The present status of the nuclear shell model

Useful though the shell model undoubtedly is for providing a correlation of the structure and properties of nuclei, theorists are still wondering why it works.

Elizabeth Urey Baranger

The nuclear shell model is the central idea of nuclear structure. Theorists work either backwards from it (by this I mean they try to justify and derive its properties by stating a basic many-body Hamiltonian) or they work forward from it (they assume it is true and try to derive and justify the wide variety and complexity of nuclear properties including the well known phenomenon of nuclear collective motion). The shell model lurks somewhere in every paper on nuclear structure. The intense interest in the shell model among experimentalists for the last fifteen years has been due to the kinds of experiments that became possible during this time. It has been an era of direct reactions that characteristically excite simple degrees of freedom of the nucleus—just those most easily explained by the shell model. Without the possibility of these experiments and their analysis, the shell model might have been left mainly to the theorists, and they would have found it a very dry subject, without the wealth of experimental data they now have.

The success of the model

The shell model, as proposed by Maria Goeppert Mayer, says that nucleons in a nucleus move independently in a central potential that has a sharp surface and a spin-orbit component. For any potential there are gaps in the spacing of single-particle levels. Nuclei with a neutron or proton number (called a "magic number") just sufficient to fill all levels up to one of the gaps are particularly stable and are referred to as "closed-shell" nuclei. With the kind of potential postulated by Mayer the magic numbers are 8, 20, 28, 50, 82 and 126. The properties of nuclei with intermediate neutron or proton numbers ("open-shell" nuclei) can be deduced through the use of an effective residual interaction. The original shell model postulated that this interaction causes an even number of identical nucleons to have a total angular momentum of zero in the lowest state, and an odd number to have the angular momentum of the filling single-particle level. (This last idea is now known to be inapplicable in the deformed region.)

There is a great variety of evidence for particularly stable nuclei. One example is shown in figure 1, which is a photograph of a model made by Gertrude Goldhaber.[1] The x coordinate is the neutron number, the y coordinate the proton number, and the z coordinate is the energy of the first 2^+ state, the first excited state for most even–even nuclei. The nuclei that are particularly stable are hard to excite. Note Pb^{208} with both neutron and proton shells closed, the tin isotopes with the proton shells closed, the $N = 82$ isotones with the neutron shell closed and doubly-closed Ca^{40}, Ca^{48}, and O^{16}. The strikingly low 2^+ energies occur for deformed "rotational" nuclei. This figure gives some indication of the enormous variety of structure that nuclei exhibit. And yet it is not random; things vary smoothly, and it is the underlying shell structure that enables us to explain the observed variations.

Knowing the proton and neutron number of any nucleus we can predict its type of structure. Figure 2a shows the very similar spectra of three closed-shell nuclei—O^{16}, Ca^{48}, Pb^{208}—where I have multiplied the excitation energies by a factor of $A^{-1/3}$ to correct for the change in spacing with size. In figure 2b are shown the spectra of three nuclei with two nucleons (or holes) in addition—O^{18}, Ca^{46}, Pb^{206}. These are similar to each other and characteristically different from those in figure 2a. The closed-shell nuclei have high first-excited states; negative-parity states occur because when you promote a particle from the levels below the gap to the levels above you most often change its parity. In the nuclei of figure 2b, most of the excited states are formed by rearranging the coupling of the valence nucleons, and they produce low states with even parity.

In figure 3 I show nuclei far from closed shells. On the left are two single-closed-shell nuclei, with many valence nucleons of one type of particle—16 neutrons for Sn^{116} and 10 protons for Nd^{142}. On the right are two nuclei with many neutrons and protons outside the closed shell, as indicated by the numbers above. Again the members of each group resemble each other and differ radically from those in the other group. The spectra of the single-closed-shell nuclei typically have a gap, followed by a high level density, with the 2^+ state lowered into this gap. The nuclei with many nucleons of both types outside the closed shell have a typical rotational spectrum; the extra nucleons have caused a deformation of the whole nucleus. These examples demonstrate that, given the neutron and proton number of a nucleus and combining this with the shell model, we know what to expect in the low spectrum of that nucleus. The shell model unifies this structure and makes the study of nuclei lying as far apart in the periodic table as Pb^{206} and O^{18} a common endeavor.

The amount of experimental information we have about the low levels of nuclei is enormous. But one of the

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more interesting ways to attack them, from a shell-model point of view, is through direct reactions. This technique, unknown in Mayer's time, has been the center of intense experimental interest in the last 20 years when machines such as cyclotrons and tandem Van de Graaff accelerators have been able to excite particles to 15–50 MeV and still get good energy resolution.

The differential cross sections have been successfully analyzed by the distorted-wave Born approximation, in which the incident and exiting particles are treated as moving independently in a central potential and the transition matrix element is computed by a Born approximation. That such analyses are so successful is again evidence for the independent-particle motion implied by the shell model, and the fact that the Born approximation is useful means that the strong interaction between nucleons can somehow be simulated by a weak effective interaction. Such reactions preferentially excite simple excitations of the target nucleus.

The most direct and elementary example is that of one-particle transfer reactions (such as d,p or d,t) on "closed-shell" targets. Clearly these reactions excite mainly those states in the final nucleus that have one particle or one hole more than the target does, and they are used to check experimentally the order of the single-particle levels proposed in Mayer's original rough model.

The experimental separation energies of states in the Pb region appear in figure 4, where the one-particle transfer experiments have been used to pick out the single-particle levels from the rest of the spectrum. The proton levels are on the left, neutron levels on the right; the nucleus in which a group of levels occurs is listed next to them.

Maria Goeppert Mayer

Maria Goeppert Mayer, who received the Nobel Prize in physics for her work on the shell model, died about a year and a half ago. I knew Maria almost all of my life as a "Friend of the Family"; the Mayers lived a few blocks away from us in Leonia, N.J., from 1939 to 1945, across the street in Chicago from 1945 to 1958 and then a half mile from my parents in La Jolla from 1960 on. I have memories of Maria from the Leonia period, when I was a teenager—but not physics memories. Maria stands out in my mind as completely different from the many wives I knew in Leonia, in that she had a strong commitment to a career and to science. My father, who likes to talk science to anyone all the time, loved talking to Maria, telling her his ideas and listening to her talk—as did all the other physicists and chemists, always talking about science at parties at our house. She was vital and lively, and gave a strong impression of living a satisfying life, in spite of problems of finding jobs and housekeepers. In looking back I realize how lucky I was to know her in this way. She gave the impression that being a theoretical physicist and a mother was possible, rewarding and worth a great deal. Also, as I did not know a very large number of physicists, and one of these happened to be a woman, I did not realize how few women physicists there really are.

I looked up the details of her physics career and was struck by the types of positions she had held. Until 1959, none of them are what I would term "regular" positions: voluntary associate at Johns Hopkins for nine years (she was paid approximately $100 per year); lecturer in chemistry at Columbia and part-time lecturer at Sarah Lawrence College; during the war, part-time at SAM Labs working on the atomic-bomb project; in the Chicago era, part-time senior physicist at Argonne while being voluntary professor at the University of Chicago.

According to her biographer, Joan Dash,* the unchallenging and unrewarding jobs she had in the early years were not particularly useful for her development, especially from the point of view of her image of herself. In spite of this, she managed through personal contacts, and through her husband, to continue research and to broaden her interests—it's lucky she was a theorist. She expressed great frustration with these early jobs, but never bitterness. Of course, she thought of herself as a research physicist, and my memories of the Leonia days are that she was regarded as such by her colleagues, although her position as part-time lecturer of chemistry is at variance with this. In the Chicago days she was certainly considered to be a professor at Chicago although she was "voluntary" because of a nepotism rule and was not paid by the University of Chicago but by Argonne. (In 1959 she was made professor; this was after the Mayers had received offers from the University of California at San Diego.) I think it is a unique career, different from any other Nobel prize winner, and that only her dedication to physics, her unique abilities and a supportive husband sustained her through it.

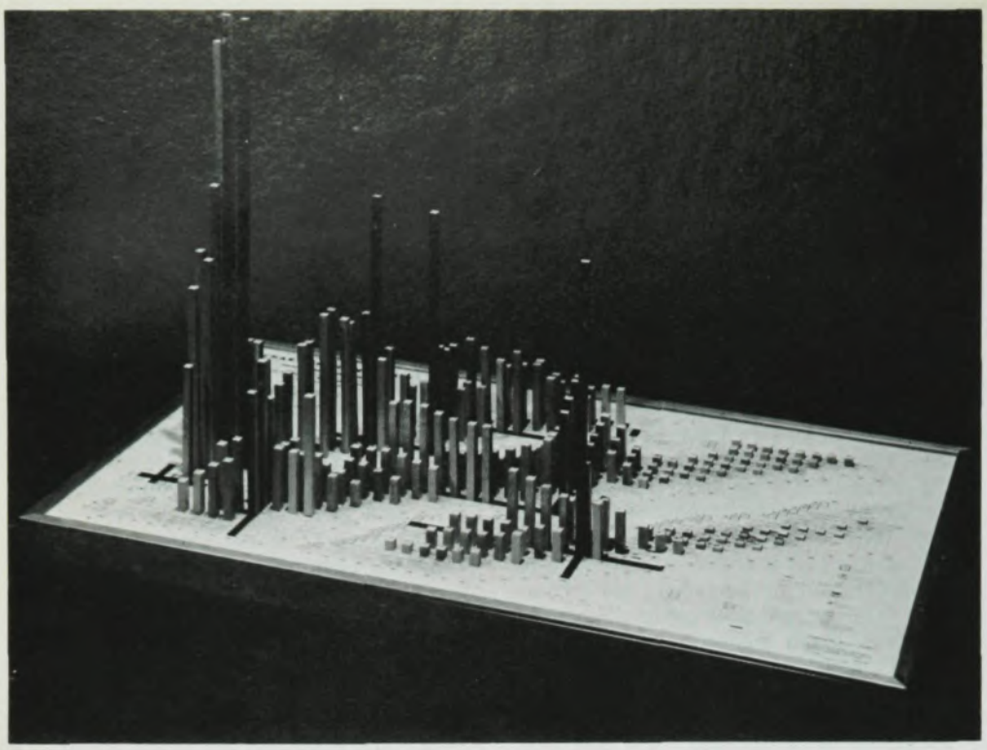
In the last conversation I had with her, at the Washington APS meeting of 1971, I told her about the APS Committee on Women in Physics, which was just being formed, and which interested her. She became a member of this committee.

She overcame quite subtle obstacles in the course of her life—she was a woman, a foreigner, she started her career in the days of the depression. How many of us could have achieved half the success that she did?

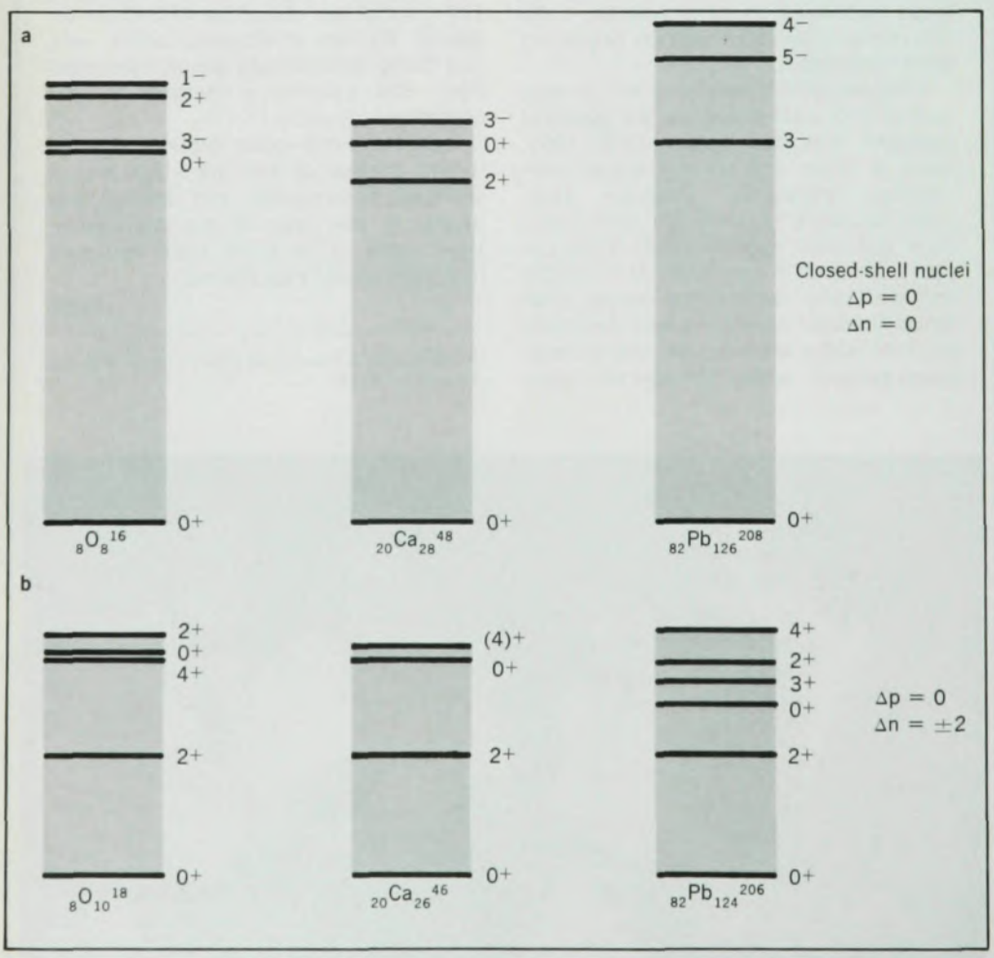
—EUB

* Joan Dash, *A Life of One's Own*, Harper and Row, New York (1973).

Maria Goeppert Mayer with shell-model theorists Ben R. Mottelson (on her right), J. Hans D. Jensen (on her left) and Aage Bohr.



Three-dimensional model of the energies of the first excited states of even–even nuclei. The dependence of excitation energy of the first 2^+ states on proton and neutron number can be seen here. The magic numbers are indicated by broad, dark bars on the Z, N plane. With very few exceptions, almost all of which occur for magic nuclei, the first excited state of an even–even nucleus is a 2^+ state; the exceptional lower states are indicated on the appropriate vertical bars. The model shows that the excitation energies are very small between magic numbers and very large at the magic numbers. (Photograph courtesy of Gertrude Scharff-Goldhaber, Brookhaven National Laboratory.) Figure 1



Lowest energy levels of three closed-shell nuclei, O^{16}, Ca^{48} and Pb^{208} (part a) and three nuclei with two nucleons (or holes) in addition, O^{18}, Ca^{46} and Pb^{206} (part b). The excitation energies are multiplied by a factor $A^{-1/3}$ to correct for the change in spacing with size. Note that the spectra of part b are similar to each other and different from those of part a. (Data from reference 16.) Figure 2

The spectroscopic factors for almost all the levels shown are approximately 1.0, indicating little fragmentation of the single-particle strength; appreciable fragmentation occurs for the starred levels. Both the orbital and total angular momentum have been measured. Let me point out that the set of quantum numbers for the levels in each group is just the same as that in the very familiar order given in Mayer and J. Hans D. Jensen's book,[2] although the order within the group is slightly different.

Why does it work?

I have tried to illustrate with these examples how useful and correct the shell model is. But why does it work? This is a subject not touched upon by Mayer in her original papers; it is a question that has received intense theoretical attention since then.

The most natural way to derive a shell model is to use Hartree-Fock theory. Then we assume the ground state is a single Slater determinant. The single-particle wavefunctions are determined by the variational principle—they are those wavefunctions that minimize the expectation value of the Hamiltonian. Low states of non-closed-shell nuclei are described as closed-shell plus valence particles in the unoccupied single-particle levels.

But although this theory leads to a shell model, we know it cannot be true. First, the nucleon–nucleon potential is known from scattering experiments, and from the requirements of nuclear saturation, to be large and repulsive at short distances; so Hartree-Fock theory cannot be used. Secondly, many experiments show the picture is not right; for instance, radiation is emitted when the nucleus makes a transition between two single-particle neutron states—clearly impossible since the neutron has no charge. The second type of discrepancy could perhaps be treated by perturbation theory; that is, by using Hartree-Fock theory and then calculating corrections and admixtures. The hard-core problem cannot be treated by perturbation theory, and Hartree-Fock must be given up.

It should be emphasized that all the experiments proving the simple shell-model nature of states (such as the one-particle transfer experiments mentioned above, which excite predominantly the single-particle states) although consistent with the Hartree-Fock picture of a single Slater-determinantal wavefunctions, do not prove this description. They merely measure overlaps between wavefunctions of various states in different nuclei. They are equally consistent with simple excitations in addition to any core, no matter how complicated.

Let me describe how the problem

has been attacked. The Hamiltonian is split into two parts

$$H = T + V$$
$$= \underbrace{T + U}_{H_0} + \underbrace{V - U}_{H_1}$$

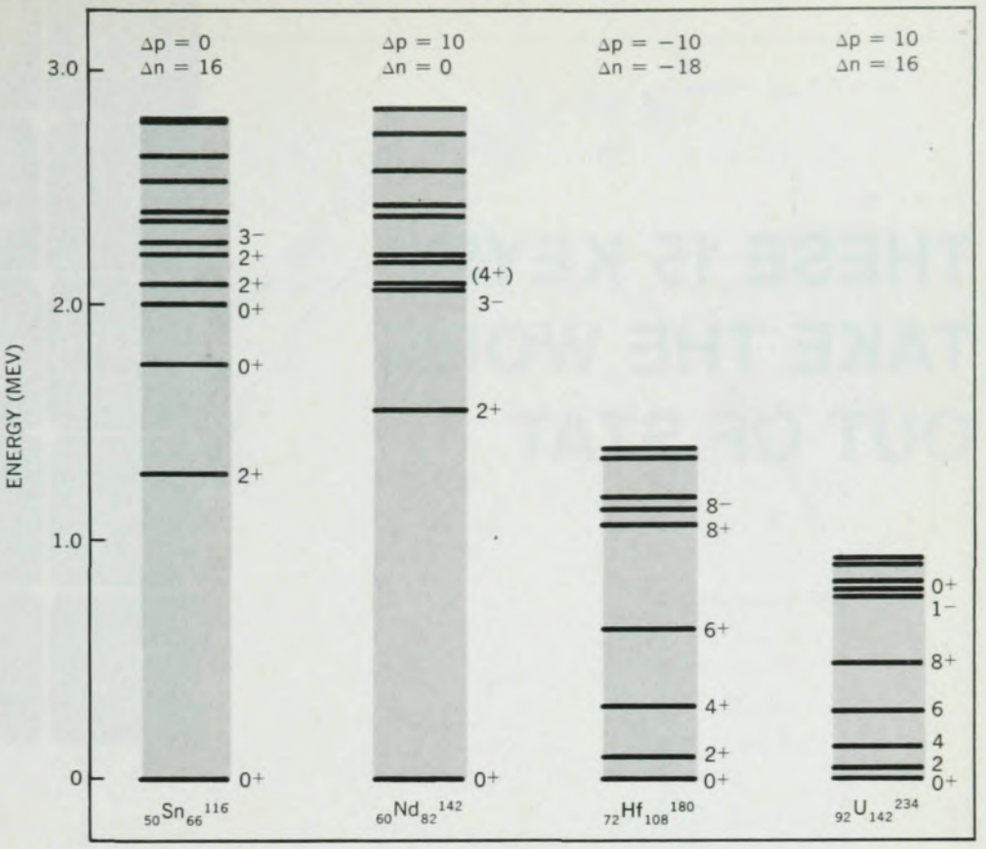
where **T** is the kinetic energy, **V** the nucleon-nucleon interaction and **U** some single-particle potential as yet undefined. One treats $\mathbf{H}_1$ as a perturbation. The perturbation expansion for the ground-state energy of the closed-shell nucleus is the well known Goldstone linked-cluster expansion. But because **V** is singular we must not treat it in perturbation theory; instead, if two particles interact, we must allow them to interact many times and to scatter into unoccupied states. Thus the interaction between two nucleons must be summed to all orders. This is done by calculating the Brueckner G-matrix from the interaction **V**. Then to first order in **G** the ground-state energy is

$$E = \sum_A \langle A|\mathbf{T}|A\rangle + \frac{1}{2}\sum_{A,B}\langle AB|\mathbf{G}|AB\rangle$$

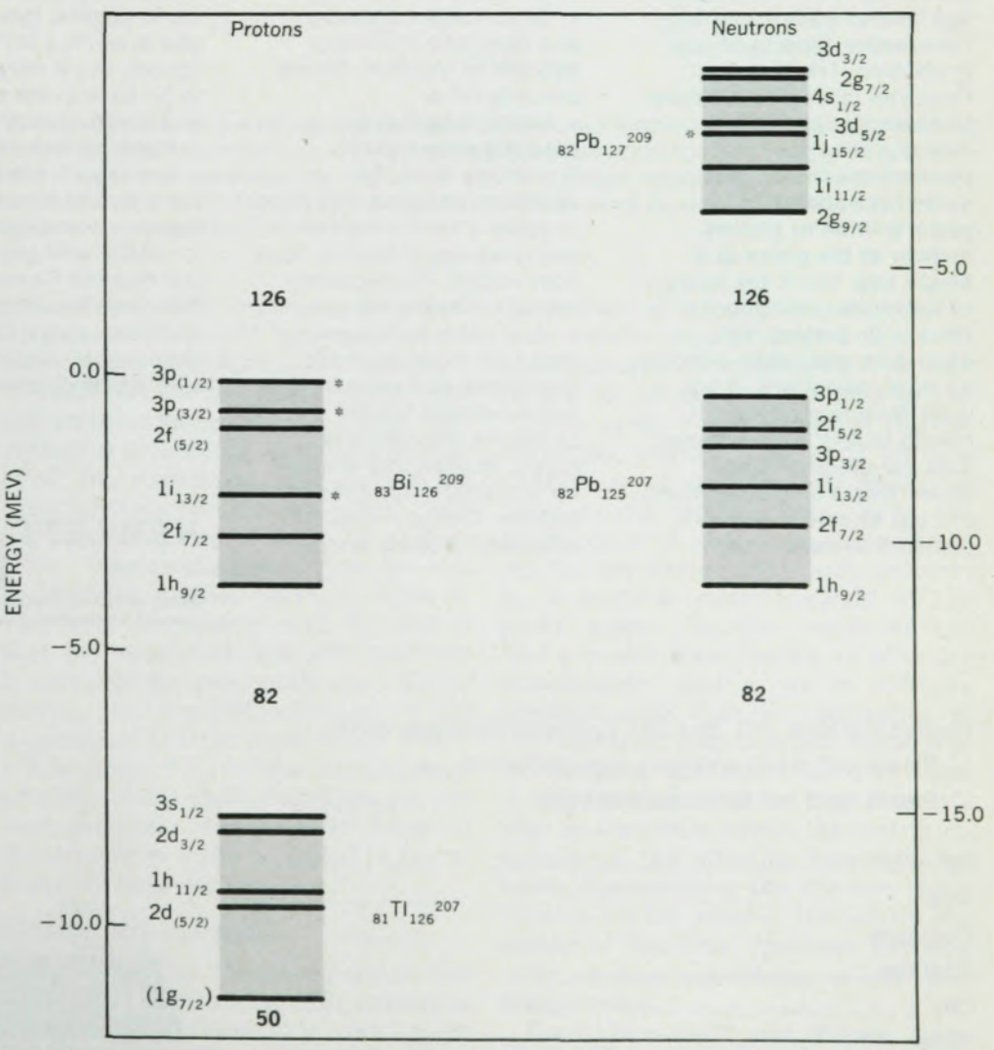
Here A, B are filled states and are eigenstates of $\mathbf{H}_0$. Exactly as in Hartree-Fock theory the second term is the sum of the interaction energies between the particles in the occupied states. But how do we choose **U**, which, after all, defines states A, B? As in Hartree-Fock theory, **U** is chosen to cancel high-order terms and thus to make the convergence fast. It is not enough to have summed to all orders the interaction between two nucleons. Clearly, once the three nucleons all come close to each other, we again need to solve the problem to all orders because the core is so strong. This three-body problem is impossibly complicated for a finite system, but it has been approximately computed in nuclear matter by Hans Bethe and his collaborators[3] using Fadeev equations, and is being tackled currently by B.D. Day, F. Coester and A. Goodman.[4] The rough calculations show that these three-body terms are small if the single-particle potential is put equal to zero for particle states. Examination of other terms shows it should be calculated self-consistently for hole states.

The results in nuclear matter are encouraging. Calculations[3] made with a soft-core nucleon–nucleon potential due to R. Reid gave 16 MeV for the binding energy per particle, close to the experimental value of 15.68 MeV. The Fermi momentum, k_F, is about 1.5 fermi, also close to the experimental value (1.36 fermi). The higher-order terms in this calculation are smaller than the two-body correlations (about 6 MeV, compared to 33 MeV), so convergence is indicated.

Calculations in finite nuclei to check the convergence are not feasible, so the



Nuclei far from closed shells. On the left are the lowest energy levels for two single-closed-shell nuclei, and on the right are two nuclei with many neutrons and protons outside the closed shell. Δp and Δn indicate the number of nucleons in addition to the closed shell. (Data from references 16 and 17.) Figure 3



Experimental single-particle energy levels in the lead region. For this figure the one-particle transfer experiments have been used to pick out the single-particle levels from the rest of the spectrum. (Data from reference 18.) Figure 4

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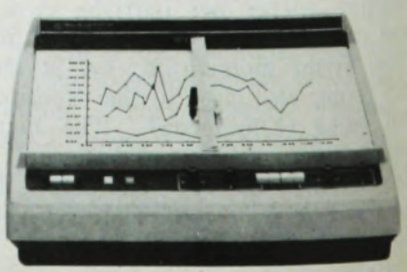

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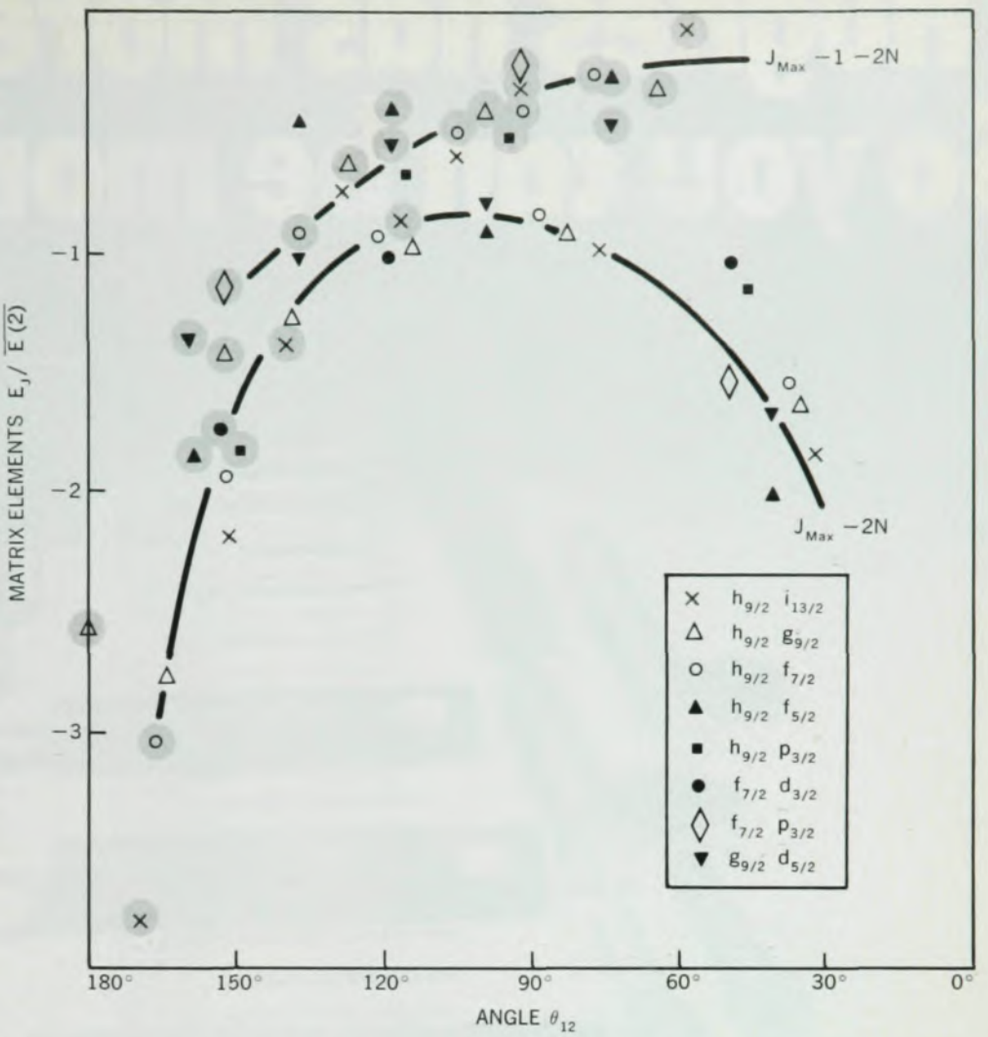
choice of **U** is thus still undetermined. Still, the results in nuclear matter encourage one to proceed to finite nuclei, keeping only the two-body correlations and using reasonable choices for **U**. Such calculations have been done, for example, on Pb^{208} by John Negele and by Tom Davies, Bob McCarthy and Peter Sauer. Negele[5] uses the local density approximation and an effective interaction, derived from the Reid potential, that is slightly adjusted to yield the experimental values in nuclear matter and thus takes the higher-order terms into account in some way. He calculates 7.83 MeV for the binding energy per nucleon in Pb^{208}, encouragingly close to the experimental value of 7.87 MeV, and 5.44 fermis for the proton rms radius—again close to the experimental figure, 5.44. Davies, McCarthy and Sauer[6] do a renormalized Brueckner–Hartree-Fock calculation that includes more terms than the usual Brueckner–Hartree-Fock, but has no adjustable parameters. The results, typical of such calculations, show too little binding (3.46 MeV nucleon) and too small a radius (4.73 fermis). They use a single-particle potential that is zero for particle states; the results are quite sensitive to the single-particle potential used, which indicates the importance of higher terms.

A closed-shell nucleus is far from being a simple Slater-determinant, because the hard core builds strong correlations into the wavefunction. If we expand the wavefunctions resulting from the above calculations, we find the amplitude of the single Slater-determinant to be negligibly small.[7]

Let me break off from this discussion of hard cores to give a more concrete example of how complicated our notion of a closed-shell nucleus is. Instead of thinking about excitations of the particles to high energy, which is what the hard core produces, we can ask about low excitations. Suppose that instead of considering O^{16} as a closer shell with the p-shell closed, we consider it as four nucleons outside of C^{12} and allow these four nucleons to be distributed among the single-particle levels $p_{1/2}$, $d_{5/2}$, $s_{1/2}$. In other words, the p-shell does not need to be completely filled nor the $d_{5/2}$ and $s_{1/2}$ completely empty. The Hamiltonian is then diagonalized within this space with phonomenological, but sensible, choices of $\mathbf{H}_0$ and $\mathbf{H}_1$. The result, obtained by A.P. Zucker, B. Buck and J.B. McGrory,[8] yields a wavefunction for O^{16} with an amplitude of only 0.71 for the closed-shell configuration. However, the same method predicts the first two levels of mass 17 in the right order and describes these two levels as the coupling of $d_{5/2}$ and $s_{1/2}$ particles to the O^{16} ground state. Hence, in this case, we see explicitly that in spite of the highly correlated nature of its ground state, O^{16} behaves in some respects as a good closed-shell nucleus.



Matrix elements of the effective interaction plotted as a function of the angle between the individual angular momentum, for eight of the cases discussed by John Schiffer in reference 13. The matrix elements are separated into two groups according to whether the total angular momentum differs from the maximum allowed value by an odd integer (gray circles) or an even integer (plain symbols). Figure 5

What can we say about nuclei with one more or less nucleon? Again, perturbation expansions have been formulated for expressing the energies of these systems relative to the core, and the core can be as complicated as possible. The result should give the single-particle energies shown in figure 4. The main discrepancy with the data is that the calculated spin-orbit splitting is too small for spin-unsaturated shells; that is, when the state with $j = l + 1/2$ is occupied and the state with $j = l - 1/2$ is empty.[3,9] So this fundamental property of the shell model has not yet been justified. Higher-order terms in the expansion must be called in to explain this behavior.

The effective interaction

How does this theory expand to the vast majority of nuclei with numerous particles in addition to a core? Our Hamiltonian is $\mathbf{H}_0 + \mathbf{H}_1$ as described above. It is a many-fermion Hamiltonian, acting between all possible configurations of a complete set of one-body orbits—eigenvectors of $\mathbf{H}_0$. An exact solution is impossible. So we pick a set of one-body orbitals in the vicinity of the Fermi surface of the unperturbed system. The set of all configurations of particle and holes, in these active orbitals only, form the model space of states. It is possible to replace the exact many-body problem by a problem stated entirely in the model space. In other words we can find a model Hamiltonian, or effective Hamiltonian, and a set of effective operators such that the eigenvalues of the effective Hamiltonian inside the model space are indentical with some of the eigenvalues of the true Hamiltonian in the entire space; the matrix elements of the effective operators between eigenstates of the effective Hamiltonian are the same as the matrix elements of the true operators between corresponding eigenstates of the true Hamiltonian.

Baird Brandow,[9] and Mikkel Johnson and Michel Baranger,[10] showed how one can write a perturbation-theory expansion for the effective interac-

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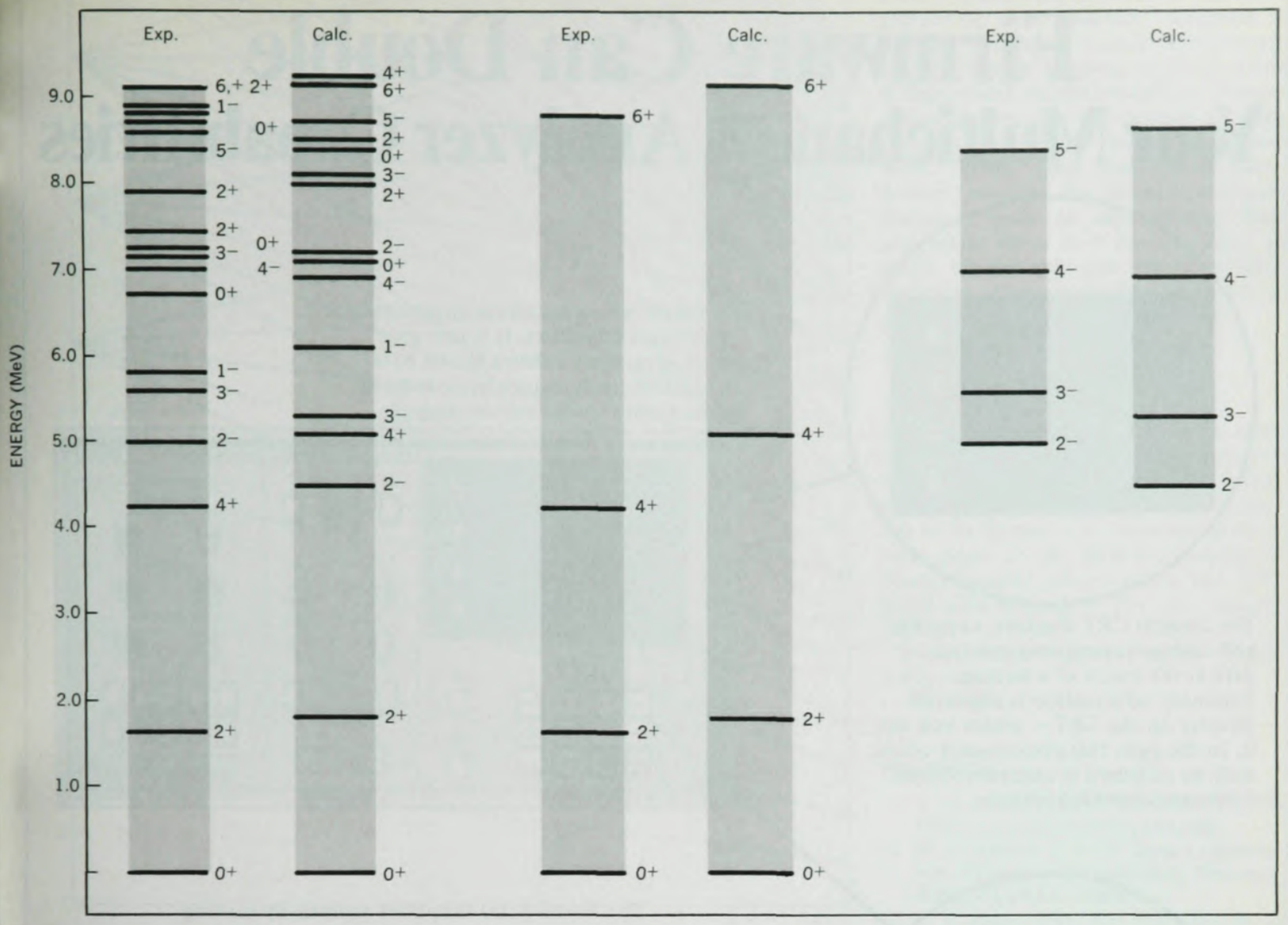

Experimental and calculated energy levels of the Ne^{20} nucleus. The first two columns show the total spectrum; the center and right-hand columns show the two lowest rotational bands separated out. (Data from reference 14.) Figure 6

tion that, in conjunction with experimental single-particle energies and wavefunctions, can be used to calculate valence properties of open-shell nuclei. As usual, an infinite set of terms must be summed to treat the hard core; so the potential gets replaced by a G-matrix. And as usual there is the problem of convergence. The convergence here has been studied in a limited way. The effective Hamiltonian in the model space has been calculated, by perturbation theory, with a very limited larger space; it includes only the next major shell above and below the model space. G. E. Brown and T. T. S. Kuo's pioneering calculation,[11] which included only first and second-order terms, yielded effective matrix elements that gave quite good agreement with experiment over a wide variety of nuclei. Since their work, M. W. Kirson, B. R. Barrett[12] and others have examined higher-order terms in O^{18} and find sizeable variations that depend on which terms are included.

But the idea of the existence of an effective interaction has pervaded shell-model calculations since the beginning. Mayer in her original papers used a delta-function force as a residual interaction in order to justify one of her original postulates—that an even number of identical particles pairs to angular momentum zero, and an odd number to the angular momentum of the filling single-particle level. But can we parametrize the effective interaction in a simple way that will be essentially the same in all parts of the periodic table? From the microscopic point of view mentioned above, it is not obvious that we can.

In the past few years John Schiffer[13] has measured and examined the spectra of nuclei for which a very reduced model space—that of two nucleons in one single-particle orbit, or two nucleons each in a different orbit—might be reasonable. The angular momenta of the two particles add vectorially to various total angular momenta. Schiffer plots the energies (which for his model space are the diagonal matrix elements of the effective interaction), corrected by a scale factor, as a function of the angle between the individual angular momentum, and he finds that they fall on a universal curve. In figure 5 are the matrix elements for eight different cases (there are more examples, but I have no space to present them all). The quantum numbers of the two single-particle levels are listed for each case. Schiffer separated the matrix elements into two groups according to whether the total angular momentum differs from the maximum allowed value by an odd or even integer. The curves are merely drawn through the data. This is the prettiest way to extract from the data the fact that there is a universal effective interaction, at least to rough approximation.

Large shell-model calculations

Most nuclei cannot be treated as two particles each in a single-model level. And this leads to what are termed "large shell-model calculations." A model space is chosen, and with experimental single-particle energies and an effective interaction, a diagonalization can be performed. The results are compared with experimentally determined excitation energies, radiative

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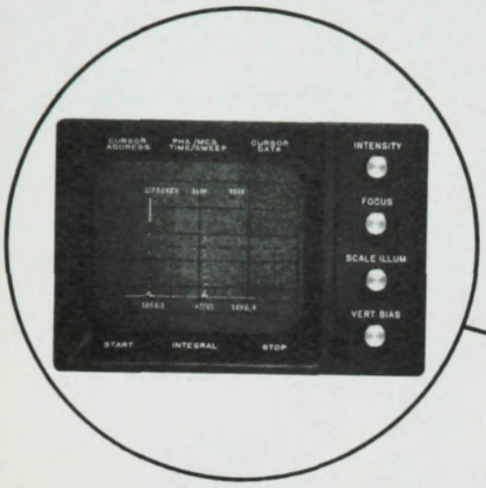

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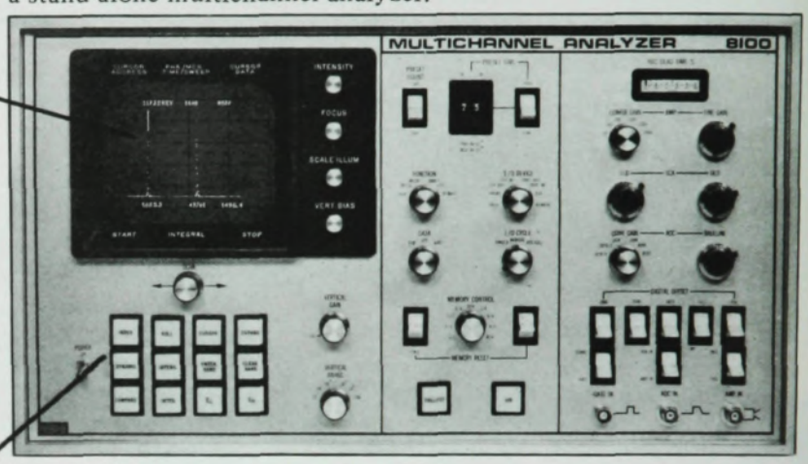

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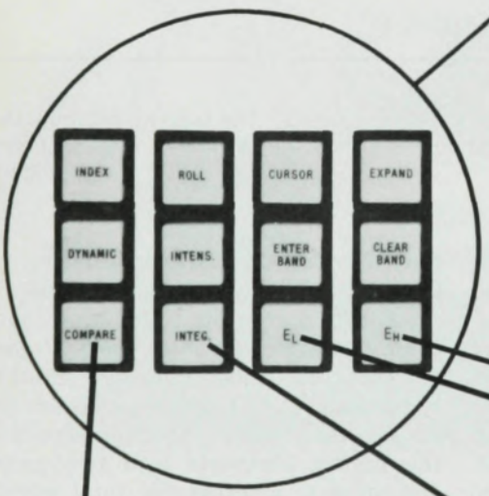

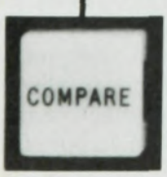

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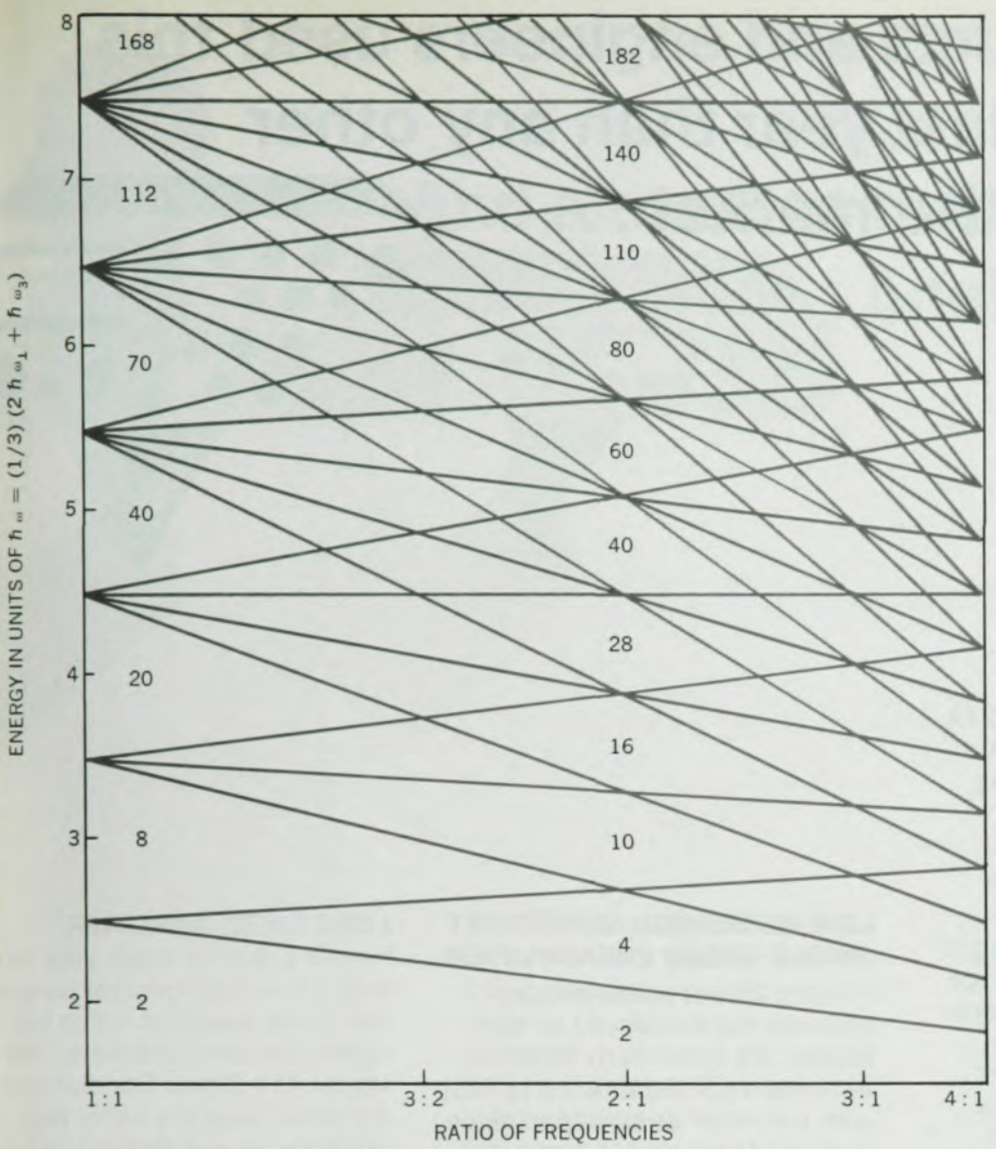

Energy levels of a deformed harmonic oscillator. The levels are plotted here as a function of the ratio of the frequencies of motion perpendicular and parallel to the symmetry axis. Gaps occur for the spherical case (ratio = 1:1) and also for other integral values of the ratio. (From reference 15.) Figure 7

transition rates, direct-reaction cross sections, magnetic moments, and so on. Data from different types of experiments are thus correlated with each other and related to a model. Examples of this procedure would be quite lengthy to present; I show one result (figure 6) from a very large calculation by Joe McGrory and Hobson Wildenthal[14] who use the Oak Ridge shell-model code. The nucleus is Ne^{20}. The model space is all states with eight nucleons distributed among the $p_{1/2}$, $d_{5/2}$ and $s_{1/2}$ levels. In more conventional shell-model calculations the p-shell would be kept completely filled. The figure shows experimental calculated energies of the levels of Ne^{20} in the first two columns; in the next two columns I have separated those levels belonging to the two lowest rotational bands. The point is that the characteristic rotational bands in Ne^{20} are reproduced by a shell-model calculation that uses a spherical basis. For the simplest description of these states we should use a deformed single-particle potential rather than a spherical one. And this is usually done for such nuclei.

A deformed potential can also have gaps in its single-particle energy levels. A simple example is shown in figure 7, which is a plot, taken from Aage Bohr and Ben Mottelson,[15] of the levels of a deformed harmonic oscillator as a function of the ratio of the frequencies of motion perpendicular and parallel to the symmetry axis. You see that gaps occur for the spherical case (ratio = 1:1); but they also occur when the ratio is 2:1. The levels that are given for this latter value of the ratio, with surface and spin-orbit effects also included, look just like the usual Mayer and Jensen levels but with different magic numbers. One evidence for the gaps is the existence of fission isomers around neutron number 148. These are metastable states that decay by fission and owe their existance to extra stability due to these shell effects.

So we see, in conclusion, that the shell model has been verified by experiment and has proved useful for a correlation of nuclear structure. However, a closer look shows that the naive picture of it is incorrect. Progress in deriving the shell model is encouraging; for further progress we need either a theoretical breakthrough on convergence problems or the courage to wade through incredibly lengthy calculations. With "large shell-model calculations" we have the means to compare different types of experimental data and relate them to a model. And, finally, we see that the effects of shell structure show up in the deformed region as well as in the spherical one.

* * *

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