Shell and pairing gaps: theory

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Nuclear Structure and Astrophysical Applications
ECT* Trento, July 8-12 2013
Mass filters

They are used

1. to identify and quantify shell closures \((S_{2n}, S_{2p}, \delta_{2n}, \delta_{2p}, \text{also } Q_\alpha)\)
2. to quantify pairing correlations \((\Delta^{(3)}, \Delta^{(4)}, \Delta^{(5)})\)
3. to quantify specific interactions ("matrix elements") \((\delta V_{pn}, \ldots)\)

- Masses are undoutably observables.
- The interpretation of the mass filters relies on simple models
- Atomic nuclei are complex systems.
- Simple models which might work for isolated systems, but will fail when describing the systematics over many 'randomly chosen) nuclei
Fig. 1. Energies of first excited intrinsic states in deformed nuclei, as a function of the mass number. The experimental data may be found in Nuclear Data Cards [National Research Council, Washington, D. C.] and detailed references will be contained in reference 1 above. The solid line gives the energy $\delta/2$ given by Eq. (1), and represents the average distance between intrinsic levels in the odd-$A$ nuclei (see reference 1).

The figure contains all the available data for nuclei with $150 < A < 190$ and $228 < A$. In these regions the nuclei are known to possess nonspherical equilibrium shapes, as evidenced especially by the occurrence of rotational spectra (see, e.g., reference 2). One other such region has also been identified around $A = 25$; in this latter region the available data on odd-$A$ nuclei is still represented by Eq. (1), while the intrinsic excitations in the even-even nuclei in this region do not occur below 4 Mev.

We have not included in the figure the low lying $K=0$ states found in even-even nuclei around $^{238}$Ra and $^{232}$Th. These states appear to represent a collective odd-parity oscillation.
The excited states with seniority 2 have an excitation energy of two times the pairing gap
\[ 2\Delta = G\Omega \]

Pairing interaction
\[ \hat{H} = -G \hat{A}^\dagger \hat{A} \]

with
\[ \hat{A}^\dagger \equiv \sum_{\alpha=1}^{\Omega} \hat{a}^+_\alpha \hat{a}^-_\alpha \]

in a single shell of degeneracy \( 2\Omega \).

For even nuclei that can be described within the model space
\[ \Delta^{(3)} = \frac{G\Omega}{2} = \Delta \]
"mass surfaces" of even-even and odd nuclei

\[ E_{\text{even-even}}(Z, N) = E_0(Z, N), \]
\[ E_{\text{odd } Z}(Z, N) = E_0(Z, N) + \Delta_p(Z, N), \]
\[ E_{\text{odd } N}(Z, N) = E_0(Z, N) + \Delta_n(Z, N). \]

where \( \Delta_q(Z, N) \) is the energy lost when "blocking" a particle.

The energy of any nucleus \( E(N) \) can be obtained by an expansion of the energy around a reference nucleus \( E(N_0) \)

\[ E(N) = \sum_{n=0}^{\infty} \frac{1}{n!} \left. \frac{\partial^n E_0}{\partial N^n} \right|_{N_0} (N - N_0)^n + D(N_0) \]

where the gap \( D \) is given by

\[ D = \begin{cases} 
0 & \text{even proton and neutron number,} \\
\Delta_n & \text{odd neutron number,} \\
\Delta_p & \text{odd proton number.} 
\end{cases} \]


1-nucleon separation energy $S_{1n}$

$$S_{1n}(N_0) = E(N_0) - E(N_0 - 1)$$

$$= \left. \frac{\partial E_0}{\partial N} \right|_{N_0} - \frac{1}{2} \left. \frac{\partial^2 E_0}{\partial N^2} \right|_{N_0} + \frac{1}{6} \left. \frac{\partial^3 E_0}{\partial N^3} \right|_{N_0} - \frac{1}{24} \left. \frac{\partial^4 E_0}{\partial N^4} \right|_{N_0} + \ldots$$

$$+ D(N_0) - D(N_0 - 1)$$

mixes everything: variation of the smooth background and pairing gap.

⇒ better use something else
3-point pairing gap $\Delta^{(3)}$

3-point gap mass difference

\[
E(N_0 + 1) - 2E(N_0) + E(N_0 - 1) = \frac{\partial^2 E_0}{\partial N^2} \Bigg|_{N_0} + \frac{1}{12} \frac{\partial^4 E_0}{\partial N^4} \Bigg|_{N_0} + \cdots + D(N_0 + 1) - 2D(N_0) + D(N_0 - 1),
\]

provides the distance of the mass surfaces if

- $E$ is a smooth function (which is not the case when not having pairing)
- $D$ does not vary when going from $N_0 - 1$ to $N_0 + 1$
- $\frac{\partial^2 E_0}{\partial N^2} \Bigg|_{N_0}$ (and higher-order derivatives) is (are) negligible

\[
\Delta^{(3)}(N_0) \equiv \frac{\pi_{N_0}}{2} \left[ E(N_0 - 1) - 2E(N_0) + E(N_0 + 1) \right]
\]

where $\pi_{N_0} = (-1)^{N_0}$ is the number parity.

(note that in the liquid drop model, $\frac{\partial^2 E_0}{\partial N^2}$ is non-zero due to the symmetry and Coulomb ($\sim Z^2$) energies)

The 4-point gap mass difference

\[
E(N_0 - 2) - 3E(N_0 - 1) + 3E(N_0) - E(N_0 + 1) = \left. \frac{\partial^3 E_0}{\partial N^3} \right|_{N_0} + \cdots + D(N_0 - 2) - 3D(N_0 - 1) + 3D(N_0) - D(N_0 + 1).
\]

can be used to define

\[
\Delta^{(4)}(N_0 = 1/2) := \frac{\pi N_0}{4} \left[ E(N_0 - 2) - 3E(N_0 - 1) + 3E(N_0) - E(N_0 + 1) \right].
\]

The 5-point gap mass difference

\[
E(N_0 + 2) - 4E(N_0 + 1) + 6E(N_0) - 4E(N_0 - 1) + E(N_0 - 2)
\]

\[
= \left. \frac{\partial^4 E_0}{\partial N^4} \right|_{N_0} + \cdots
\]

\[
= +D(N_0 - 2) - 4D(N_0 - 1) + 6D(N_0) - 4D(N_0 + 1) - D(N_0 + 2)
\]

can be used to define

\[
\Delta^{(5)}(N_0) := -\frac{\pi N_0}{8} \left[ E(N_0 + 2) - 4E(N_0 + 1) + 6E(N_0) 
-4E(N_0 - 1) + E(N_0 - 2) \right].
\]

Odd-Even Staggering of Nuclear Masses: Pairing or Shape Effect?

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(Received 20 April 1998)

The odd-even staggering of nuclear masses was recognized in the early days of nuclear physics. Recently, a similar effect was discovered in other finite fermion systems, such as ultrasmall metallic grains and metal clusters. It is believed that the staggering in nuclei and grains is primarily due to pairing correlations (superconductivity), while in clusters it is caused by the Jahn-Teller effect. We find that, for light- and medium-mass nuclei, the staggering has two components. The first originates from pairing while the second, comparable in magnitude, has its roots in the deformed mean field.

- "Values of $\Delta^{(3)}(N)$ calculated at odd $N$ can be, roughly, associated with the pairing gap."
- "the differences of $\Delta^{(3)}$ at adjacent even and odd values of $N$ give information about the single-particle spectra"

$$e_{n+1} - e_n = 2[\Delta^{(3)}(N = 2n) \quad - \Delta^{(3)}(N = 2n + 1)]$$

FIG. 2. Schematic illustration of various contributions to the OES. The odd-even energy difference, $\Delta_{0-e}$, is decomposed into the pairing part, $\Delta$, and the mean-field part, $\delta e/2$. 
Mean-field models. Analysis II

FIG. 9. $\Delta^{(3)}_{\text{BCS}}, \Delta^{(5)}_{\text{BCS}},$ and $\Delta$ as a function of $A$. From top to bottom, the pairing gap increases from 0 to 1200 keV. Left column: calculation with an equidistant doubly degenerate spectrum. Right column: calculation using the self-consistent neutron HF spectrum of $^{152}$Ce. In addition to $\Delta$, the lowest qp in odd nuclei is shown. Results are displayed between $^{148}$Ce and $^{156}$Ce.

"Equi Spect" denotes a schematic model:

- equidistant two-fold degenerate single-particle levels with level spacing $\delta \epsilon = 400$ keV
- constant gap pairing varied between $\Delta = 0$ and 1200 keV
BCSE: calculating odd nuclei as if they were even ones without blocking

FIG. 10. Energy differences $\Delta_{\text{BCSE}}^{(3)}$, $\Delta_{\text{BCSE}}^{(5)}$, and $\Delta_{\text{BCS}}^{(3)} - \Delta_{\text{BCS}}^{(5)}$. Left and right panels: same as for Fig. 9. The results are displayed between $^{148}\text{Ce}$ and $^{156}\text{Ce}$.

FIG. 11. Binding energy as a function of $N$ for the even part (squares joined by dashed line) and for the full odd states (circle). Left panel: no pairing. Right panel: realistic-pairing case.

some conclusions relevant for the present discussion:

- $\Delta^{(3)}(N = 2n - 1)$ gives the pairing gap (+polarization effects) only in the no-pairing limit

- for realistic pairing, $\Delta^{(5)}$ gives the pairing gap (+polarization effects), while values for $\Delta^{(3)}$ alternate around it as the 2nd derivative of the smooth background energy is not zero
FIGURE 1. Experimental three-point mass differences (crosses) for neutrons along the tin isotopic chain versus several theoretical measures of the OEMS: $\Delta_{LCS}^n$(even) (dashed-line), $\Delta_{LCS}^n$(odd) (dashed-dotted line) and $\Delta_{th}^{(3)}(N)$ (full line). Theoretical three-point mass differences are also shown for odd-even nuclei computed using an even-number-parity vacuum as a reference state, i.e. a HFB state without any quasi-particle blocking as if odd-even nuclei had the same structure as even-even ones (dotted line) [33, 34].
Mean-field models. Analysis III

Shell and pairing gaps: theory

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Shell and pairing gaps: theory

\( \Delta^{(5)} \) provides better measure for the distance between mass surfaces of even and odd nuclei than \( \Delta^{(3)} \) as all contributions from the smooth surface are suppressed up to terms that go as the power \( N^4 \) or \( Z^4 \) . . .

\[ \Delta^{(5)} \]

. . . provided there is no discontinuity in the mass surface as it happens at shell closures

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**Fig. 3.** Five-point gaps \( \Delta^{(5)} \) computed using either blocked calculations of the odd-mass nuclei (dashed lines) or their BCS ground states (dotted lines) for the chain of tin isotopes with BCS+DF pairing. Non-zero \( \Delta^{(5)} \) from not blocked calculations appear only at closed shells and are caused by a spurious contribution of the mean field to \( \Delta^{(5)} \). The difference of both curves (solid line) gives the contribution from the blocking to \( \Delta^{(5)} \).

How is the evolution of shell structure related to systematics of masses?

1-nucleon separation energy $S_{1n}$

\[ S_{1n}(N_0) = E(N_0) - E(N_0 - 1) \]

\[ = \left. \frac{\partial E_0}{\partial N} \right|_{N_0} - \frac{1}{2} \left. \frac{\partial^2 E_0}{\partial N^2} \right|_{N_0} + \frac{1}{6} \left. \frac{\partial^3 E_0}{\partial N^3} \right|_{N_0} - \frac{1}{24} \left. \frac{\partial^4 E_0}{\partial N^4} \right|_{N_0} + \ldots \]

\[ + D(N_0) - D(N_0 - 1) \]

mixes everything: variation of the smooth background and pairing gap.

⇒ better use something else
2-nucleon separation energies and "shell gaps"

Two-nucleon separation energy

\[ S_{2n}(N_0) = E(N_0) - E(N_0 - 2) \]

\[ = 2 \frac{\partial E_0}{\partial N} \bigg|_{N_0} - 2 \frac{\partial^2 E_0}{\partial N^2} \bigg|_{N_0} + \frac{4}{3} \frac{\partial^3 E_0}{\partial N^3} \bigg|_{N_0} - \frac{2}{3} \frac{\partial^4 E_0}{\partial N^4} \bigg|_{N_0} \]

"Shell gap"

\[ \delta_{2n}(N_0) = S_{2n}(N_0) - S_{2n}(N_0 + 2) \]

\[ = E(N_0 - 2) - 2E(N_0) + E(N_0 + 2) \]

\[ = 4 \frac{\partial^2 E_0}{\partial N^2} \bigg|_{N_0} + \frac{4}{3} \frac{\partial^4 E_0}{\partial N^4} \bigg|_{N_0} + \ldots \]
How is the evolution of shell structure related to systematics of masses?

Evolution of the $N = 50$ Shell Gap Energy towards $^{78}\text{Ni}$


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(Received 20 March 2008; published 31 July 2008)

$$
\delta_{2n}(N, Z) = S_{2n}(Z, N) - S_{2n}(Z, N + 2) = E(N - 2, Z) - 2E(N, Z) + E(N + 2, Z)
$$
Eigenvalues of the single-particle Hamiltonian vs. $S_{2q}$

lower panel: $-S_{2p}(Z=50, N)/2$

The global linear trend is taken out subtracting

$$\frac{N-82}{2} [S_{2p}(Z=50, N=50) - S_{2p}(Z=50, N=82)]$$

using the spherical mean-field $S_{2p}$


lower panel: $-S_{2n}(Z, N=50)/2$

The global linear trend is taken out subtracting

$$\frac{N-50}{2} [S_{2n}(Z=28, N=50) - S_{2n}(Z=50, N=50)]$$

using the spherical mean-field $S_{2n}$
Eigenvalues of the single-particle Hamiltonian vs. $S_{2q}$

lower panel: $-S_{2p}(Z=50, N)/2$
The global linear trend is taken out subtracting

$$\frac{N-82}{2} [S_{2p}(Z=50, N=50) - S_{2p}(Z=50, N=82)]$$

using the spherical mean-field $S_{2p}$


lower panel: $-S_{2n}(Z, N=50)/2$
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using the spherical mean-field $S_{2n}$
Eigenvalues of the single-particle Hamiltonian vs. $S_{2q}$

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$$\frac{N-82}{2} [S_{2p}(Z=50, N=50) - S_{2p}(Z=50, N=82)]$$

using the spherical mean-field $S_{2p}$


lower panel: $-S_{2n}(Z, N=50)/2$

The global linear trend is taken out subtracting

$$\frac{N-50}{2} [S_{2n}(Z=28, N=50) - S_{2n}(Z=50, N=50)]$$

using the spherical mean-field $S_{2n}$
Two-nucleon gaps

\[ \delta_2 p(N, Z) = S_{2p}(Z, N) - S_{2p}(Z - 2, N) \]

\[ \delta_2 n(N, Z) = S_{2n}(Z, N) - S_{2n}(Z, N - 2) \]

- In spite of their name, the two-nucleon shell gaps do not measure the gap in the single-particle spectrum in self-consistent mean-field model.

experimental values shown here include more recent data than the plots in the papers.
Collectivity-enhanced quenching of signatures of shell closures


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Collectivity-enhanced quenching of signatures of shell closures

Collectivity-enhanced quenching of signatures of shell closures

same effect seen in 5-dimensional collective Hamiltonian from Gogny D1s

It is customary to discuss shell structure in terms of the spectrum of eigenvalues of the single-particle Hamiltonian $\epsilon_\mu$ in even-even nuclei

$$\hat{h} \psi_\mu = \epsilon_\mu \psi_\mu$$

Koopman's theorem states that $\epsilon_\mu$ is equal to the one-nucleon separation energy if
- The nucleus is perfectly described by a HF state (i.e. that there are no correlations of any kind whatsoever)
- rearrangement and polarization effects changing the single-particle wave functions when adding or removing a particle are negligible

The structure of the mean-field state of an even- even and an odd-$A$ nucleus is different (blocking, additional mean fields that originate from interactions involving currents and spin densities in the odd-$A$ nucleus, ...), there always are correlations and they will give a different contribution to the binding in even-even and odd-$A$ nuclei, etc.

Mutually enhanced magicity

MUTUAL SUPPORT OF MAGICITIES
AND RESIDUAL EFFECTIVE INTERACTIONS NEAR $^{208}$Pb

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Received 1 November 1982

Abstract: We summarize experimental evidence in the lead region on the increased stability associated with neutron magic number when the proton number is magic, and vice versa. The effect is interpreted in the framework of the nuclear shell model with empirical effective interactions. Its relation to spherical Hartree-Fock calculations is pointed out and used to test Skyrme-type forces. None of the considered Skyrme interactions reproduce the effect.


Fig. 1. (a) Excitation energies of single-neutron $\frac{3}{2}^+$ levels in $N = 125$ nuclei and of single neutron-hole $\frac{1}{2}^-$ levels in $N = 127$ nuclei. Data from Table of Isotopes (4) and more recent literature ($^{211}$Po, ref. 5). (b) $S_n$ systematics of odd-$N$ nuclei near $^{208}$Pb. Data from The 1977 Atomic Mass Evaluation (4) and more recent literature ($^{207}$Hg, ref. 7).
$Q_\alpha$ values of even-even nuclei

$Q_\alpha$ values calculated from

- spherical liquid drop with parameters derived from SLy4 (a)
- spherical self-consistent mean field with SLy4 (b)
- deformed self-consistent mean field with SLy4 (c)
- $J = 0$, $N$ and $Z$ projected GCM of axial states with SLy4 (d)
- isotopic chains $Z = 90, 100, 110, 120$ shown in red
What is represented by $\delta V_{pn}$?

$\delta V_{pn}(N, Z) = -\frac{1}{4} [E(Z, N) - E(Z, N - 2) - E(Z - 2, N) + E(Z - 2, N - 2)]$

M. B., P.-H. Heenen, PRC 83 (2011) 064319
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M. B., P.-H. Heenen, PRC 83 (2011) 064319
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- $N - Z = 32$ chain across the rare-earth region
- deformation well reproduced
- contribution from deformation is the key ingredient to describe fine structure of $\delta V_{pn}$
- contribution from fluctuations in deformation is important in transitional regions

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M. B., P.-H. Heenen, PRC 83 (2011) 064319
What is represented by $\delta V_{pn}$?
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What is represented by $\delta V_{pn}$?

$$\delta V_{pn} = \frac{1}{4} \left( \frac{1}{4} \right)$$
What is represented by $\delta V_{pn}$?

$\delta V_{pn} = \frac{1}{4} (\text{red} + \text{green} - \text{blue})$

Comparison of
- frozen HF: calculation without pairing using the same single-particle states of the HF solution of $^{208}\text{Pb}$ for all 4 nuclei
- HF: calculation without pairing using self-consistent states
- HF+BCS+LN: calculation with pairing using self-consistent states
- J=0 GCM: calculation with pairing using the mixing of symmetry-restored self-consistent states with different quadrupole deformation
The interpretation of observables in terms of simple models leads to a model-dependent interpretation of observables. This is a constant source of confusion and misunderstanding when comparing different models.

- the simplicity of the model assumptions made when interpreting mass filters as gaps of some kind clashes with the realities of complex systems

- It is recommended to compare only calculated mass filters with experimental mass filters, not some model-dependent ingredient of the model used (spectral gaps, . . .)