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THE SIMPLE SHELL MODEL VERSUS MANY-BODY CALCULATIONS*

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In spite of the heading, these approaches to nuclear structure physics are not in any contrast. They approach the problem of nuclear structure from opposite directions. We believe, however, that when many-body calculations will achieve their final goal, we will eventually understand why the simple shell model works so well and where it fails. The shell model has been used extensively and successfully for almost 60 years. It is still not understood why it is such a good approximation.

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The aim of this talk is to demonstrate by rather old examples how the shell model can be simple and elegant and yet efficient. This situation will be compared with some results of many-body theory which is much more fundamental and ambitious but is still making its first steps on a very difficult road.

Why so far, has nuclear many body theory not reached a complete solution? Its input is the interaction between free nucleons. This interaction has been studied for more than 50 years and there is still no theory from which it may be derived. Of course, not resorting to string theory, QCD is considered to be a sufficiently exact theory of protons and neutrons. For nuclear structure, however, it is needed for rather low energies where perturbation theory does not work. Perhaps QCD on a lattice will give a satisfactory solution. So far, various models have been constructed which reproduce rather exactly many results of scattering experiments but their off-shell behavior is arbitrary to a large extent. Another point is the relative importance of 3-body forces. Many of the calculations introduce them as input but their strength is determined only from bound 3 and 4 body systems.

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When the second generation shell model was introduced in 1949, it was clear to Maria Mayer that a mutual interaction between nucleons is necessary to explain ground state spins of nuclei [1]. The interactions which followed were taken from various versions of free nucleon interaction published in those days. After a few years it was found that this interaction is rather singular and cannot be used with shell model wave functions. It became clear that the bare nuclear interaction must be strongly renormalized to be used in the shell model. This was attempted by Brueckner theory of the G-matrix and later by a long list of authors who refined it and tried to make it useful for shell model calculations.

It should be made clear that these attempts which finally seem to have succeeded, as described by Covello [2], start from the shell model. They do not attempt to calculate binding energies of nuclei with closed shells. Nor do they attempt to calculate separation energies of single nucleons outside closed shells (single nucleon energies). Their aim is to calculate the effective interactions between nucleons outside closed shells, valence nucleons. The idea is that the bare interaction introduces strong short range correlations between nucleons. These mix into the shell model wave functions of independent motion, states of high lying configurations to which nucleons are excited by the interaction. It is possible to continue using shell model wave functions if the effects of mixing of high lying states are attributed to a change of the mutual interaction. The resulting effective interaction should be much more tame and could be used as a perturbation.

Recently, more ambitious attempts were initiated. They start *ab initio*, from the bare interaction between free nucleons and use shell model wave functions only as basis for their calculations. One of these approaches is the No Core Shell Model (NCSM) which uses harmonic oscillator wave functions as basis functions. Due to computational complexity they are able to use oscillator functions up to $6h\omega$. Some of their results will be discussed in the following. The resulting wave functions are very complicated and it is not clear how the simple shell model will emerge from them. In fact, their results so far, seem to show that the shell model could not possibly be a good approximation ...

Since early many-body calculations did not produce reliable values for the effective interaction, an alternative approach was developed [3]. In it, matrix elements of the effective interaction were determined from measured energies of nuclei. To obtain meaningful results, some limitations on the effective interaction had to be imposed. In the many-body theory the resulting effective interaction is a complicated operator. Even if the bare interaction acts only between two nucleons, the effective interaction contains not only two-body terms but also 3-body terms and higher order ones. There was no way to determine how big those terms should be.

If the effective interaction is assumed to be a two-body one, matrix elements of a configuration with $n > 2$ nucleons are linear combinations of matrix elements of two-body configurations. Hence, a set of measured energies in a group of nuclei can be expressed in terms of a smaller number of two-body matrix elements. If such two-body matrix elements are found, this gives confidence that the choice of configuration was correct. It also means that the matrix elements so obtained may be used to calculate energies of other states, not yet measured. Examples of this approach will be presented in the following.

The first successful application of this method which demonstrated its power, is the relation between the spectra of ^{38}Cl and ^{40}K. According to the simple shell model, in ^{40}K there are three $1d_{3/2}$ protons coupled to $J_p = 3/2$ (one $d_{3/2}$ hole) and one $1f_{7/2}$ neutron. In such a configuration there are 4 states with spins $J = 2, 3, 4, 5$. If these are taken to belong to the 4 nucleon configuration, their interaction energies are linear combinations of the interaction energies of the 2 nucleon $d_{3/2}f_{7/2}$ $J = 2, 3, 4, 5$ states. Hence, spacings of the ^{40}K levels are linear combinations of the spacings of the two-nucleon configuration expected in ^{38}Cl. Since the ^{40}K levels were known, we calculated the spacings of the ^{38}Cl levels. There was no resemblance between them and published data. When new measurements were published, the agreement with our predicted energies turned out to be very good [4] as shown in Fig. 1. Such a calculation was carried out independently by Pandya and published a little later [5].

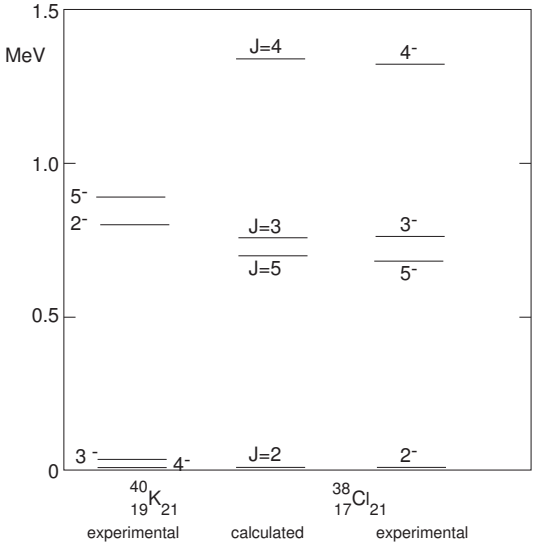

Fig. 1. Prediction of ^{38}Cl levels from those of ^{40}K.

This good agreement indicated that in ^{40}K and ^{38}Cl, the states considered do not mix appreciably with other states. Moreover, it indicates that the $J = 3/2$ state in ^{37}Cl is due to a single $1d_{3/2}$proton outside closed shell of $1d_{5/2}$ and $2s_{1/2}$ orbits. This fact was noticed, but unlike the practice of these days, no discovery of a new magic number, $Z = 16$, was announced.

The (3 spacings of) two-body matrix elements of the effective interaction determined in this way satisfy consistency conditions of nicely reproducing 6 experimental data (3 level spacings in ^{38}Cl and in ^{40}K). Hence, they may be safely adopted and be used in calculating spectra of other nuclei. Another very important result was that matrix elements, or differences thereof, do not change appreciably when going from one nucleus to its neighbors. This rather regular behavior is an important ingredient in applications of this method.

This was the first shell model calculation with significant quantitative agreement with experiment. It was followed by other such calculations which became more and more complicated, culminating in calculations with many millions of shell model states. In all these calculations, only two-body interactions have been used.

It is a fact that in all shell model calculations carried out so far, no evidence of explicit 3-body effective interaction was found. This is interesting and perhaps significant. It may be that these interactions are either rather weak or independent of the state considered, or both. Also two-body matrix elements between states of $1d_{3/2}$ protons and $1f_{7/2}$ neutrons are affected by possible 3-body interactions with nucleons in the core. Similarly, interactions of a valence nucleon with two core nucleons could contribute to single nucleon energies which are taken from experiment. Even if those contributions are relatively weak, the large number of core nucleons may lead to significant contributions. In the present way of determination of matrix elements from experiment it is impossible to distinguish such contributions from those of genuine two-body interactions.

Most nuclear spectra are complex and mixing of several configurations is necessary. Still, there are several simple cases, like the one described above. Each such case yields information only about a limited set of matrix elements but it has been possible to extract from them some general properties of the effective interaction. These are:

> The $T = 1$ part of the effective interaction, between identical nucleons, is *strong* and *attractive* in $J = 0$ states. In other states it is rather *weak* and *repulsive* on the *average*.
>
> The $T = 0$ part, included in the proton–neutron effective interaction, is *strong* and *attractive* on the *average*.

An important conclusion from these properties is that the central potential well of the shell model is created by the proton–neutron effective interaction. It determines its depth as well as its shape, thereby it determines positions and spacings of single nucleon orbits. A direct consequence is that positions of single proton orbits depend on the occupation numbers of neutrons and *vice versa*.

This realization led us 48 years ago to look at isotones with neutron number 7 and predict that the ground state of ^{11}Be should be $1/2^+$ rather than the expected $1/2^-$ state whose excitation energy was also predicted [6]. The shell model space which we used was rather limited but the shell model calculation was exact. More elaborate calculations can be made but none could be simpler.

We started from levels of ^{13}C, the $1p_{1/2}$ ground state and the $1/2^+$ excited state at about 3 MeV taken to be the $2s_{1/2}$ single neutron state (Fig. 2). To reach $J = 1/2$ states of ^{11}Be, two $1p_{3/2}$ protons coupled to $J = 0$ should

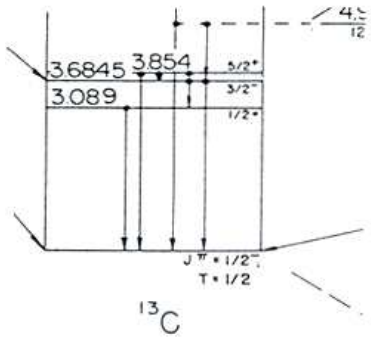

Fig. 2. Single neutron levels in ^{13}C.

be removed. The interaction of the latter with a $1p_{1/2}$ neutron is naturally expected to be stronger than their interaction with a $2s_{1/2}$ neutron. Information about these interactions may be provided by levels of ^{12}B obtained from ^{13}C by removing one $1p_{3/2}$ proton. Its lowest measured levels have spins 1^+, 2^+ and 1^-, 2^-, taken to be due to the $1p_{3/2}$ proton hole coupled to the $1p_{1/2}$ and $2s_{1/2}$ neutrons (Fig. 3). Actually only the centers-of-mass of these levels are required. The interaction energy of a pair of j-protons coupled to $J = 0$ with a j'-neutron is equal to *twice* the average interaction of a j-proton with a j'-neutron. The average interaction energy (it has now a fancier name — the *monopole interaction*) is defined by

$$V\left(jj'\right) = \Sigma(2J+1)\left\langle jj'J|V|jj'J\right\rangle / \Sigma(2J+1)\,.$$

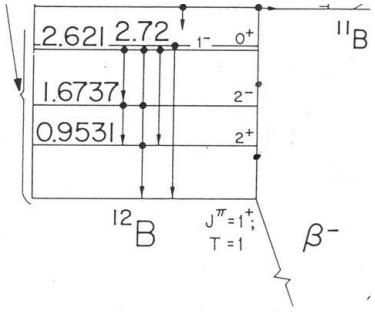

Fig. 3. States of proton $1p_{3/2}$ hole-neutrons in $1p_{1/2}$ and $2s_{1/2}$ orbits in ^{12}B.

Comparing the spacing in ^{13}C with the spacing of centers-of-mass in ^{12}B we can directly find out the effect of removing *two* $1p_{3/2}$ protons from ^{13}C to obtain ^{11}Be. A graphic solution of the exact shell model calculation described above is presented in Fig. 4. This is not a simple extrapolation, it yields an *exact* solution of the shell model calculation using the simple jj-coupling configurations mentioned above [6].

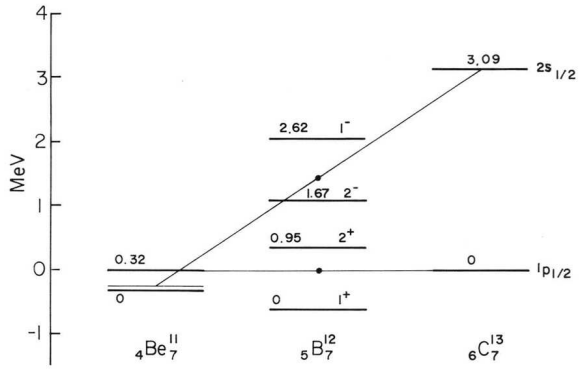

Fig. 4. Prediction of the $1/2^+$ ground state of ^{11}Be.

The ^{11}Be case clearly demonstrated that the proton–neutron interaction may interchange the position of orbits in different major shells. An obvious point about which we did not make any fuss, is that for 4 protons the number of 8 neutrons is no longer a magic number. The $2s$ orbit from the next major shell becomes lower than the $1p_{1/2}$ orbit. It is often questioned whether models which are useful for stable nuclei can be used for unstable ones. Here, the $p_{1/2}$ neutron is only slightly bound and yet, its energy was predicted from the more stable ^{12}B and ^{13}C.

A similar behavior was observed experimentally for the neutron magic number 20. As explained above, in ^{36}S and higher mass nuclei mentioned there, the neutron s, d shell is fairly closed and $N = 20$ is magic. With $N = 20$ and removing protons, down to ^{33}Al and ^{32}Na, the s, d neutrons lose more interaction energy than the $1f_{7/2}$ neutrons. Hence, the single neutron $1f_{7/2}$ orbit becomes sufficiently close to s, d orbits so that neutron configurations are mixtures of neutrons in f and s, d orbits. The resulting spectra become complicated and much more collective than in heavier $N = 20$ isotones. This situation is referred to as the disappearance of the $N = 20$ magic number as is the case with the $N = 8$ magic number in ^{11}Be and neighboring nuclei.

In rather light nuclei, like those in which valence nuclei occupy the $1p$ shell, it is possible to see how well *ab initio* calculations, like the NCSM, reproduce measured energies. In such nuclei, the many-body calculations are simpler, although still very complicated. Results of such calculations for $A = 14$ nuclei were presented and compared with experimental data [7]. In that paper, the 39 authors present measurements of Gamow–Teller transitions from the ^{14}N ground state, with $J = 1, T = 0$ to levels in ^{14}C and ^{14}O. These are compared with NCSM calculations. There are some agreements and some disagreements and the authors present the latter as a challenge to the shell model. It is, however, a challenge to NCSM since in the simple shell model there are certainly no gross discrepancies with experiment.

The results reported in Ref. [7] are presented in Fig. 5. The most important discrepancy is the appearance, at rather low excitation, of a 0^+ state (another 0^+ state a bit higher was not reached by those experiments) and three rather than one 2^+ states. The fact that the Gamow–Teller strength is shared by the three 2^+ states is not surprising. They are rather close and most probably mixed. Still, the summed strength is less than the expected one. This, however, is a common feature of the shell model and will not

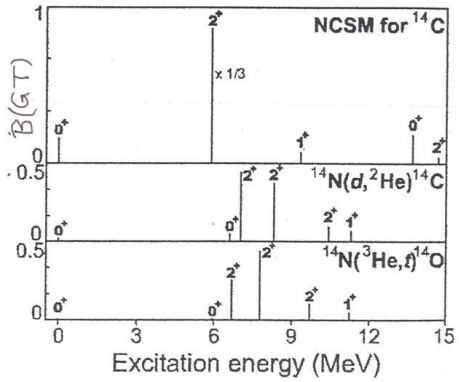

Fig. 5. NCSM calculations for $A = 14$ nuclei compared with experiment.

be further discussed. It is interesting to see that the calculation predicts a rather large transition strength to the ground state of ^{14}C. This Gamow–Teller strength has been measured many years ago by the highly quenched ^{14}C beta decay. It is barely seen in the ^{14}C levels and not at all in the ^{14}O levels in Fig. 5. This quenching makes the well known ^{14}C dating possible. In the simple shell model, such quenching within the p-shell was shown to be possible if tensor forces are included [8].

To find the interpretation of those extra levels in the simple shell model, it is necessary to look at the predicted positions of p-shell levels. Many years ago, Cohen and Kurath determined the effective interactions in the p-shell from some measured energies and used them to calculate positions of other levels [9]. Their results for ^{14}C are shown in Fig. 6 where also the NCSM results are indicated. It is significant that the NCSM *ab initio* calculations are in fair agreement with the Cohen–Kurath ones. Thus, in the simple shell model, the extra levels are intruders, due to excitation of p-neutrons into the higher s, d-shell. This should not be a big surprise since a more drastic intrusion was seen in ^{11}Be. This assignment can be justified in a more quantitative fashion.

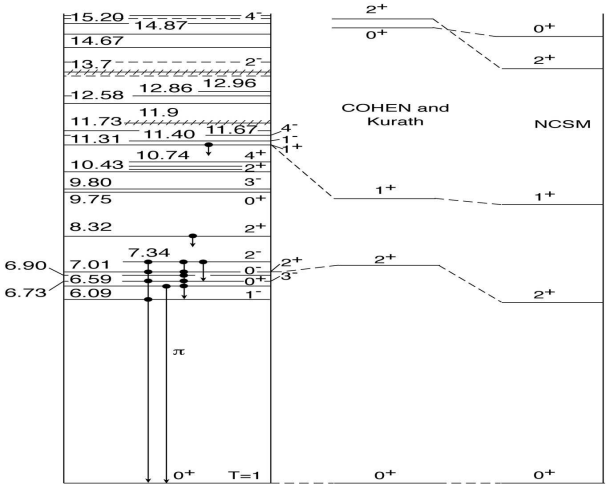

Fig. 6. ^{14}C levels compared with Cohen–Kurath and NCSM calculations.

In Fig. 2 it is seen that the neutron $2s_{1/2}$ orbit lies at 3.09 MeV above the $1p_{1/2}$ orbit. The $1d_{5/2}$ orbit lies rather close to it, at 3.85 MeV. Two neutrons in these orbits can couple to yield two 0^+ states ($s^2_{1/2}$ and $d^2_{5/2}$ configurations) and two 2^+ states ($s_{1/2}d_{5/2}$ and $d^2_{5/2}$ configurations). The single neutron energies can be obtained from the ^{13}C spectrum in Fig. 2. Before taking into account mutual interactions, the $s^2_{1/2}$ state should lie

$2\times3.09 = 6.18$ MeV about the ^{14}C ground state, rather close to the measured value of 6.59 MeV. The $s_{1/2}d_{5/2}$ states should lie at $3.09 + 3.85 = 6.94$ MeV and the single neutron contribution to $d^2_{5/2}$ excitation energies is equal to $2 \times 3.85 = 7.7$ MeV. These energies are in the right energy domain but to calculate the exact positions of these levels it is necessary to take into account the mutual interactions. To do this, it is necessary to know the values of diagonal and non-diagonal matrix elements between these states as well as the non-diagonal matrix elements of them with p-shell states. There were some attempts to determine these matrix elements from experimental data. Here, it is sufficient to look at the analogous situation in ^{16}C.

In ^{15}C the neutron p-shell is closed and the single valence neutron should be in the s, d-shell. Indeed, the ground state has spin $1/2^+$, due to a $2s_{1/2}$ neutron and above it, at 0.74 MeV, there is a spin $5/2^+$ state due to a $1d_{5/2}$ neutron. The order of these two states is the same as in ^{13}C and their spacing is almost equal to 0.76 MeV, the spacing in ^{13}C. The lowest levels in ^{16}C are expected to be due to two neutrons in these orbits and their relative positions should be equal to those in ^{14}C if their interactions with p-shell states is not taken into account. This observation was made long ago by Fortune [10] whose experimental level scheme is shown in Fig. 7. In addition to level spacings, the lowest excited 0^+ state is calculated to lie at 6.38 MeV, very close to the experimental 6.59 MeV. The slight difference may become even smaller if the interaction of this state with the ^{14}C ground state will be taken into account. The agreement between the spectra of ^{14}C and ^{16}C in Fig. 7 is impressive indeed.

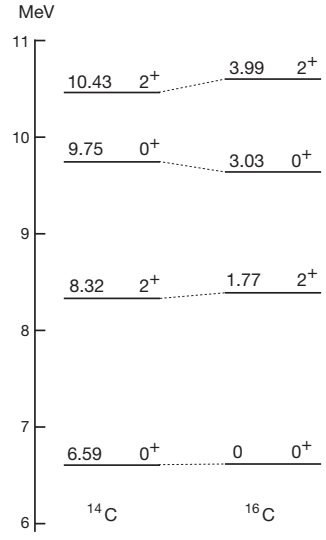

Fig. 7. ^{16}C levels and corresponding ^{14}C levels.

In addition to the energies of the extra levels considered above, there is another indication that these are intruder states. It is related to the wave functions of these states in the simple shell model. It is obtained by considering the Coulomb energy differences between them and rather pure p-shell states. Looking at the ^{14}C level scheme in Fig. 6, several negative parity levels can be seen between 6 and 8 MeV. No negative parity states can arise from an even number of p-nucleons. In the simple shell model these levels are obtained by raising one $1p_{1/2}$ neutron into the s, d shell. Indeed, these levels have spins $0^-, 1^-, 2^-$ and 3^- which are due to coupling of the ground state of ^{13}C with one $2s_{1/2}$ and one $1d_{5/2}$ nucleon respectively.

In Fig. 8, positions of these levels above the ^{14}C ground state are compared with positions of corresponding $T = 1$ levels above the 0^+, $T = 1$ state of ^{14}N which lies 2.31 MeV above its 1^+, $T = 0$ ground state. The Coulomb energy differences of these negative energy states are considerably smaller than that of the p-shell ground state. The larger change is seen for states with a $2s_{1/2}$ nucleon which is due to its wave function having a larger spatial extension. A $2s_{1/2}$ proton has no centrifugal barrier to keep it closer to the core protons. Such reduced Coulomb energy differences can be seen in positions of the first excited 0^+ state and following three 2^+ states in ^{14}C and ^{14}O in Fig. 5. The 2^+ states are admixtures of a p-shell state and the two s, d-shell states discussed above. It is interesting to note that the 1^+ state which is a pure p-shell state, has practically the same Coulomb energy shift as the ground state, even though it lies more than 11 MeV above it.

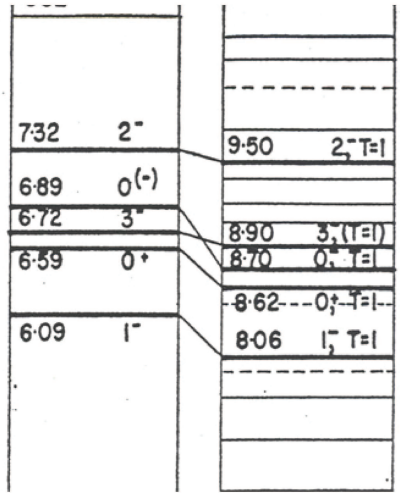

Fig. 8. Coulomb energy differences of some nuclear states.

Thus, it seems that NCSM reproduces reasonably well (spacings of) states due to p-shell nucleons. The calculated positions of intruder states, however, seem to be much higher than the experimental ones. The $A = 14$ nuclei are thus, a challenge not to this (simple) shell model but to the NCSM calculations. Why does NCSM miss intruder states? In schematic models, where a shell model potential well is determined by charge distributions of nuclei, large gaps emerge between major shells. As a result, intruder states turn out to be rather high and certainly not ground states as in ^{11}Be. In the simple shell model, energies of single nucleon orbits are taken from experiment and intruder states are calculated to be where they are. Still, in no core calculations, as suggested by their name, no *a priori* potential well is assumed so what is the reason?

In NCSM calculations, harmonic oscillator wave functions are used just as basis functions. The $h\omega$ of the wave functions adopted in the calculations reported in Ref. [7] is about 14 MeV. Hence, the difference in *kinetic energy* of these basis states is half of $h\omega$ which is about 7 MeV. This is a rather large energy difference which is apparently difficult to reduce by the mutual interactions. It is true that oscillator functions form a complete set and a complete calculation will yield correct results independent of the value of $h\omega$. Computational complexities, however, prevent for the time being, reaching a satisfactory solution. The results reported in Ref. [7] were obtained by using oscillator functions only up to $6h\omega$.

Ab initio calculations of nuclear states and energies are of great importance provided the input, the bare interaction is sufficiently correct and the approximations made are satisfactory. Then accurate energies of nuclear states will be obtained, also of nuclei which are inaccessible experimentally. More important would be the knowledge of the real nuclear wave functions. This will enable accurate calculation of various moments and transitions, electromagnetic and weak ones, including double beta decay. This will eliminate the need to resort to effective charges, effective magnetic moments *etc.* As we saw, there are still many difficulties to overcome.

Some example of the simplicity of the shell model were presented above. From the early days it was clear that shell model wave functions could not be the exact real ones. States of individual nucleons do not include short range correlations which are due to the strong interactions observed in scattering of free nucleons. The bare interaction is fully taken into account in *ab initio* calculations. It leads to strong admixtures of basis states involving excitations to several higher major shells. The higher the shells involved, the better the approximation obtained. This raises the important question whether the shell model will emerge from these calculation as a good approximation. The shell model has been so simple, useful and elegant to such an extent that it would be illogical to abandon it. A simple example above

showed that single nucleon wave functions have some reality in nuclei. Reliable many-body theory of the nucleus could and should explain why the shell model works so well, which interactions lead to it and where it becomes useless. The question still remains whether *simplicity* (shell model) will emerge from *complexity* (many-body theory).

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