, \quad \alpha = 1, 2, 3. \tag{98}$$

Multiplying together the  $N$  equations (88), the  $(2N^2 - 2N)$  equations (89), and the  $3N$  equations (98), we obtain the relation

$$\mu(dS) \mu(dG) = \left\{ \prod_{i < j} |e^{i\theta_i} - e^{i\theta_j}|^4 \right\} \mu(dE) \mu(dR), \tag{99}$$

which establishes Theorem 8 for  $\beta = 4$ .

The most obvious physical consequence of Theorem 8 is the so-called "repulsion of energy levels." The probability of finding an unusually small separation  $\Delta = (\theta_i - \theta_j)$  between two levels tends to zero with  $\Delta$  like  $\Delta^\beta$ . According to Theorem 7 this phenomenon occurs also in the Gaussian model (where effectively  $\beta = 1$ ), a fact which was well known to Wigner and others. What

is new and unexpected in Theorem 8 is that the level repulsion is so drastically stronger in the symplectic ensemble, going with  $\Delta^4$  instead of  $\Delta$ . Qualitatively speaking, one may say that the presence of the Kramers degeneracy makes any additional accidental degeneracy enormously more unlikely.

It is possible to understand the different powers  $\beta$  which appear in Eq. (79) by a simple mathematical argument based on counting dimensions. The dimension of the space  $T_1$  is  $\frac{1}{2}(N^2+N)$ , while the dimension of the subspace  $T_1'$  composed of matrices in  $T_1$  with two equal eigenvalues is  $[\frac{1}{2}(N^2+N)-2]$ . The difference in dimension, being 2 instead of 1, accounts for a factor in Eq. (79) linear in  $\Delta$ . Similarly, when  $\beta=2$ , the dimension of  $T_2$  is  $N^2$  while that of  $T_2'$  is  $[N^2-3]$ . When  $\beta=4$ , the dimension of  $T_4$  is  $[2N^2-N]$  while that of  $T_4'$  is  $[2N^2-N-5]$ .

VI. ELECTROSTATIC ANALOG

Consider an infinitely thin circular conducting wire of radius 1. Let  $N$  unit charges be free to move on the wire, the positions of the charges being identified by angular variables  $[\theta_1, \dots, \theta_N]$ . The universe is supposed to be two-dimensional, being merely the plane in which the circle lies. The charges repel each other, according to the Coulomb law of two-dimensional electrostatics, with a potential energy

$$W = - \sum_{i < j} \ln |e^{i\theta_i} - e^{i\theta_j}|. \tag{100}$$

We shall study the statistical mechanics of this Coulomb gas, considered as a classical system.

In classical statistical mechanics the velocity distribution of the charges is trivial and can be separated from the position distribution. We shall simply discard the velocity-dependent factors and their (easily calculable) contributions to the thermodynamics of the problem. The probability distribution of the angles  $[\theta_1, \dots, \theta_N]$ , when the Coulomb gas is in thermal equilibrium at temperature  $T$ , is then given by

$$Q_{N\beta}(\theta_1, \dots, \theta_N) = C_{N\beta} \exp[-\beta W], \tag{101}$$

with

$$\beta = 1/T. \tag{102}$$

The nontrivial contributions to the thermodynamic variables are to be calculated from the positional partition-function

$$\Psi_N(\beta) = (2\pi)^{-N} \int \dots \int_0^{2\pi} \exp[-\beta W] d\theta_1 \dots d\theta_N. \tag{103}$$

The reader will probably have observed that the distributions (79) and (101) are identical. We have therefore established

*Theorem 9. There is a precise mathematical identity between the distribution of eigenvalues of a random matrix*

*S and the distribution of positions of charges in a finite Coulomb gas at a finite temperature T. When S is taken from the orthogonal ensemble, the unitary ensemble, or the symplectic ensemble, the corresponding temperature of the gas is  $T=1$ ,  $T=\frac{1}{2}$ , or  $T=\frac{1}{4}$ , respectively.*

The beauty of Theorem 9 is that it shows the expression "repulsion of energy levels" to be more than an empty phrase. Energy levels do indeed behave exactly as if they were like charges, repelling each other with a force varying inversely with the first power of the distance. Another consequence of Theorem 9 is that the thermodynamic notions of entropy, specific heat, etc., can be transferred from the Coulomb gas to the eigenvalue series. This will prove very useful, as it gives us a precise and well-understood language in which to describe the statistical properties of the eigenvalue series.

It may seem strange that the temperature in Theorem 9 is a dimensionless quantity. The reason for this is that we have chosen the magnitude of the charges to be unity. In two-dimensional electrostatics, the dimensions of charge are [energy]<sup>1/2</sup>. If the charges had been taken to be equal to  $e$ , then the temperatures in Theorem 9 would be  $T=e^2$ ,  $T'=\frac{1}{2}e^2$ ,  $T=\frac{1}{4}e^2$ , giving  $T$  the dimensions of energy.

VII. CALCULATION OF THE PARTITION FUNCTION

In this section we use a simple group-theoretical argument to evaluate the partition function

$$\Psi_N(\beta) = (2\pi)^{-N} \int \dots \int_0^{2\pi} \left\{ \prod_{i < j} |e^{i\theta_i} - e^{i\theta_j}|^\beta \right\} \times d\theta_1 \dots d\theta_N, \tag{104}$$

for the physical values 1, 2, and 4 of  $\beta$ . The result can be checked easily by a direct calculation in the case  $\beta=2$ ; for  $\beta=1$  a direct calculation is very difficult but possible, using the methods of Mehta<sup>5</sup>; for  $\beta=4$  no method of direct calculation has yet been found.

The method of procedure is to integrate over all the variables  $dS$ ,  $dG$ ,  $dE$ , and  $dR$  in Eqs. (90), (92), and (99). The relation (80) shows that  $S$  is fixed when  $E$  and  $R$  are given. However, when  $S$  is given,  $E$  and  $R$  are still subject to freedom of choice in two respects. (i) The order of the  $N$  angles  $\theta_j$  may be permuted in any of  $(N!)$  ways, provided that the rows of  $R$  are simultaneously permuted in the same way. (ii)  $R$  may be multiplied on the left by the diagonal matrix  $G$ , each of whose  $N$  diagonal elements may be chosen independently. The elements of  $G$  belong to a space  $\sum_\beta$  which is geometrically the surface of a sphere of unit radius in a space of  $\beta$  dimensions. When  $\beta=1$ ,  $\sum_\beta$  consists of the two points  $\pm 1$  only. When  $\beta=2$ ,  $\sum_\beta$  consists of the complex numbers with unit modulus. When  $\beta=4$ ,  $\sum_\beta$  consists of the unimodular real quaternions.

The integration of Eqs. (90), (91), and (99) then gives

$$N!V_\beta[S_\beta]^N = (2\pi)^N \Psi_N(\beta)\Omega_\beta. \tag{105}$$

Here  $V_\beta$  is the volume of the ensemble space  $T_\beta$ , defined by the measure  $\int \mu(dS)$ .  $S_\beta$  is the surface area of the  $\beta$ -dimensional sphere  $\sum_\beta$ , namely,

$$S_\beta = [2 \cdot \pi^{\beta/2} / \Gamma(\frac{\beta}{2})]. \tag{106}$$

In particular, when  $\beta=1$ ,  $S_\beta=2$ , which is correct since  $\int \mu(dG)$  then reduces to a summation over  $N$  independent choices of  $\pm 1$ . Finally,

$$\Omega_\beta = \int \mu(dR) \tag{107}$$

is the volume of the orthogonal group  $O(N)$  for  $\beta=1$ , of the unitary group  $U(N)$  for  $\beta=2$ , and of the symplectic group  $Sp(N)$  for  $\beta=4$ . The value of  $\Omega_\beta$  is

$$\Omega_\beta = S_{N\beta} S_{(N-1)\beta} \cdots S_\beta, \tag{108}$$

with  $S_\beta$  given by Eq. (106). To prove Eq. (108), consider for example  $\Omega_4$ . The general matrix in  $Sp(N)$  consists of  $N$  vectors each having  $N$  quaternion components; these vectors are of unit length and pair-wise orthogonal in the quaternion sense. We can choose the first vector to be any set of  $N$  quaternions such that the sum of the squares of their  $4N$  real coefficients is unity. The first vector then is free to move on a  $4N$ -dimensional sphere of measure  $S_{4N}$ . The remaining  $(N-1)$  vectors are all perpendicular to the first and form a symplectic matrix in  $Sp(N-1)$ . Therefore

$$\Omega_4(N) = S_{4N} \Omega_4(N-1), \tag{109}$$

and this proves Eq. (108) for  $\beta=4$ . The proof for  $\beta=1, 2$  is the same. Note that here  $O(N)$  is the full orthogonal group, including reflections, so that the last factor  $S_1=2$  occurs correctly in Eq. (108) when  $\beta=1$ .

It remains only to determine the  $V_\beta$ . Take first  $\beta=1$  and go back to the definition of  $\mu(dS)$  by Eqs. (4)-(6). Let us define a neighborhood of  $U$  in the unitary group  $U(N)$  by

$$dU = idHU, \tag{110}$$

with  $dH$  Hermitian. Writing  $dH_{ij} = dH_{ij}^1 + idH_{ij}^2$ , the measure  $\mu(dU)$  is given by Eq. (75). Assembling Eqs. (4), (5), and (110), we find

$$dM_{ij} = dH_{ij} + dH_{ji} = 2dH_{ij}^1. \tag{111}$$

The antisymmetric components  $dH_{ij}^2$  of  $dH$  do not appear in Eq. (111). In fact, when  $S$  is fixed, the matrix  $U$  is undetermined by a transformation (20) with  $R$  orthogonal, and the measure of a neighborhood of  $R$  is given precisely by

$$dR = -dH^2R, \tag{112}$$

$$\mu(dR) = \prod_{i<j} dH_{ij}^2. \tag{113}$$

Assembling Eqs. (6), (75), and (113), we find

$$\mu(dS)\mu(dR) = 2^{iN(N+1)}\mu(dU). \tag{114}$$

Integrating this over all the variables gives the desired result,

$$V_1 = 2^{iN(N+1)}[\Omega_2/\Omega_1]. \tag{115}$$

In the case  $\beta=2$  the evaluation of  $V_\beta$  is trivial, since  $T_2$  is  $U(N)$  and therefore

$$V_2 = \Omega_2. \tag{116}$$

Lastly let  $\beta=4$ . The measure  $\mu(dS)$  in  $T_4$  is defined by Eqs. (62), (65), (66), and (68), where  $U$  now belongs to the group  $U_q(N)$  of unitary  $(N \times N)$  matrices with complex quaternion elements. A neighborhood of  $U$  in  $U_q(N)$  is given by Eq. (110), with  $dH$  a Hermitian quaternion matrix. An element of  $dH$  has the form

$$dH_{ij} = dH_{ij}^{10} + idH_{ij}^{20} + \sum_{\alpha=1}^3 (dH_{ij}^{1\alpha} + idH_{ij}^{2\alpha})\tau^\alpha, \tag{117}$$

with eight independent real coefficients  $dH_{ij}^{k\alpha}$ . The measure in  $U_q(N)$  is given by

$$\mu(dU) = \prod_{i,j,k,\alpha} dH_{ij}^{k\alpha}. \tag{118}$$

Assembling Eqs. (62), (65), and (110) gives

$$dM_{ij}^\alpha = 2dH_{ij}^{1\alpha}, \quad \alpha=0, 1, 2, 3, \tag{119}$$

the components  $dH_{ij}^{2\alpha}$  again not appearing. When  $S$  is fixed,  $U$  is undetermined by a symplectic transformation (64), and the measure of a neighborhood of  $B$  in the symplectic group  $Sp(N)$  is given by

$$dB = -dH^2B, \tag{120}$$

$$\mu(dB) = \prod_{i,j,\alpha} dH_{ij}^{2\alpha}. \tag{121}$$

Since the number of equations (119) is  $(2N^2-N)$ , Eqs. (68), (118), and (121) give

$$\mu(dS)\mu(dB) = 2^{N(2N-1)}\mu(dU). \tag{122}$$

Integrating this over all variables gives

$$V_4 = 2^{N(2N-1)}[\Omega_8/\Omega_4], \tag{123}$$

where  $\Omega_8$  is the volume of  $U_q(N)$ , and  $\Omega_4$  that of  $Sp(N)$ .

Although Eq. (108) holds for  $\beta=1, 2, 4$ , it does not hold for  $\beta=8$ , since the complex quaternions do not form a division algebra. Instead,  $U_q(N)$  is merely a different parametrization of the ordinary unitary group  $U(2N)$ . The group measure in  $U(2N)$  is given by

$$dU = idKU, \quad dK = dK^1 + idK^2, \tag{124}$$

$$\mu(dU) = \prod_{i,j} dK_{ij}^1 dK_{ij}^2, \tag{125}$$

where  $dK^1$  and  $dK^2$  are real  $(2N \times 2N)$  matrices, symmetric and antisymmetric, respectively. The matrices  $dH$  and  $dK$  must be identical, only  $dH$  is expressed in quaternion components by Eq. (117) while  $dK$  is expressed in ordinary matrix components by Eq. (124). The relation between the  $dH_{ij}^{k\alpha}$  and the  $dK_{ij}^k$  is then the following. A complex quaternion (117), which may be written for brevity

$$a^1 + ia^2 + (b^1 + ib^2)\tau^1 + (c^1 + ic^2)\tau^2 + (d^1 + id^2)\tau^3, \quad (126)$$

appears in the  $dK$  matrix as a  $(2 \times 2)$  block

$$\begin{bmatrix} a^1 + d^2 + i(a^2 - d^1) & b^2 - c^1 + i(-b^1 - c^2) \\ b^2 + c^1 + i(c^2 - b^1) & a^1 - d^2 + i(a^2 + d^1) \end{bmatrix}. \quad (127)$$

For each nondiagonal  $dH_{ij}$ , all eight components are present in Eqs. (126) and (127). For the diagonal elements  $dH_{jj}$ ,  $a^2 = b^1 = c^1 = d^1 = 0$  and only  $a^1$ ,  $b^2$ ,  $c^2$ , and  $d^2$  survive.

The Jacobian of the transformation from the components  $a^1, b^1, c^1, d^1, a^2, b^2, c^2, d^2$  to the linear combinations appearing in Eq. (127) is  $2^4$  for each of  $\frac{1}{2}(N^2 - N)$  nondiagonal  $dH_{ij}$ , and 2 for each of  $N$  diagonal  $dH_{jj}$ . Hence the Jacobian of the total transformation from the  $dH_{ij}^{k\alpha}$  to the  $dK_{ij}^k$  is

$$J = \det |\partial dK_{mn}^p / \partial dH_{ij}^{k\alpha}| = 2^{N(2N-1)}. \quad (128)$$

According to Eqs. (118) and (125), the volume of  $U(2N)$  is just  $J$  times the volume of  $U_q(N)$ . Therefore, Eq. (123) reduces to

$$V_4 = [\Omega_2(2N) / \Omega_4(N)]. \quad (129)$$

It is now only a matter of simple arithmetic to compute  $\Psi_N(\beta)$  from Eqs. (105), (106), (108), (115), (116), and (129). We find

$$\Psi_N(1) = N! \pi^{-N} 2^{\frac{1}{2}N(N+1)} [\Omega_2 / \Omega_1^2] = \Gamma(1 + \frac{1}{2}N) / [\Gamma(\frac{3}{2})]^N, \quad (130)$$

$$\Psi_N(2) = N!, \quad (131)$$

$$\Psi_N(4) = N! \pi^{-N} \{ \Omega_2(2N) / [\Omega_4(N)]^2 \} = 2^{-N} (2N)!. \quad (132)$$

These results lead to the following general statement:

*Conjecture A. For every integer  $N$  and real or complex  $\beta$ , we have identically*

$$\Psi_N(\beta) = \Gamma(1 + \frac{1}{2}N\beta) / [\Gamma(1 + \frac{1}{2}\beta)]^N. \quad (133)$$

The evidence for the truth of this conjecture is overwhelmingly strong. We have proved it for  $\beta = 1, 2$ , or  $4$ , and for many other special cases to be described in the following section. But a general proof is still lacking. The failure of our strenuous efforts to find a proof has led us to surmise that some novel and interesting mathematics is lurking behind this innocent-looking identity.

### VIII. MATHEMATICAL STATUS OF THE CONJECTURE

In this section we marshal the mathematical evidence in favor of conjecture A.

We first examine the analytic behavior of  $\Psi_N(\beta)$  as a function of the complex variable  $\beta$ . It is easy to verify (and physically intuitive) that the maximum value of the quantity

$$y = \prod_{i < j} |e^{i\theta_i} - e^{i\theta_j}| \quad (134)$$

is attained when the points  $e^{i\theta_j}$  are arranged at the vertices of a regular  $N$ -sided polygon, and that the maximum is equal to

$$Y = N^{\frac{1}{2}N}. \quad (135)$$

Therefore

$$\Psi_N(\beta) = \int_0^Y P(y) y^\beta dy, \quad (136)$$

where  $P(y)$  is a positive weight function. In other words,  $\Psi_N(\beta)$  is a moment-function defined on a finite interval.<sup>17</sup> Such a function must possess very special analytic properties. It must be analytic in the half-plane ( $\text{Re}\beta > 0$ ), and it must satisfy there the inequality

$$|\Psi_N(\beta)| < C |Y^\beta|. \quad (137)$$

Now the function

$$\psi_N(\beta) = \Gamma(1 + \frac{1}{2}N\beta) / [\Gamma(1 + \frac{1}{2}\beta)]^N \quad (138)$$

certainly satisfies these conditions. It has singularities only on the negative real axis, and its asymptotic behavior for large  $|\beta|$  is

$$\psi_N(\beta) \sim N^{\frac{1}{2}} (\pi\beta)^{-\frac{1}{2}(N-1)} Y^\beta. \quad (139)$$

The function

$$\Delta_N(\beta) = Y^{-\beta} [\Psi_N(\beta) - \psi_N(\beta)] \quad (140)$$

is thus regular and bounded in  $\text{Re}\beta > 0$ .

Now a theorem of Carlson<sup>18</sup> states:

*Carlson's Theorem. If a function of  $\beta$  is regular and bounded in  $\text{Re}\beta > 0$ , and if it is zero for  $\beta = 2, 4, 6, \dots$ , then it is identically zero.*

Applying this theorem to the function  $\Delta_N(\beta)$ , we deduce that conjecture A, for any fixed value of  $N$ , must hold identically in  $\beta$  if it holds for every even integer  $\beta = 2k$ . For  $\beta = 2k$ , the integrand in Eq. (104) reduces to a finite polynomial in the variables  $z_j = \exp(i\theta_j)$ . We have thus proved that conjecture A is equivalent to the following purely algebraic statement:

<sup>17</sup> J. A. Shohat and J. D. Tamarkin, *The Problem of Moments* (The American Mathematical Society, Providence, Rhode Island, 1943), p. 8.

<sup>18</sup> See E. C. Titchmarsh, *Theory of Functions* (Oxford University Press, Oxford, England, 1939), 2nd Ed., p. 186.

Conjecture B. For positive integer values of  $N$  and  $k$ , the coefficient of

$$[z_1 z_2 \cdots z_N]^{(N-1)k} \tag{141}$$

in the polynomial

$$\prod_{i \neq j} [z_i - z_j]^k \tag{142}$$

is equal to

$$(Nk)!/[k!]^N. \tag{143}$$

Note that each pair  $(i, j)$  in the product (142) is counted twice. This way of writing the product eliminates an unaesthetic minus sign from Eq. (143).

This algebraic form of the conjecture looks so simple that it ought to be provable by elementary combinatorial methods. However, the illusion of simplicity is quickly dispelled if one looks at the previous history of the problem.

When  $N=1$  or  $2$ , the conjecture is indeed trivial. So far as we have been able to discover, the only nontrivial case of the conjecture that has been previously known is the case  $N=3$ . The case  $N=3$  appears, in heavily disguised form, as Eq. VI, (3) in the first letter<sup>19</sup> written by Ramanujan to Hardy in 1913, the letter which resulted in Ramanujan being discovered as a mathematical genius. Like all Ramanujan's statements, this one is very far from being trivial; however, it was not new in 1913. An equivalent form of conjecture B for  $N=3$  is the identity

$$\sum_{j=-k}^k (-1)^j \binom{2k}{k+j}^3 = \frac{(3k)!}{(k!)^3}, \tag{144}$$

where

$$\binom{2k}{k+j}$$

is a binomial coefficient. In this form the statement was first proposed as a conjecture by Morley,<sup>20</sup> and was proved by Dixon<sup>21</sup> in 1891. Subsequently, Dixon<sup>22</sup> found and proved a natural generalization of Eq. (144), namely

$$\sum_j (-1)^j \binom{a+b}{a+j} \binom{b+c}{b+j} \binom{c+a}{c+j} = \frac{(a+b+c)!}{a!b!c!}, \tag{145}$$

valid for any positive integers  $a, b$ , and  $c$ . As is often the case in such problems, an inductive proof of Eq. (145) is easier than a direct proof of the special case (144).

In trying to deal with the case of general  $N$  by

<sup>19</sup> S. Ramanujan, *Collected Papers* (Cambridge University Press, Cambridge, England, 1927), p. 26 of the Introductory Notice. The same equation appears as Eq. (1.1) in G. H. Hardy, *Ramanujan* (Cambridge University Press, Cambridge, England, 1940), p. 7.

<sup>20</sup> By private communication. See, also, F. Morley, *Proc. London Math. Soc.* 34, 397 (1902).

<sup>21</sup> A. C. Dixon, *Messenger of Math.* 20, 79 (1891).

<sup>22</sup> A. C. Dixon, *Proc. London Math. Soc.* 35, 285 (1903).

algebraic methods, one is led to the following generalized conjecture:

Conjecture C. Let  $(a_1, a_2, \dots, a_N)$  be any set of  $N$  positive integers. Then the constant term in the expansion of the polynomial

$$\prod_{i \neq j} \left[ 1 - \frac{z_j}{z_i} \right]^{a_i} \tag{146}$$

in powers of  $(z_1, \dots, z_N)$  is

$$(a_1 + \dots + a_N)!/[a_1! a_2! \cdots a_N!]. \tag{147}$$

In the case  $N=3$ , conjecture C reduces to Eq. (145) and is thus known to be correct. For general  $N$ , conjecture C reduces to conjecture B when  $a_1 = a_2 = \dots = a_N = k$ .

The evidence in favor of conjecture C is again overwhelming. We have succeeded in proving it (and hence also conjectures A and B) for the cases  $N=4$  and  $5$ . The proof for  $N=4$  is given in Appendix B of this paper. It is based on the "evergreen proof," a combination of the principles of induction and symmetry, first invented in a different connection by Dougall.<sup>23</sup> The same method works, with greater complications of detail, when  $N=5$ . Beyond  $N=5$ , these algebraic devices seem to fail utterly.

To summarize the evidence for conjecture A, it is known to be true for all  $\beta$  if it is true for  $\beta=2k$ ; it is known to be true for all  $N$  with  $\beta=1, 2$ , or  $4$ ; and it is known to be true for all  $\beta$  with  $N=1, 2, 3, 4$ , or  $5$ . The simplest case in which it could conceivably be false is  $N=\beta=6$ , and even to test it in this special case would require a prohibitive amount of numerical computation.

In the next section we shall find some additional independent evidence. Namely, conjecture A makes definite predictions concerning the thermodynamic behavior of the Coulomb gas in both the high-temperature limit  $\beta \rightarrow 0$  and the low-temperature limit  $\beta \rightarrow \infty$ . These predictions can be checked against perturbation-theory expansions in powers of  $\beta$  and  $\beta^{-1}$ , respectively. In all cases which have been examined, the agreement is exact.

*Note added in proof.* Conjecture C has now been proved by Dr. Kenneth Wilson of Harvard University and by Dr. J. Gunson of the University of Birmingham, England. Wilson's proof will shortly be published in this journal. Gunson's proof is essentially the same as Wilson's, but was found independently.

### IX. PHYSICAL CONSEQUENCES OF THE CONJECTURE

Conjecture A specifies precisely the statistical properties of a finite Coulomb gas of  $N$  particles. For physical applications, and in particular for describing the statistical properties of eigenvalues of complex systems, we are only interested in the limit  $N \rightarrow \infty$ . We study in

<sup>23</sup> J. Dougall, *Proc. Edinburgh Math. Soc.* 25, 114 (1907).

TABLE I. Values of the thermodynamic quantities  $F$ ,  $U$ ,  $S$ , and  $C$  as functions of  $\beta = T^{-1}$ .  $\gamma$  is Euler's constant.

	$\beta \rightarrow 0$	$\beta = 1$	$\beta = 2$	$\beta = 4$	$\beta \rightarrow \infty$
$F$	$\frac{1}{2}(1 - \gamma - \ln(\frac{1}{2}\beta)) + (\pi^2/48)\beta$	$\frac{1}{2}(1 + \ln\frac{1}{2}\pi) = 0.726$	$\frac{1}{2} = 0.500$	$\frac{1}{2} - \frac{1}{4}\ln 2 = 0.327$	$(1/2\beta)\ln(\pi\beta) + (1/6\beta^2)$
$U$	$\frac{1}{2}(-\gamma - \ln(\frac{1}{2}\beta)) + (\pi^2/24)\beta$	$1 - \frac{1}{2}(\gamma + \ln 2) = 0.365$	$\frac{1}{2}(1 - \gamma) = 0.211$	$\frac{3}{4} - \frac{1}{2}(\gamma + \ln 2) = 0.115$	$1/2\beta - 1/6\beta^2$
$S$	$-\frac{1}{2}\beta + (\pi^2/48)\beta^2$	$\frac{1}{2}(1 - \gamma - \ln\pi) = -0.361$	$-\gamma = -0.577$	$1 - 2\gamma - \ln 2 = -0.848$	$\frac{1}{2}(1 - \ln(\pi\beta)) - 1/3\beta$
$C$	$\frac{1}{2}\beta - (\pi^2/24)\beta^2$	$\frac{3}{2} - \frac{1}{2}\pi^2 = 0.266$	$2 - \frac{1}{2}\pi^2 = 0.355$	$7 - \frac{3}{2}\pi^2 = 0.420$	$\frac{1}{2} - 1/3\beta$

this section the thermodynamics of the infinite Coulomb gas, or equivalently the statistics of an infinitely long series of eigenvalues.

The partition function (104) is normalized so that the potential energy of the gas is zero at infinite temperature ( $\beta = 0$ ). The potential energy at zero temperature ( $\beta = \infty$ ) is then the ground-state energy

$$W_0 = -\ln Y = -\frac{1}{2}N \ln N. \tag{148}$$

In order to obtain well-defined limits for the thermodynamic variables as  $N \rightarrow \infty$ , we must first change the zero of energy to the position  $W_0$ . The gas has then by definition zero energy at zero temperature, and a positive energy at any positive temperature. The partition function defined on the new energy-scale is

$$\Phi_N(\beta) = Y^{-\beta} \Psi_N(\beta). \tag{149}$$

The free energy per particle  $F_N(\beta)$  is

$$F_N(\beta) = -[\beta N]^{-1} \ln \Phi_N(\beta). \tag{150}$$

Taking the limit  $N \rightarrow \infty$  in conjecture A, we deduce

*Conjecture D. As  $N \rightarrow \infty$ , the free energy per particle of the Coulomb gas at temperature  $T = \beta^{-1}$  tends to the limiting value*

$$F(\beta) = \beta^{-1}L(\frac{1}{2}\beta) + \frac{1}{2}[1 - \ln(\frac{1}{2}\beta)], \tag{151}$$

$$L(z) = \ln \Gamma(1+z). \tag{152}$$

In what follows we shall always assume that conjecture D is correct.

From Eq. (151) the values of the other thermodynamic quantities follow. These are:

Energy per particle:

$$U = F + \beta(\partial F / \partial \beta) = \frac{1}{2}[L'(\frac{1}{2}\beta) - \ln(\frac{1}{2}\beta)]. \tag{153}$$

Entropy per particle:

$$S = \beta^2(\partial F / \partial \beta) = \frac{1}{2}\beta[L'(\frac{1}{2}\beta) - 1] - L(\frac{1}{2}\beta). \tag{154}$$

Specific heat per particle:

$$C = -\beta^2(\partial U / \partial \beta) = -\frac{1}{4}\beta^2 L''(\frac{1}{2}\beta) + \frac{1}{2}\beta. \tag{155}$$

Note that although Eq. (151) has been rigorously proved for  $\beta = 1, 2, 4$ , the same is not true of Eqs. (153), (154), and (155). These last equations depend on the validity of conjecture D for general  $\beta$ . However, in the case  $\beta = 2$ , the first two derivatives of  $F(\beta)$  can be directly computed. This has been done, and the results

agree with Eqs. (153), (154), and (155) at  $\beta = 2$ . So we have yet another independent check on conjecture D. The values of the thermodynamic functions for physically interesting values of  $\beta$  are summarized in Table I.

There follow some miscellaneous remarks concerning the interpretation of these results.

### A. Physical Nature of the Coulomb Gas

The thermodynamic functions are analytic over the whole range from  $\beta = 0$  to  $\beta = \infty$ . The Coulomb gas is a single-phase system with no thermodynamic transition at any finite temperature. In a later paper we will prove that the system possesses a long-range order of crystalline type at all temperatures. Thus it might be appropriate to call it a "crystal" rather than a gas. In a one-dimensional system the distinction between crystal and gas is somewhat arbitrary.

At low temperatures ( $\beta \rightarrow \infty$ ) the charges are regularly spaced in a crystalline lattice arrangement, and the thermal excitations are compressional waves of small amplitude (phonons) running through the lattice. As the temperature is raised, the local disorder becomes greater, although some degree of long-range lattice structure always persists. At high temperatures ( $\beta \rightarrow 0$ ) we can define a Debye length  $\Lambda$ , with the property that all charge fluctuations are neutralized by correlated motions of other charges within a distance of the order of  $\Lambda$ . The system then behaves approximately like a gas of independent particles, each particle carrying with it a neutralizing "charge cloud" of size  $\Lambda$ . The energy  $U$  is the electrostatic energy of a particle interacting with its induced charge cloud. Since  $U$  is normalized to be zero at low temperatures, when  $\Lambda$  is equal to the level spacing

$$\Delta = 2\pi/N, \tag{156}$$

we may define  $\Lambda$  in general by the equation

$$U = \frac{1}{2} \ln(\Lambda/\Delta). \tag{157}$$

The factor  $\frac{1}{2}$  appears because the interaction includes the self-energy of the induced charge itself. At high temperatures we have then from column 1 of the table

$$\Lambda = 2e^{-\gamma}[\Delta/\beta] \sim \Delta T. \tag{158}$$

In other words, the induced charge cloud is spread out over about  $(2T)$  neighboring particles.

For  $\beta = 1$ , the value of chief interest in applications to the eigenvalue problem, the Debye length is only of the order of one level spacing. In this case the notion of

a Debye length hardly applies, and all violations of charge neutrality involving more than one or two particles are highly improbable. The long-range regularity of the eigenvalues is extremely rigid, and the eigenvalue series looks qualitatively more like a "wobbly crystal" than a classical plasma. The same remark applies even more strongly to the cases  $\beta=2$  and 4.

## B. Entropy as a Measure of Information Content

The entropy  $S$  provides us with a quantitative and exact notion of the "degree of irregularity" of an arrangement of atoms. Because of the existence of the analogy between Coulomb gas and eigenvalue series, the same quantity  $S$  gives a precise measure of the degree of irregularity of a long sequence of eigenvalues. It is appropriate here to use the language of information theory.<sup>24</sup>

A perfectly random sequence of  $N$  numbers, with mean spacing  $\Delta$  and with values determined within some observational limit of accuracy  $\delta$ , can carry a quantity of information

$$I_0 = [1 + \ln(\Delta/\delta)][N/\ln 2], \quad (159)$$

measured in the practical unit of binary digit or bit. A series of  $N$  eigenvalues taken from the statistical ensemble  $E_\beta$  can carry only a reduced amount of information

$$I(\beta) = I_0 + S(\beta)[N/\ln 2]. \quad (160)$$

This loss of information content is a direct measure of the statistical regularity of the eigenvalue series. According to the numbers in the table, the loss of information is

0.521 bit per level in the even-spin case ( $\beta=1$ ),

0.833 bit per level in the case without time-reversal symmetry ( $\beta=2$ ),

1.223 bits per level in the odd-spin case ( $\beta=4$ ).

It would be quite feasible to compute the entropy of an observed sequence of levels and see whether the result agreed with these numbers. However, for a practical test of the statistical model the quantities  $U$  and  $C$  would undoubtedly be more convenient.

## C. Statistical Interpretation of $U$ and $C$

Denoting by  $\langle \rangle$  an ensemble-average, we have by Eqs. (103) and (149)

$$NU = \langle W - W_0 \rangle, \quad (161)$$

$$NC = \langle (W - \langle W \rangle)^2 \rangle, \quad (162)$$

where  $W$  is the electrostatic energy given by Eq. (100),

<sup>24</sup> C. E. Shannon, Bell System Tech. J. 27, 379 and 623 (1948). Reprinted in book form, C. E. Shannon and W. Weaver, *The Mathematical Theory of Communication* (University of Illinois, Urbana, Illinois, 1949).

and  $W_0 = -\frac{1}{2}N \ln N$  is the value of  $W$  for a uniformly spaced series. Thus  $U$  is, apart from normalization, the ensemble average of the logarithm of the geometric mean of all distances between pairs of eigenvalues. And  $C$  is the statistical mean-square fluctuation of the same quantity.

As a statistic for analyzing the properties of observed eigenvalue series,  $W$  seems to be the best expression to use. It has two great advantages over other possible statistics such as  $F$  and  $S$ ; (i)  $W$  can be computed from the eigenvalue pair-correlation function alone, without analyzing higher order correlations, and (ii) the statistical uncertainty of  $W$  is known from the value of  $C$ .

We summarize the situation in the following

*Theorem 10. Let  $(z_1, \dots, z_N)$  be the eigenvalues of a random matrix taken from one of the ensembles  $E_1, E_2, E_4$ . The statistic*

$$W - W_0 = \frac{1}{2}N \ln N - \sum_{i < j} \ln |z_i - z_j| \quad (163)$$

*has the expectation value  $NU$  and the root-mean-square deviation  $(NC)^{\frac{1}{2}}$ , with the values of  $U$  and  $C$  given in the table above.*

This theorem is unfortunately not yet adapted to practical use. In practice we never have a complete series of  $N$  eigenvalues all round the unit circle. We have a comparatively small number  $n$  of observed levels, which are supposed to be a small section of a complete eigenvalue series of order  $N \gg n$ . In order to analyze the statistics of the observed levels, it is necessary to work out in detail the predicted behavior of a section of  $n$  levels chosen at random from a matrix of one of the basic ensembles. We shall find that a statement substantially identical with Theorem 10 can be proved, with the summation in  $W$  restricted to the observed levels, and with  $NU, (NC)^{\frac{1}{2}}$  replaced by  $nU, (nC)^{\frac{1}{2}}$ . A full discussion of this and other properties of partial level series will be given in later papers of the series.

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## APPENDIX A

### Proof That a Hermitian Self-Dual Matrix Can Be Diagonalized in Quaternion Algebra

Let  $H$  be a Hermitian self-dual ( $N \times N$ ) quaternion matrix. Let  $(q_1, \dots, q_N)$  be an  $N$ -component vector

whose components are real quaternions. The expression

$$Q = \sum_{ij} \tilde{q}_i H_{ij} q_j \tag{A1}$$

is a scalar (because  $H$  is self-dual) and is real (because  $H$  is Hermitian). The ratio

$$R = (Q/P), \quad P = \sum_i \tilde{q}_i q_i \tag{A2}$$

is a bounded real scalar function of the  $q_j$ . For some set of real quaternions

$$q_j = A_{j1} \tag{A3}$$

$R$  attains its maximum value  $D_1$ . The fact that  $R$  is stationary at the point (A3) implies

$$\sum_j H_{ij} A_{j1} = D_1 A_{i1} \tag{A4}$$

Proceeding in the same way through the successive stationary values of  $R$ , we find  $N$  real scalar quantities  $D_i$  and  $N$  real quaternion vectors  $A_{jk}$  such that

$$\sum_j H_{ij} A_{jk} = D_k A_{ik} \tag{A5}$$

Writing  $B$  for the matrix  $A^{-1}$ , we have

$$H = B^{-1} D B, \tag{A6}$$

with  $D$  real, scalar, and diagonal, while  $B$  is quaternion real.

From Eq. (A6) we deduce

$$D B B^R = B B^R D. \tag{A7}$$

Thus  $B B^R$  either is diagonal, or (if several of the  $D_j$  are equal) can be chosen to be diagonal. Since the normalization of each vector  $B_{jk}$  is arbitrary, we can choose them all to have unit length. Then

$$B B^R = 1, \tag{A8}$$

i.e.,  $B$  is symplectic.

APPENDIX B

Proof of Conjecture C for  $N=4$

Let the function  $F(a_1, \dots, a_N)$  of the non-negative integer variables  $(a_1, \dots, a_N)$  be defined by

$$F = \sum_{\lambda_{jk}} \prod_{i < k} \left\{ (-1)^{\lambda_{jk}} \binom{a_j + a_k}{a_j + \lambda_{jk}} \right\}. \tag{B1}$$

The summation variables  $\lambda_{jk}$  are integers subject to the conditions

$$\lambda_{jk} = -\lambda_{kj}, \quad j, k = 1, \dots, N, \tag{B2}$$

$$-a_j \leq \lambda_{jk} \leq a_k, \tag{B3}$$

$$\sum_k \lambda_{jk} = 0, \quad j = 1, \dots, N. \tag{B4}$$

We also define  $f(a_1, \dots, a_N)$  by

$$f = [a_1 + \dots + a_N]! / [a_1! \dots a_N!]. \tag{B5}$$

When all the factors in Eq. (146) are expanded by the binomial theorem, conjecture C reduces to the statement

$$F = f. \tag{B6}$$

Suppose next that  $(a_1, \dots, a_{N-1})$  are non-negative integers with

$$a_1 + \dots + a_{N-1} = m, \tag{B7}$$

while  $x = a_N$  is free to be non-integral. A function  $F(x) = F(a_1, \dots, a_{N-1}, x)$  can then be defined by Eq. (B1), the conditions (B3) with  $j=N$  or  $k=N$  being omitted. This  $F(x)$  is a polynomial in  $x$  of degree  $m$ , and is therefore well defined for all positive or negative  $x$ . Moreover, when  $x$  is a non-negative integer the new definition reduces to the old one. Similarly,

$$f(x) = (m+x)! / [a_1! \dots a_{N-1}! x!] \tag{B8}$$

has an obvious meaning as a polynomial in  $x$  of degree  $m$ . Conjecture C is thus equivalent to the statement that Eq. (B6) holds as an identity in  $x$  for non-negative integer values of  $(a_1, \dots, a_{N-1})$ .

The essential step in the proof is the following Lemma which holds for all  $N$ .

*Lemma 1.  $F(x)$  has the symmetry property*

$$F(x) = (-1)^m F(-m-1-x). \tag{B9}$$

*Note:* It is trivial that  $f(x)$  has the same symmetry. To prove the lemma, we go back to Eq. (146). We can represent  $F$  by the contour integral

$$F = \frac{1}{(2\pi i)^N} \int \dots \int dz_1 \dots dz_N \left\{ \prod_{i \neq j} (z_i - z_j)^{a_j} \right\} \times \prod_j z_j^{-m-1-a_N+a_j}. \tag{B10}$$

So long as all the  $a_j$  are non-negative integers, the paths of integration can be chosen in any way provided that each variable  $z_j$  circles the origin once in the positive direction. When  $a_N = x$  is allowed to be nonintegral, the contours for  $(z_1, \dots, z_{N-1})$  are still arbitrary, but the contour for  $z_N$  must be chosen to circle the origin inside all the other contours. This gives the correct value for  $F$ , since for  $|z_N| \ll |z_j|$  all the nonterminating binomial series  $(z_j - z_N)^{a_j+x}$  can be expanded in ascending powers of  $z_N$  as required by Eq. (B1).

Now make in Eq. (B10) the transformation of variables

$$z_N = -y_N, \tag{B11}$$

$$z_j = y_j - y_N, \quad j = 1, \dots, N-1. \tag{B12}$$

The rule for choosing the contours of integration is the same for the  $y_j$  as it was for the  $z_j$ . In terms of the variables  $y_j$ , the expression for  $F$  is identical with Eq. (B10) except for an over-all sign  $(-1)^m$  and the replacement of  $x$  by  $(-m-1-x)$ . This proves Lemma 1.

The second Lemma also holds for all  $N$ .



*Lemma 2.* Let  $0 \leq a_1 \leq a_2 < \dots \leq a_{N-1}$ . Then  $F(x) = f(x) = 0$  when  $x$  is any negative integer in the range

$$-a_1 \leq x < 0. \tag{B13}$$

To prove Lemma 2, observe that  $F(x)$  contains, in every term of the expansion (B1), a product of  $(N-1)$  factors

$$\binom{a_j+x}{a_j+\lambda_{jN}}. \tag{B14}$$

A factor (B14) will vanish whenever  $x$  satisfies Eq. (B13) and

$$\lambda_{jN} > x. \tag{B15}$$

But in view of Eq. (B4), not all  $\lambda_{jN}$  can be negative, and so at least one factor (B14) will always vanish. This proves Lemma 2.

We now complete the proof of the conjecture for  $N=4$ , following the method of Dougall.<sup>23</sup> We suppose  $a_1, a_2$ , and  $a_3$  to be non-negative integers with

$$0 \leq a_1 \leq a_2 \leq a_3, \quad a_1 + a_2 + a_3 = m. \tag{B16}$$

Let it be assumed as an inductive hypothesis that  $F(x) = f(x)$  holds as an identity in  $x$  whenever  $a_1 + a_2 + a_3 < m$ . Because  $F(a_1, a_2, a_3, a_4)$  is formally symmetric between  $a_3$  and  $a_4$ , the inductive hypothesis implies

$$F(a_1, a_2, a_3, x) = f(a_1, a_2, a_3, x) \tag{B17}$$

for the integer values of  $x$

$$x = 0, 1, \dots, a_3 - 1. \tag{B18}$$

Lemma 2 states that Eq. (B17) holds for

$$x = -a_1, -a_1 + 1, \dots, -1. \tag{B19}$$

Lemma 1 in combination with Eqs. (B18) and (B19)

implies that Eq. (B17) holds for

$$x = -a_1 - a_2 - 2a_3, \dots, -a_2 - a_3 - 1. \tag{B20}$$

The three ranges (B18), (B19), and (B20) do not overlap, and they contain altogether

$$2(a_1 + a_3) \geq m + a_1 \tag{B21}$$

distinct values of  $x$ . But the two sides of Eq. (B17) are polynomials in  $x$  of degree  $m$ . If  $a_1 > 0$ , Eq. (B17) must hold as an identity in  $x$ . If  $a_1 = 0$ , Eq. (B17) reduces to the statement

$$F(a_2, a_3, x) = f(a_2, a_3, x), \tag{B22}$$

which is true since conjecture C has already been proved for  $N=3$ . Therefore Eq. (B17) always holds, and the conjecture is proved for  $N=4$ .

The same proof also applies in the case  $N=3$ , when instead of Eq. (B21) we obtain

$$2(a_1 + a_2) = 2m > m \tag{B23}$$

distinct values of  $x$ .

When we try to extend the argument to  $N=5$ , we have  $2(a_1 + a_4)$  values of  $x$  for which the analog of Eq. (B17) is proved, and this is not necessarily greater than  $m = a_1 + a_2 + a_3 + a_4$ . Two further steps are then required. (i) By using all the inequalities (B3) and (B4), we can strengthen Lemma 2 so that it holds for negative integers  $x$  down to  $(-a_2)$  instead of  $(-a_1)$ . We then have instead of Eq. (B21)

$$2(a_2 + a_4) \geq m, \tag{B24}$$

which is better but still not quite good enough.

(ii) Equation (B17) can be directly verified for one more value of  $x$ , namely,  $x = -a_1 - 1$ . The argument for  $N=5$  then just squeezes through. There is clearly no hope of obtaining by such piecemeal methods enough  $x$  values to deal with  $N \geq 6$ .