Nuclear structure II (global properties, shells)

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National Nuclear Physics Summer School 2014
William & Mary, VA

• Global properties of atomic nuclei
• Shell structure
• Nucleon-nucleon interaction
• Deuteron, Light nuclei
Global properties of atomic nuclei
Sizes

\[ \rho(0) = 0.17 \text{nucleons/fm}^3 \]

\[ \rho(r) = \rho_0 \left[ 1 + \exp\left( \frac{r - R}{a} \right) \right]^{-1} \]

\[ R \approx 1.2A^{1/3} \text{ fm}, \quad a \approx 0.6 \text{ fm} \]
Calculated and measured densities
Binding

\[ m(N, Z) = \frac{1}{c^2} E(N, Z) = N M_n + Z M_H - \frac{1}{c^2} B(N, Z) \]

The binding energy contributes significantly (~1%) to the mass of a nucleus. This implies that the constituents of two (or more) nuclei can be rearranged to yield a different and perhaps greater binding energy and thus points towards the existence of nuclear reactions in close analogy with chemical reactions amongst atoms.
The sharp rise of B/A for light nuclei comes from increasing the number of nucleonic pairs. Note that the values are larger for the 4n nuclei (\(\alpha\)-particle clusters!). For those nuclei, the difference

\[
\Delta E \equiv B(N, Z) - nB(2, 2)
\]

divided by the number of alpha-particle pairs, \(n(n-1)/2\), is roughly constant (around 2 (MeV)). This is nice example of the saturation of nuclear force. The associated symmetry is known as SU(4), or Wigner supermultiplet symmetry.

Table 1-3: Binding energies (MeV) for some stable light nuclei.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>(E_B)</th>
<th>(E_B/A)</th>
<th>(\Delta E)</th>
<th>Symbol</th>
<th>(E_B)</th>
<th>(E_B/A)</th>
<th>Symbol</th>
<th>(E_B)</th>
<th>(E_B/A)</th>
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<td>2.22</td>
<td>1.11</td>
<td>—</td>
<td>(^3\text{H})</td>
<td>8.48</td>
<td>2.83</td>
<td>(^3\text{He})</td>
<td>7.72</td>
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<td>(^4\text{He})</td>
<td>28.30</td>
<td>7.07</td>
<td>—</td>
<td>(^5\text{He})</td>
<td>27.41</td>
<td>5.48</td>
<td>(^5\text{Li})</td>
<td>26.33</td>
<td>5.27</td>
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<td>32.00</td>
<td>5.33</td>
<td>—</td>
<td>(^7\text{Li})</td>
<td>39.25</td>
<td>5.61</td>
<td>(^7\text{Be})</td>
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<td>(^8\text{Be})</td>
<td>56.50</td>
<td>7.06</td>
<td>-0.09</td>
<td>(^9\text{Be})</td>
<td>58.17</td>
<td>6.46</td>
<td>(^9\text{B})</td>
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<td>6.48</td>
<td>—</td>
<td>(^{11}\text{B})</td>
<td>76.21</td>
<td>6.93</td>
<td>(^{11}\text{C})</td>
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<td>(^{13}\text{C})</td>
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<td>7.47</td>
<td>(^{13}\text{N})</td>
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<td>7.48</td>
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<td>(^{16}\text{O})</td>
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<td>(^{17}\text{F})</td>
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<td>7.54</td>
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<td>137.37</td>
<td>7.63</td>
<td>—</td>
<td>(^{19}\text{F})</td>
<td>147.80</td>
<td>7.78</td>
<td>(^{19}\text{Ne})</td>
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<td>160.65</td>
<td>8.03</td>
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<td>198.26</td>
<td>8.26</td>
<td>28.48</td>
<td>(^{25}\text{Mg})</td>
<td>205.59</td>
<td>8.22</td>
<td>(^{25}\text{Al})</td>
<td>200.53</td>
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</tr>
</tbody>
</table>
The most tightly bound nucleus

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In many textbooks,\textsuperscript{1-3} we are told that $^{56}\text{Fe}$ is the nuclide with the greatest binding energy per nucleon, and therefore is the most stable nucleus, the heaviest that can be formed by fusion in normal stars.

But we calculate the binding energy per nucleon $BE/A$, for a nucleus of mass number $A$, by the usual formula,

\begin{equation}
BE/A = (1/A)(Zm_H + Nm_n - M_{\text{atom}})c^2,
\end{equation}

where $m_H$ is the hydrogen atomic mass and $m_n$ is the neutron mass, for the nuclides $^{56}\text{Fe}$ and $^{62}\text{Ni}$ (both are stable) using data from Wapstra and Audi.\textsuperscript{4} The results are 8.790 MeV/nucleon for $^{56}\text{Fe}$ and 8.795 MeV/nucleon for $^{62}\text{Ni}$. The difference,

\begin{equation}
(0.005 \text{ MeV/nucleon}) \approx 60 \text{ nucleons) = 300 keV},
\end{equation}

is much too large to be accounted for as the binding energy of the two extra electrons in $^{62}\text{Ni}$ over the 26 electrons in $^{56}\text{Fe}$.

To accomplish this with a single fusion requires a nuclide with $Z = 2, A = 6$. But no such stable nuclide exists. The other possibility is two sequential fusions with $^3\text{H}$, producing first $^{59}\text{Co}$ then $^{62}\text{Ni}$. However, the $^3\text{H}$ nucleus is unstable and is not expected to be present in old stars synthesizing heavy elements. We are aware that there are element-generating processes other than charged-particle fusion, such as processes involving neutron capture, which could generate nickel. However, these processes apparently do not occur in normal stars, but rather in supernovas and post-supernova phases, which we do not address.

We conclude that $^{56}\text{Fe}$ is the end product of normal stellar fusion not because it is the most tightly bound nucleus, which it is not, but that it is in close, but unbridgeable, proximity to $^{62}\text{Ni}$, which is the most tightly bound nucleus.

\begin{itemize}
  \item \textsuperscript{4}\textit{A. H. Wapstra and G. Audi, Nucl. Phys. A 432, 1 (1985).}
\end{itemize}
For most nuclei, the binding energy per nucleon is about 8MeV. Binding is less for light nuclei (these are mostly surface) but there are peaks for $A$ in multiples of 4. (But note that the peak for $^{8}\text{Be}$ is slightly lower than that for $^{4}\text{He}$.

- The most stable nuclei are in the $A\sim 60$ mass region
- Light nuclei can gain binding energy per nucleon by fusing; heavy nuclei by fissioning.
- The decrease in binding energy per nucleon for $A>60$ can be ascribed to the repulsion between the (charged) protons in the nucleus: the Coulomb energy grows in proportion to the number of possible pairs of protons in the nucleus $Z(Z-1)/2$
- The binding energy for massive nuclei ($A>60$) thus grows roughly as $A$; if the nuclear force were long range, one would expect a variation in proportion to the number of possible pairs of nucleons, i.e. as $A(A-1)/2$. The variation as $A$ suggests that the force is saturated; the effect of the interaction is only felt in a neighborhood of the nucleon.
Nuclear liquid drop

The semi-empirical mass formula, based on the liquid drop model, considers five contributions to the binding energy (Bethe-Weizacker 1935/36)

\[ B = a_{vol} A - a_{surf} A^{2/3} - a_{sym} \frac{(N - Z)^2}{A} - a_{c} \frac{Z^2}{A^{1/3}} - \delta(A) \]

15.68  -18.56  -28.1  -0.717

pairing term

\[ \delta(A) = \begin{cases} 
-34A^{-3/4} & \text{for even - even} \\
0 & \text{for even - odd} \\
34A^{-3/4} & \text{for odd - odd} 
\end{cases} \]

Leptodermous expansion
The semi-empirical mass formula, based on the liquid drop model, compared to the data.
Pairing energy

\[ \Delta_n = B(N,Z) - \frac{B(N+1,Z) + B(N-1,Z)}{2} \]
\[ \Delta_p = B(N,Z) - \frac{B(N,Z+1) + B(N,Z-1)}{2} \]

A common phenomenon in mesoscopic systems!
Neutron star, a bold explanation

Let us consider a giant neutron-rich nucleus. We neglect Coulomb, surface, and pairing energies. Can such an object exist?

\[
B = a_{vol} A - a_{surf} A^{2/3} - a_{sym} \frac{(N - Z)^2}{A} - a_{c} \frac{Z^2}{A^{1/3}} - \delta(A) + \frac{3}{5} \frac{G}{r_0 A^{1/3}} M^2
\]

More precise calculations give \( M(\text{min}) \) of about 0.1 solar mass (\( M_\odot \)). Must neutron stars have

\[
R \approx 10 \text{ km}, \quad M \approx 1.4 M_\odot
\]
• All elements heavier than $A=110-120$ are fission unstable!
• But… the fission process is fairly unimportant for nuclei with $A<230$. Why?
The classical droplet stays stable and spherical for $x<1$. For $x>1$, it fissions immediately. For $^{238}\text{U}$, $x=0.8$. 

The fissibility parameter is defined as:

$$E_{LDM}^{\text{def}} = E_S(0) \left[ B_S^{\text{def}} - 1 + 2x \left( B_C^{\text{def}} - 1 \right) \right]$$

$$B_S^{\text{def}} = \frac{E_S^{\text{def}}}{E_S(0)}, \quad B_C^{\text{def}} = \frac{E_C^{\text{def}}}{E_C(0)}$$

$$x = \frac{E_C(0)}{2E_S(0)} = \frac{Z^2 / A}{\left( Z^2 / A \right)_{\text{crit}}} \approx \frac{Z^2}{50A}$$
Realistic calculations

1938 - Hahn & Strassmann
1939 Meitner & Frisch
1939 Bohr & Wheeler
1940 Petrzhak & Flerov
Nuclear shapes

The first evidence for a non-spherical nuclear shape came from the observation of a quadrupole component in the hyperfine structure of optical spectra. The analysis showed that the electric quadrupole moments of the nuclei concerned were more than an order of magnitude greater than the maximum value that could be attributed to a single proton and suggested a deformation of the nucleus as a whole.

• Schüler, H., and Schmidt, Th., Z. Physik 94, 457 (1935)

The question of whether nuclei can rotate became an issue already in the very early days of nuclear spectroscopy

• Thibaud, J., Comptes rendus 191, 656 (1930)
• Bohr, N., Nature 137, 344 (1936)
Figure I.1: Matter density contours for the deuteron (left) and the $^{154}$Gd nucleus (right) deduced from experiment.

Shape of a charge distribution in $^{154}$Gd
LINES CONNECT ISOTOPES

Neutron Number $N$

Energy of $\gamma^2$ (MeV)

(a)

LINES CONNECT ISOTOPES

(b)

$\beta(E2) (e^2 \text{b}^2)$

$\sim 400$ s.p.u.

$\sim 1$ s.p.u.
Coexistence of collective and noncollective motion

152Dy

Triaxial band
Noncollective states
Superdeformed bands

E
t
Q

Fission/fusion exotic decay heavy ion coll.

E

Shape coexistence

Q_0  Q
Q_1  Q_2  Q
Nucleonic Shells
Nobel Prize 1922
Bohr’s picture still serves as an elucidation of the physical and chemical properties of the elements.

Nobel Prize 1963
We know now that this picture is very incomplete…
Harmonic oscillator + flat bottom + spin-orbit oscillator
Average one-body Hamiltonian

$$\hat{H}_0 = \sum_{i=1}^{A} h_i, \quad h_i = -\frac{\hbar^2}{2M} \nabla_i^2 + V_i$$

$$h_i \phi_k(i) = \varepsilon_k \phi_k(i)$$

$$\phi = \frac{1}{\sqrt{A!}} \begin{bmatrix} \phi_i(r_1) & \phi_i(r_2) & \ldots & \phi_i(r_A) \\ \phi_j(r_1) & \phi_j(r_2) & \ldots & \phi_j(r_A) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_l(r_1) & \phi_l(r_2) & \ldots & \phi_l(r_A) \end{bmatrix}$$

$$= a_i^+ \ldots a_j^+ a_i^+ |0\rangle$$
Product (independent-particle) state is often an excellent starting point

Localized densities, currents, fields

Typical time scale: babyseconds ($10^{-22}$s)

Closed orbits and s.p. quantum numbers

But...

Nuclear box is not rigid: motion is seldom adiabatic

The walls can be transparent

In weakly-bound nuclei, residual interaction may dominate the picture: shell-model basis does not govern the physics!

Shell-model basis not unique (many equivalent Hartree-Fock fields)
Shell effects and classical periodic orbits

Balian & Bloch, Ann. Phys. 69 (1971) 76
Bohr & Mottelson, Nuclear Structure vol 2 (1975)
Strutinski & Magner, Sov. J. Part. Nucl. 7 (1976) 138


\[ g(\varepsilon) = \tilde{g}(\varepsilon) + \sum_{\gamma} A_{\gamma}(\varepsilon) \cos \left[ \frac{S_{\gamma}(\varepsilon)}{\varepsilon - \alpha_{\gamma}} \right] \]

\[ S_{\gamma}(\varepsilon) = \int_{\gamma} p\, dq \]

The action integral for the periodic orbit \( \gamma \)

\[ \varepsilon(n_1, n_2, n_3) = \varepsilon(n_{10}, n_{20}, n_{30}) + (n_1 - n_{10}) \left( \frac{\partial \varepsilon}{\partial n_1} \right)_0 + \]
\[ + (n_2 - n_{20}) \left( \frac{\partial \varepsilon}{\partial n_2} \right)_0 + (n_3 - n_{30}) \left( \frac{\partial \varepsilon}{\partial n_3} \right)_0 + \ldots \]

\[ \frac{\partial \varepsilon}{\partial n_1}_0 : \frac{\partial \varepsilon}{\partial n_2}_0 : \frac{\partial \varepsilon}{\partial n_3}_0 = k_1 : k_2 : k_3 \]

\[ N_{\text{shell}} = k_1 n_1 + k_2 n_2 + k_3 n_3, \quad \varepsilon_0_{\text{shell}} = \frac{1}{k_1} \left( \frac{\partial \varepsilon}{\partial n_1} \right)_0 \]

Principal shell quantum number

Distance between shells (frequency of classical orbit)
Pronounced shell structure (quantum numbers)

Shell structure absent

shell ———

gap

shell ———

gap

shell ———

closed trajectory (regular motion)

trajectory does not close
Sodium Clusters

- Jahn-Teller Effect (1936)
- Symmetry breaking and deformed (HF) mean-field
Revising textbooks on nuclear shell model…

2\(^+\) levels in neutron-rich nuclei

- N=20
- N=28
- New gaps N=32,34?

Energy (MeV) vs Neutron number

Forces
- Many-body dynamics
- Open channels

from A. Gade
Living on the edge… Correlations and openness

Light drip line nuclei

Forces

Many-body dynamics

Open channels
Neutron Drip line nuclei

HUGE
Diffused
PAIRED

4He  5He  6He  7He  8He  9He  10He
The Force
Nuclear force

A realistic nuclear force force: schematic view

- Nucleon r.m.s. radius \( \sim 0.86 \text{ fm} \)
- Comparable with interaction range
- Half-density overlap at max. attarction
- \( V_{\text{NN}} \) not fundamental (more like inter-molecular van der Waals interaction)
- Since nucleons are composite objects, three-and higher-body forces are expected.
There are infinitely many equivalent nuclear potentials!

\[ \hat{H} \Psi = E \Psi \]
\[ (\hat{U} \hat{H} \hat{U}^{-1}) \hat{U} \Psi = E \hat{U} \Psi \]

Reid93 is from V.G.J. Stoks et al., PRC 49, 2950 (1994).
nucleon-nucleon interactions

Effective-field theory potentials

Renormalization group (RG) evolved nuclear potentials

$V_{\text{low-k}}$ unifies NN interactions at low energy

$\text{N}^3\text{LO: Entem et al., PRC68, 041001 (2003)}$

Epelbaum, Meissner, et al.

The computational cost of nuclear 3-body forces can be greatly reduced by decoupling low-energy parts from high-energy parts, which can then be discarded.

Three-body forces between protons and neutrons are analogous to tidal forces: the gravitational force on the Earth is not just the sum of Earth-Moon and Earth-Sun forces (if one employs point masses for Earth, Moon, Sun)

Recently the first consistent Similarity Renormalization Group softening of three-body forces was achieved, with rapid convergence in helium. With this faster convergence, calculations of larger nuclei are possible!
The challenge and the prospect: NN force

Ishii et al. PRL 99, 022001 (2007)

Optimizing the nuclear force
input matters: garbage in, garbage out

- The derivative-free minimizer POUNDERS was used to systematically optimize NNLO chiral potentials
- The optimization of the new interaction NNLO \(^{2\text{nd}}/\text{datum} \approx 1\) for laboratory NN scattering energies below 125 MeV. The new interaction yields very good agreement with binding energies and radii for A=3,4 nuclei and oxygen isotopes
- Ongoing: Optimization of NN + 3NF


<table>
<thead>
<tr>
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<th>Emp./Rec. [36–41]</th>
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<td>(\eta)</td>
<td>0.02473(4)</td>
<td>0.0256(5)</td>
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<td>0.8854(2)</td>
<td>0.8845(8)</td>
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<td>(\langle r^{-1}\rangle) (fm(^{-1}))</td>
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Deuteron, Light Nuclei
Deuteron

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<tr>
<th>Property</th>
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<td>Binding energy</td>
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<td>Isospin</td>
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<td>Magnetic moment</td>
<td>$\mu = 0.857 \mu_N$</td>
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<tr>
<td>Electric quadrupole moment</td>
<td>$Q = 0.282 \text{ e fm}^2$</td>
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\[ \mu_p + \mu_n = 2.792\mu_N - 1.913\mu_N = 0.879\mu_N \]

\[ |\psi_d\rangle = 0.98|^{3}S_1\rangle + 0.20|^{3}D_1\rangle \]

produced by tensor force!
GFMC calculations tell us that:

\[ \langle V_\pi \rangle / \langle V \rangle \sim 70 \text{ -- } 80\% \]
\[ \langle V_\pi \rangle \sim -15 \text{ MeV/pair} \]
\[ \langle V^R \rangle \sim -5 \text{ MeV/pair} \]
\[ \langle V^3 \rangle \sim -1 \text{ MeV/three} \]
\[ \langle T \rangle \sim 15 \text{ MeV/nucleon} \]
\[ \langle V_C \rangle \sim 0.66 \text{ MeV/pair of protons} \]
Few-nucleon systems
(theoretical struggle)

A=2: many years ago...

3H: 1984 (1% accuracy)
  • Faddeev
  • Schroedinger

3He: 1987

4He: 1987

5He: 1994 (n-α resonance)

A=6,7,..12: 1995-2014