Statistics and the Shell Model or Chaotic Motion in Atomic Nuclei

Quantum Chaos is a very young field. It relates to such diverse phenomena as the behavior of the hydrogen atom in a strong magnetic field, the dissipation of energy in large atoms and molecules, the magnetic properties of small metallic clusters at low temperature, the statistical features of atomic nuclei, and to theoretical issues like semiclassical quantization. It is hotly debated and controversial, much in contrast to its older cousin Classical Chaos which is well investigated and known to play a fundamental role in nonlinear systems, both conservative and dissipative.¹

I wish to discuss a few select topics of this field. These relate to statistical properties of nuclei and their interpretation in terms of chaotic motion. This choice is neither accidental nor based on personal prejudice. Because of the available (relative) energy resolution, nuclei have so far provided the most numerous and the best data on the chaotic behavior of finite quantum systems. (The data base in atomic and molecular physics will soon grow rapidly, however.)

The discussion will center on the very different features of averages and fluctuations in nuclei, and in other many-body systems. I will put forward arguments to show that averages are determined by the dynamics and therefore carry dynamical information, while fluctuations reflect chaotic behavior, are generic for finite quantum systems, and carry no information content.

Only a few years separate the discovery of the neutron (and the beginning of nuclear physics) from the first surfacing of stochasticity, today understood as a manifestation of chaotic motion. Then, novel data on neutron capture led N. Bohr in 1936 to the concept of the compound nucleus, a system of strongly interacting nucleons, not amenable to a mean-field approach and therefore very different from the many-body system defined by the motion of electrons in an atom. Bohr's idea of a neutron-nucleus collision is depicted in Fig. 1. (This is a photograph of a mechanical set-up actually built at the time in Bohr's institute). The picture and the underlying concept are truly astonishing in their depth of understanding and vision. Indeed, one of the standard models for chaotic motion in classical and quantum physics of today is nearly identical to Bohr's model. This is the Sinai billiard of Fig. 4, modelled after Boltzmann's idea of a hard-sphere gas.

Bohr's view dominated nuclear physics for nearly 15 years. In its wake Wigner was led to the concept of a random-matrix model to which I return below. This dominance finally gave way to the shell model, to the collective model and, more generally speaking,

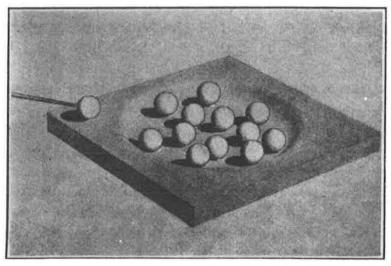
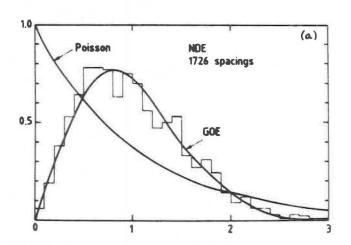


FIGURE 1 Bohr's model of a neutron-nucleus collision [taken from Nature 137, 351 (1936)].

to the understanding of nuclear dynamics as regular motion in terms of a mean-field approach. Nevertheless, Bohr's view did not become obsolete. The dichotomy between his picture and a mean-field approach, or between stochasticity and dynamics, or, in modern terms, between chaotic and regular motion, has continued to exist. Only recently have we begun to understand the resolution of this puzzle. In describing this development, I confine myself to data taken at low energies (typical excitation energies are around 10 MeV), although evidence for stochastic behavior also exists outside this domain.

The resolution hinges on the distinction between average properties and fluctuations about the average.² Average properties are defined as mean values over many excited states of fixed spin and parity. Examples are the average level spacing, the strength function (the ratio of mean partial width and mean level spacing), and the mean value of an element of the S-matrix, averaged over many compound-nucleus resonances. Average properties can be calculated reliably using mean-field techniques or other semiclassical approximations, irrespective of whether the system shows chaotic features or not. For the average level spacing, the Weyl formula proves the point. For the average S-matrix, the uncertainty principle implies that averaging over a large energy interval (in comparison to the mean level spacing) removes all but the fast part of the collision process which involves only a few degrees of freedom and can therefore be modelled in terms of the shell model and the collective model (optical model and coupled channels calculations). Whenever the shell model, the collective models, or meanfield theories have been used outside the ground-state domain (to which I return below), this was done to calculate average properties of nuclei.

Chaotic Motion manifests itself in the *fluctuations* about the average values. To make this point, I introduce two examples. Figure 2 displays the distribution of level spacings about their mean values. The data involve 1726 spacings (the "nuclear data ensemble," NDE), i.e., the totality of all resonance spacings measured either by time-of-flight neutron spectroscopy or by high-resolution proton scattering. On the left-hand part of the figure, the histogram shows the frequency of occurrence of a given spacing between neighboring levels of the same spin and parity versus the size of



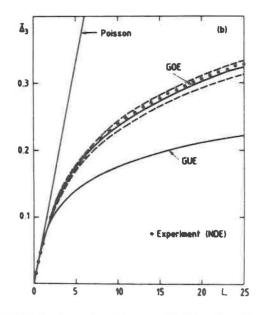


FIGURE 2 Nearest-neighbor spacing distribution (left) and average Δ_3 statistic (right) for the nuclear data ensemble [taken from R. U. Haq, A. Pandey and O. Bohigas, Phys. Rev. Lett. 48, 1086 (1982)].

the spacing (in units of the average level spacing). On the righthand part the dots with error bars show the Δ_3 statistic versus L. This is a measure of the mean square deviation of the actual integrated level density from the integrated mean level density over an interval of length L (in units of the mean level spacing). I wish to emphasize that most of the data used in the figure have become available only in the last dozen years or so through the determined effort of a few groups who have chosen to work outside the established trends, and who have contributed significantly to a revolution in our understanding of nuclear dynamics. The data in Fig. 2 all relate to isolated compound-nucleus resonances (mean spacing large compared to mean decay width) which are typically encountered near neutron threshold. With increasing excitation energy the average level spacing decreases exponentially, the average decay width increases exponentially, and a few MeV above neutron threshold the resonances overlap strongly (average decay width large compared to average level spacing). A typical inelastic cross section in this domain is shown in Fig. 3. The peaks are not due to isolated resonances. The rapid energy dependence of the cross section is rather due to the fact that at one value of the energy, many overlapping resonances add coherently while at another they interfere destructively. This pattern can be qualitatively understood and was in fact predicted by Ericson and by Brink and

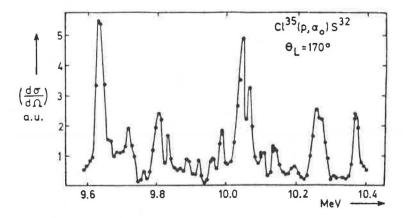


FIGURE 3 Fluctuations of the compound-nucleus cross section [taken from T. Ericson and T. Mayer-Kuckuk, Ann. Rev. Nucl. Sci. 16, 183 (1966)].

Stephens more than two decades ago on the basis of the postulate that the amplitudes of the interfering resonances are uncorrelated random variables. Thus, the differential cross section versus energy should be a random process. This can be verified by statistical tests on the experimental data.

It is perhaps intuitively obvious that the random fluctuations of the cross section relate to chaotic motion (although this point deserves to be, and will be, clarified further). But what is the significance of the level fluctuations shown in Fig. 2? On a phenomenological level, a first answer can be given in terms of the randommatrix model introduced by Wigner. To model the complexity of (and our lack of information on) nuclear states at ≈10 MeV excitation energy. Wigner envisaged a matrix representation of the nuclear Hamiltonian in which the individual matrix elements are considered to be independent random variables. A particular matrix ensemble obeying time-reversal invariance consists of real symmetric matrices in which the independent elements are uncorrelated random variables with a Gaussian probability distribution and zero mean values. The further requirement that the probability density be orthogonally invariant (so that no basis plays a preferred role) uniquely determines the ensemble. For obvious reasons, this ensemble is referred to as the Gaussian orthogonal ensemble (GOE). The level fluctuations predicted by this ensemble are shown as solid lines labelled GOE in Fig. 2. More precisely: The solid lines correspond to Hamiltonian matrices, the dimension of which goes to infinity. The dashed curves in the right-hand part of Fig. 2 show the deviations expected because of the finite size of the nuclear data ensemble. Figure 2 suggests that the GOE correctly reproduces the fluctuation properties of nuclear levels. This impression is confirmed by extensive statistical tests. This agreement and the fact that the GOE can be derived from a maximum-entropy approach (and thus carries zero information content) together suggest that the observed fluctuation properties may indeed relate to chaotic motion.

This surmise receives strong support from the study of simple chaotic systems.³ The evidence is based mainly on numerical results. Figure 4 shows a version of the Sinai billiard mentioned earlier. A massive point-like particle moves in two dimensions within the confines of a rectangle (on the surface of which it is

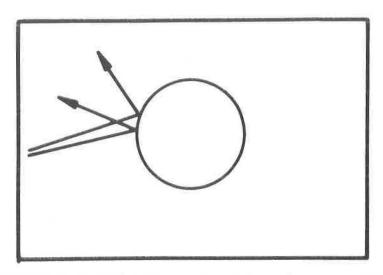


FIGURE 4 The Sinai billiard. The two trajectories have a distance which grows exponentially with time. This is due to the defocussing caused by the reflection on the circle.

reflected elastically). The rectangle encloses a circle which likewise reflects the particle elastically. (This model is an idealization of a hard-sphere gas and is actually very similar to Bohr's model of Fig. 1.) It is known that the Sinai billiard is a completely chaotic classical system (a K-system). Quantization of the Sinai billiard leads to the time-independent Schrödinger equation for a free particle, subject to the boundary conditions that the wave function be zero on the surfaces of the rectangle and circle. A sample of 740 eigenvalues calculated numerically for this problem has been used to construct the histogram for the nearest-neighbor spacing distribution shown in the upper part of Fig. 5 and the Δ_3 statistic shown with error bars in the lower part. The solid lines correspond to the GOE predictions. The dashed lines in Fig. 5 labelled Poisson, and the solid curves labelled likewise in Fig. 2, show the behavior of level fluctuations characteristic of a regular (integrable) classical system upon quantization.

The agreement between the numerical results presented in Fig. 5 and the GOE predictions is certainly very impressive. Equally impressive is the agreement between the GOE predictions and the

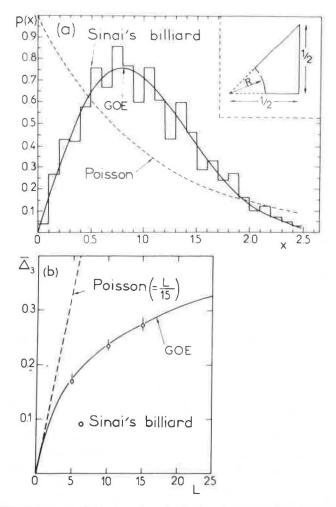


FIGURE 5 Nearest-neighbor spacing distribution (upper part) and average Δ_3 statistic (lower part) for the Sinai billiard [taken from O. Bohigas, M. J. Giannoni and C. Schmit, Phys. Rev. Lett. **52**, 1 (1984)].

nuclear data ensemble in Fig. 2. In fact, without being told, nobody could tell which of the two histograms shown in Figs. 2 and 5 refers to which situation. This agreement suggests the following hypothesis.

The quantum analogue of a completely chaotic classical system

exhibits level fluctuations which coincide with those of the GOE. These fluctuations are generic and do not depend on particular features of the Hamiltonian. The fluctuations observed in nuclear spectra signal that the nucleus is a chaotic system.

Although there exists no data to contradict it, this hypothesis—attractive because of its universality and simplicity—must certainly be qualified. Using semiclassical arguments, Berry has shown in Ref. 1 that the logarithmic increase of $\overline{\Delta_3}(L)$ versus L predicted by the GOE is a generic feature of completely chaotic systems up to a maximum value L_0 . For $L > L_0$, the function $\overline{\Delta_3}(L)$ levels off and no longer follows the logarithmic pattern of the GOE. The value of L_0 depends on the number of degrees of freedom. In nuclei (and probably also in atoms and molecules) L_0 is so large that this qualification has no practical consequences. It is not known whether a qualification must also be made with regard to the nearest-neighbor spacing distribution, since nothing is known analytically about it. But the universality claimed in the hypothesis could be checked if more data on atoms and molecules were available.

Another qualification concerns the use of the GOE. In the framework of nuclear physics, matrix ensembles different from the GOE are physically more reasonable and yield better average properties.² However, these ensembles cannot be dealt with analytically so far. Moreover—and this is the decisive point—the available numerical evidence suggests that the fluctuation properties of these ensembles are identical to those of the GOE, indicating once again the universality of the GOE fluctuations.

Classical chaotic systems are characterized by the Kolmogorov entropy. Qualitatively speaking, this is a measure of the speed with which the system "mixes," i.e., loses track of the initial conditions. It is striking that the hypothesis introduced above does not involve a similar parameter in the quantum context—the GOE fluctuations are parameter-free and thus universal. The analysis of Berry suggests that the Kolmogorov entropy is only relevant for the behavior of $\overline{\Delta_3}(L)$ near $L=L_0$ and thus practically without interest.

The GOE predicts the fluctuation properties of eigenvalues and of eigenfunctions. For the latter the prediction is: The inner product of the GOE eigenfunctions with an arbitrary (but fixed) vector in Hilbert space has a Gaussian probability distribution centered

at zero. This prediction can be tested² by sampling, for instance, the distribution of reduced partial widths of slow-neutron resonances: Every reduced partial width is the square of a matrix element; the latter can be viewed as an inner product. The agreement with the nuclear data set is again very good. For lack of evidence (either analytical or, with sufficient statistics, numerical) on eigenfunction distributions of chaotic systems like the Sinai billiard, our hypothesis does not refer to this aspect and is therefore certainly incomplete. In the discussion of the compound-nucleus problem I shall assume that the GOE also correctly describes the fluctuations of the eigenvectors.

In spite of these qualifications, the picture which emerges is simple and convincing. Outside the ground-state domain, we distinguish average properties from fluctuations. The former reflect dynamical properties of the system and can be calculated reliably, for instance within the mean-field approach. The latter are generic for chaotic systems, quite independent of the dynamics, carry no information, and can be simulated by the GOE. This partially resolves the dichotomy between Bohr's picture and the success of dynamical models.

In classical mechanics, chaotic motion is an expression of the instability of the system against small changes of the initial conditions. The fluctuations of chaotic quantum systems can be viewed similarly. In the absence of conserved quantum numbers, every state of the system interacts with every other one. It is precisely this feature which is modelled by the GOE. It leads to levelrepulsion (via the Wigner-von Neumann theorem), and to the linear rise of the nearest-neighbor spacing distribution versus spacing visible for small spacings in Figs. 2 and 5. It likewise leads to the "stiffness" of the spectrum, displayed in the same figures by the fact that the Δ_3 values of the GOE are appreciably smaller than those of an integrable system. Moreover, any small change of the Hamiltonian would qualitatively change the positions of the eigenvalues and, more importantly, the composition of the eigenfunctions. It follows that outside the ground-state domain, both the information content of nuclear spectra and the predictive power of nuclear models are limited.

These facts suggest a new view of the nuclear (and many other) many-body problem(s), and lead to intriguing and unresolved

questions concerning the nuclear dynamics. In concluding this Comment, I briefly touch upon both subjects.

The new view of the many-body problem suggested by the abovementioned facts is based on the realization that it is both futile and useless to calculate details of a spectrum outside the groundstate domain. Only average properties are required; the fluctuations are simulated by the GOE.

A case in point is the cross-section fluctuations shown in Fig. 3. If the compound-nucleus resonances do indeed have the fluctuation properties typical of chaotic motion, then the cross section is a random process, and it is impossible (and also without any interest) to predict theoretically the value of the cross section at any given energy. What is required instead are the average value, the variance, and the correlation width of the cross section. (These quantities are actually of interest in applications of nuclear science to reactor techniques and astrophysics.) Can we calculate these quantities, assuming that the average value of the S-matrix is given, and that the stochastic behavior of the compound-nucleus resonances is modelled by the GOE?

There are two aspects to this question. First, the problem just posed is well-defined (the number of parameters is equal to the number of input data), and it is mathematically quite similar to the problem of working out analytically the curves labelled GOE in Figs. 2 and 5. This latter problem was solved two decades ago by Dyson and Mehta. Second, the problem of cross-section fluctuations is sufficiently different from the Dyson–Mehta problem to render their special method of solution inapplicable. Inasmuch as the problem of cross-section fluctuations is only a special case in a wider class (defined by the postulate that the fluctuation properties of any observable can be simulated by the GOE), a general method of solution is called for. This difficulty has delayed the solution of the compound-nucleus problem by several decades; the problem was solved only quite recently.⁴

The solution is found by realizing that this problem is closely linked to problems investigated in the statistical mechanics of disordered systems, and that the methods developed there can be modified and applied. Random Hamiltonians are widely used to simulate disordered systems. I recall some cases of fundamental interest: The problem of Anderson localization in dirty conductors;

the integer quantum Hall effect; and the problem of spin glasses. One approach to these problems consists of mapping them onto a nonlinear sigma model. The problem of compound-nucleus scattering can be viewed formally as an Anderson model for a dirty conductor in zero dimensions. It can be mapped onto a zerodimensional nonlinear sigma-model. Because of its particularly simple structure, the latter can be worked out exactly. The method of solution is quite general; it is presently being applied to other physical situations and to other observables. [As a spin-off, one can use the exact solution to investigate the validity of an approximation scheme (the replica trick) widely used in statistical mechanics.] It thus appears that the new view of the many-body problem defined above can be implemented. In the case of compound-nucleus scattering, the exact solution agrees with solutions found earlier for limiting cases, with the results of Monte Carlo simulations, and with numbers resulting from a maximum-entropy approach to the scattering matrix. There is no doubt that the problem has been solved. The solution has meanwhile found useful and interesting applications in nuclear physics, in reactor technology, and in astrophysics.

It remains to discuss some intriguing open problems. So far, we have been concerned with the fluctuation properties of levels of fixed spin and parity or, in the case of the Sinai billiard, levels of the same symmetry properties outside the ground-state domain. There is mounting evidence that in nuclei these fluctuation properties persist all the way down into the ground-state domain, at least for some values of spin and parity, and for odd-odd nuclei. suggesting complete chaoticity. This fact has to be contrasted with the phenomenal success of the nuclear models in the ground-state region which suggests completely regular behavior. In contemplating this dilemma, one notices that in the overwhelming number of cases, the nuclear models relate properties of nuclear levels which differ in one or several quantum numbers (spin, parity, nucleon number, etc.). Is it possible that chaotic behavior within a family of states having identical quantum numbers occurs simultaneously with completely regular behavior of data (transition matrix elements, energy level correlations) relating states of different quantum numbers? Or is the ground-state domain an intermediate regime between complete regularity and complete chaos?

Do the fluctuation properties depend on the quantum numbers? Are they affected by the collective nuclear motion?

These questions are important for our general understanding of chaoticity versus regularity in many-body systems. I believe that the answers must be sought by a two-pronged approach. On the one hand, the study of chaoticity in systems having more integrals of motion than the energy is called for. Such systems would be a little closer to actual nuclei than is the Sinai billiard. On the other hand, more data in the ground-state domain are badly needed. In particular, a thorough study of states with different (and up to very high) spins in the vicinity of the ground state (the Yrast line) should be most interesting. Such a study could reveal the opposite actions of strong collectivity and of chaoticity.

These questions are not confined to nuclear physics. In atoms and molecules, there is strong evidence for regular motion in the ground-state domain; in units of the mean level spacing, this domain is perhaps more extended in these systems than in nuclei. There is also growing evidence for chaotic behavior at sufficiently high excitation energies.

In summary, I have argued that nuclei, aside from their strong regular features, also display chaotic behavior. This behavior is generic for small quantum systems; the fluctuations can faithfully be modelled by the GOE. An adaptation and extension of methods developed in the theory of disordered systems make it possible to calculate fluctuation properties of observables in terms of their average values. A more complete understanding of the interplay between regular and chaote features, especially in the ground-state region, remains an open problem. Viewed in this way, the nuclear many-body problem is intimately linked with both ergodic theory and with the theory of disordered systems. Its study forms part of the statistical mechanics of finite quantum systems.

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