



The Abdus Salam
International Centre for Theoretical Physics



1939-19

**Joint ICTP-IAEA Workshop on Nuclear Structure and Decay Data:
Theory and Evaluation**

28 April - 9 May, 2008

**Theory Nuclear Structure
(I) Single-particle models**

P. VAN ISACKER
*GANIL, Group Physique
F-14076 Caen
France*

Nuclear Structure

(I) Single-particle models

P. Van Isacker, GANIL, France

Overview of nuclear models

- *Ab initio* methods: Description of nuclei starting from the bare nn & nnn interactions.
- Nuclear shell model: Nuclear average potential + (residual) interaction between nucleons.
- Mean-field methods: Nuclear average potential with global parametrisation (+ correlations).
- Phenomenological models: Specific nuclei or properties with local parametrisation.

Nuclear shell model

- Many-body quantum mechanical problem:

$$\begin{aligned}\hat{H} &= \sum_{k=1}^A \frac{p_k^2}{2m_k} + \sum_{k<l}^A \hat{V}_2(\mathbf{r}_k, \mathbf{r}_l) \\ &= \underbrace{\sum_{k=1}^A \left[\frac{p_k^2}{2m_k} + \hat{V}(\mathbf{r}_k) \right]}_{\text{mean field}} + \underbrace{\left[\sum_{k<l}^A \hat{V}_2(\mathbf{r}_k, \mathbf{r}_l) - \sum_{k=1}^A V(\mathbf{r}_k) \right]}_{\text{residual interaction}}\end{aligned}$$

- Independent-particle assumption. Choose V and neglect residual interaction:

$$\hat{H} \approx \hat{H}_{\text{IP}} = \sum_{k=1}^A \left[\frac{p_k^2}{2m_k} + \hat{V}(\mathbf{r}_k) \right]$$

Independent-particle shell model

- Solution for one particle:

$$\left[\frac{p^2}{2m} + \hat{V}(\mathbf{r}) \right] \phi_i(\mathbf{r}) = E_i \phi_i(\mathbf{r})$$

- Solution for many particles:

$$\Phi_{i_1 i_2 \dots i_A} (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A) = \prod_{k=1}^A \phi_{i_k}(\mathbf{r}_k)$$

$$\hat{H}_{\text{IP}} \Phi_{i_1 i_2 \dots i_A} (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A) = \left(\sum_{k=1}^A E_{i_k} \right) \Phi_{i_1 i_2 \dots i_A} (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A)$$

Independent-particle shell model

- Anti-symmetric solution for many particles (Slater determinant):

$$\Psi_{i_1 i_2 \dots i_A}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_{i_1}(\mathbf{r}_1) & \phi_{i_1}(\mathbf{r}_2) & \dots & \phi_{i_1}(\mathbf{r}_A) \\ \phi_{i_2}(\mathbf{r}_1) & \phi_{i_2}(\mathbf{r}_2) & \dots & \phi_{i_2}(\mathbf{r}_A) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{i_A}(\mathbf{r}_1) & \phi_{i_A}(\mathbf{r}_2) & \dots & \phi_{i_A}(\mathbf{r}_A) \end{vmatrix}$$

- Example for $A=2$ particles:

$$\Psi_{i_1 i_2}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} [\phi_{i_1}(\mathbf{r}_1)\phi_{i_2}(\mathbf{r}_2) - \phi_{i_1}(\mathbf{r}_2)\phi_{i_2}(\mathbf{r}_1)]$$

Hartree-Fock approximation

- Vary ϕ_i (ie V) to minimize the expectation value of H in a Slater determinant:

$$\delta \frac{\int \Psi_{i_1 i_2 \dots i_A}^*(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A) \hat{H} \Psi_{i_1 i_2 \dots i_A}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A) d\mathbf{r}_1 d\mathbf{r}_2 \dots d\mathbf{r}_A}{\int \Psi_{i_1 i_2 \dots i_A}^*(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A) \Psi_{i_1 i_2 \dots i_A}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A) d\mathbf{r}_1 d\mathbf{r}_2 \dots d\mathbf{r}_A} = 0$$

- Application requires choice of H . Many global parametrizations (Skyrme, Gogny,...) have been developed.

Poor man's Hartree-Fock

- Choose a simple, analytically solvable V that approximates the microscopic HF potential:

$$\hat{H}_{\text{IP}} = \sum_{k=1}^A \left[\frac{p_k^2}{2m} + \frac{m\omega^2}{2} r_k^2 - \zeta \mathbf{l}_k \cdot \mathbf{s}_k - \kappa l_k^2 \right]$$

- Contains
 - Harmonic oscillator potential with constant ω .
 - Spin-orbit term with strength ζ .
 - Orbit-orbit term with strength κ .
- Adjust ω , ζ and κ to best reproduce HF.

Harmonic oscillator solution

- Energy eigenvalues of the harmonic oscillator:

$$E_{nlj} = \left(N + \frac{3}{2}\right)\hbar\omega - \kappa\hbar^2 l(l+1) + \zeta\hbar^2 \begin{cases} -\frac{1}{2}l & j = l + \frac{1}{2} \\ \frac{1}{2}(l+1) & j = l - \frac{1}{2} \end{cases}$$

$N = 2n + l = 0, 1, 2, \dots$: oscillator quantum number

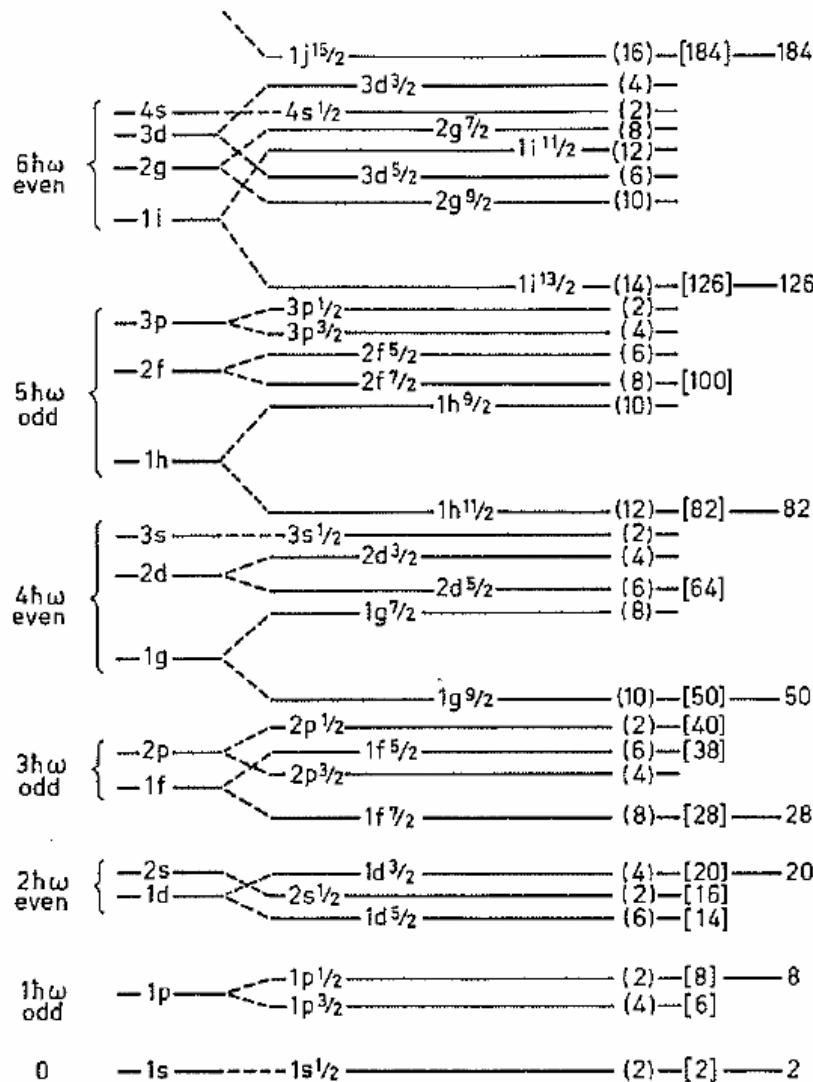
$n = 0, 1, 2, \dots$: radial quantum number

$l = N, N-2, \dots, 1 \text{ or } 0$: orbital angular momentum

$j = l \pm \frac{1}{2}$: total angular momentum

$m_j = -j, -j+1, \dots, +j$: z projection of j

Energy levels of harmonic oscillator



- Typical parameter values:

$$\hbar\omega \approx 41 A^{-1/3} \text{ MeV}$$

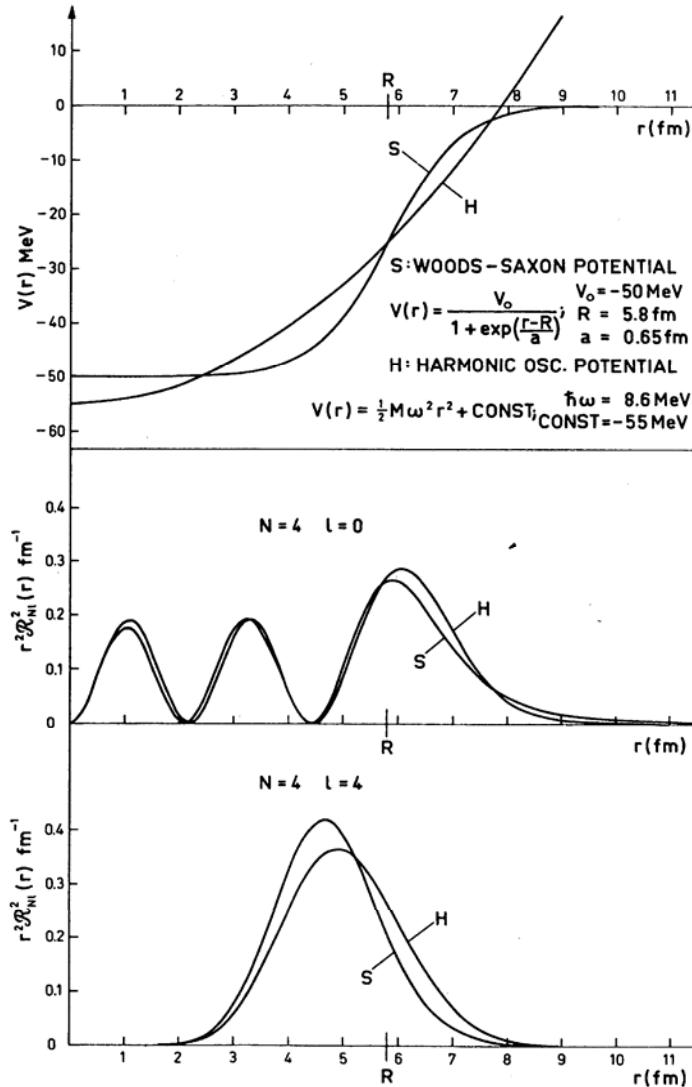
$$\zeta \hbar^2 \approx 20 A^{-2/3} \text{ MeV}$$

$$\kappa \hbar^2 \approx 0.1 \text{ MeV}$$

$$\therefore b \approx 1.0 A^{1/6} \text{ fm}$$

- ‘Magic’ numbers at 2, 8, 20, 28, 50, 82, 126, 184,...

Why an orbit-orbit term?



- Nuclear mean field is close to Woods-Saxon:

$$\hat{V}_{\text{WS}}(r) = \frac{V_0}{1 + \exp \frac{r - R_0}{a}}$$

- $2n+l=N$ degeneracy is lifted $\Rightarrow E_l < E_{l-2} < \dots$

Why a spin-orbit term?

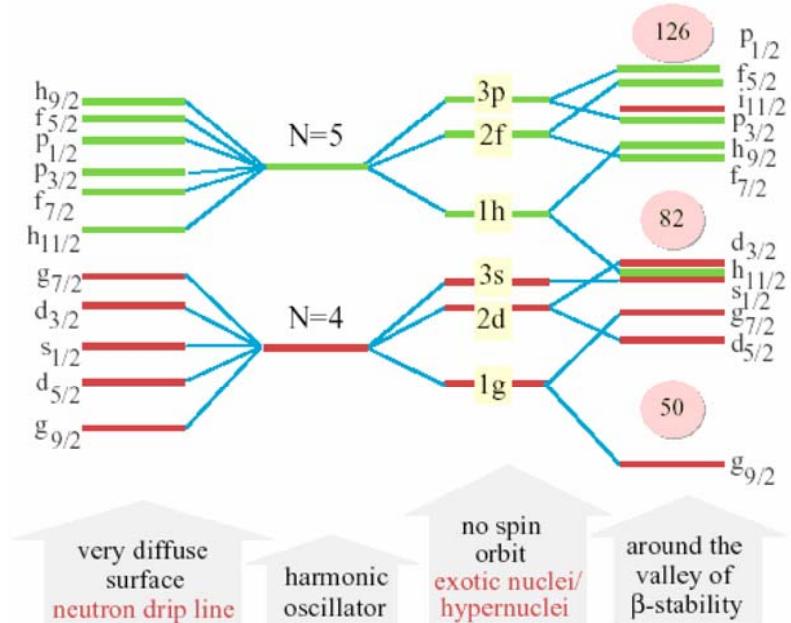
- Relativistic origin (*ie* Dirac equation).
- From general invariance principles:

$$\hat{V}_{\text{SO}} = \zeta(r) \mathbf{l} \cdot \mathbf{s}, \quad \zeta(r) = \frac{r_0^2}{r} \frac{\partial V}{\partial r} [= \zeta \text{ in HO}]$$

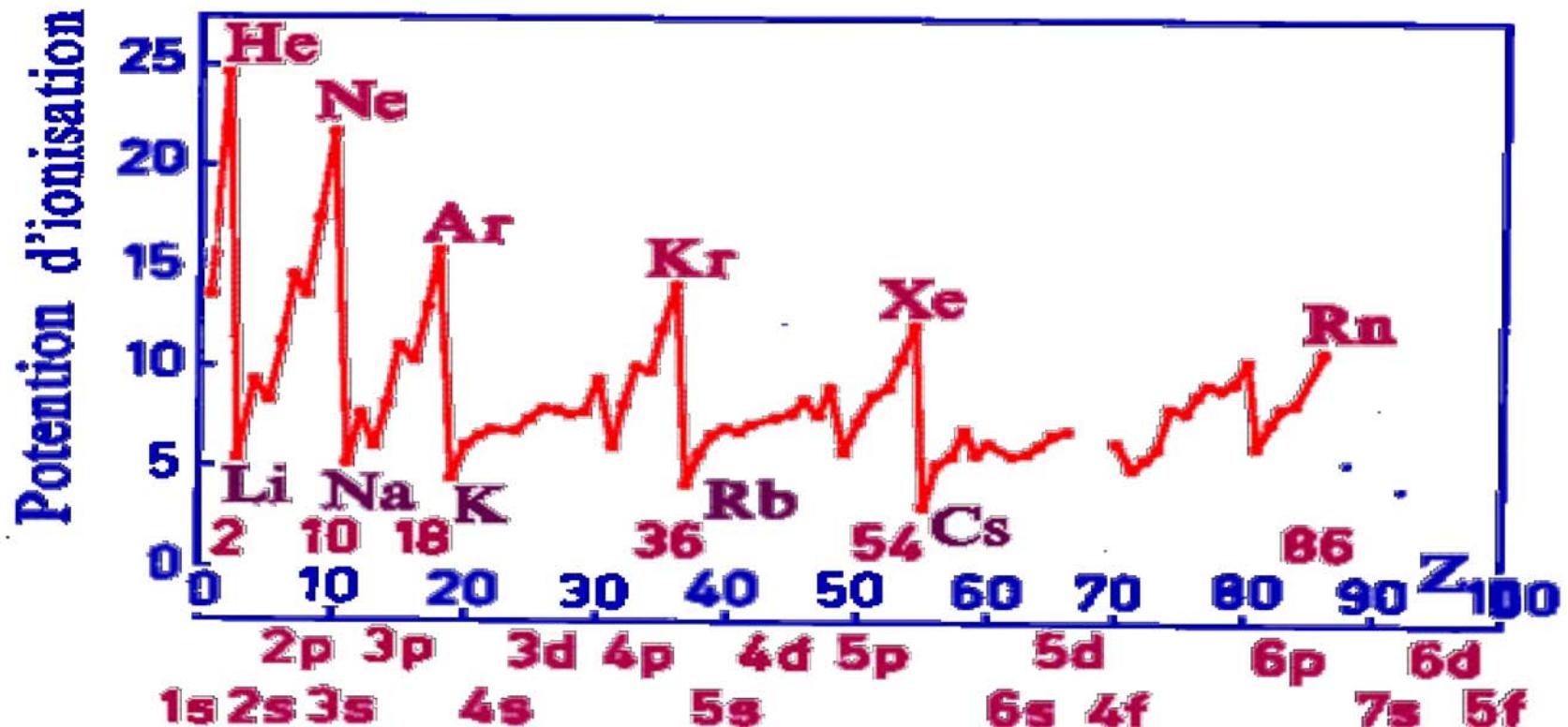
- Spin-orbit term is surface peaked \Rightarrow diminishes for diffuse potentials.

Evidence for shell structure

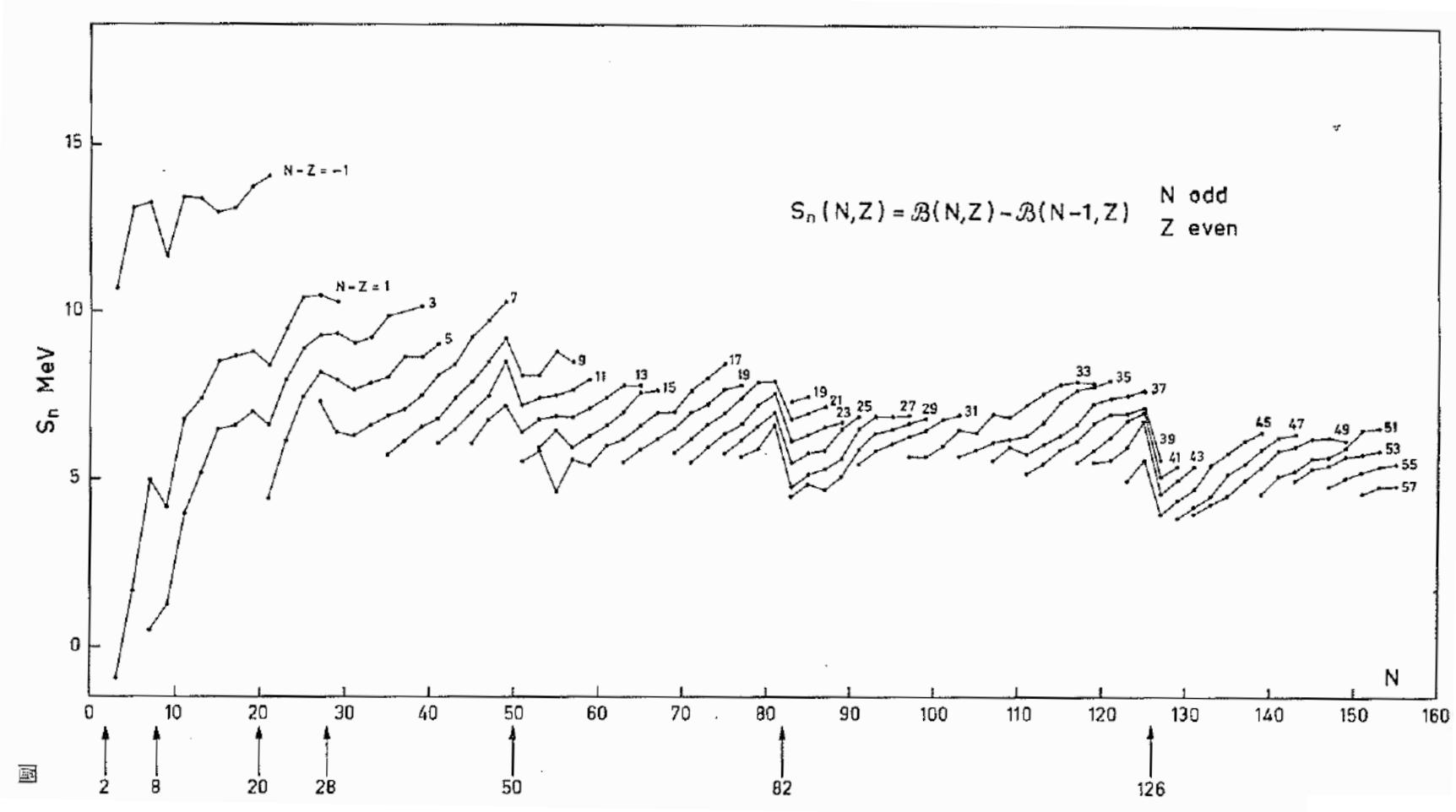
- Evidence for nuclear shell structure from
 - 2^+ in even-even nuclei [E_x , $B(E2)$].
 - Nucleon-separation energies & nuclear masses.
 - Nuclear level densities.
 - Reaction cross sections.
- *Is nuclear shell structure modified away from the line of stability?*



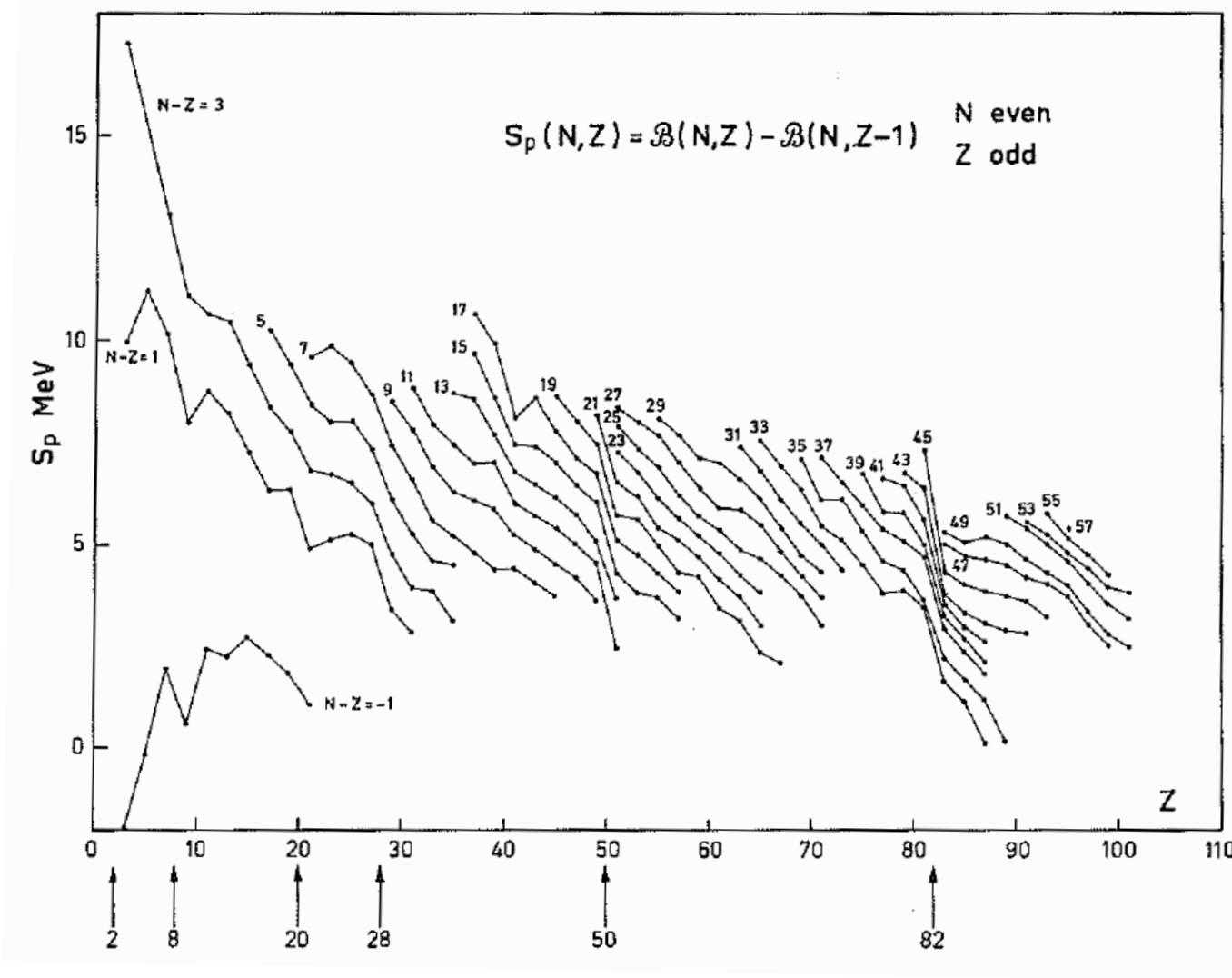
Ionisation potential in atoms



Neutron separation energies



Proton separation energies



Liquid-drop mass formula

- Binding energy of an atomic nucleus:

$$B(N,Z) = a_v A - a_s A^{2/3} - a_c \frac{Z(Z-1)}{A^{1/3}} - a'_s \frac{(N-Z)^2}{A} + a_p \frac{\Delta(N,Z)}{A^{1/3}}$$

- For 2149 nuclei ($N, Z \geq 8$) in AME03:

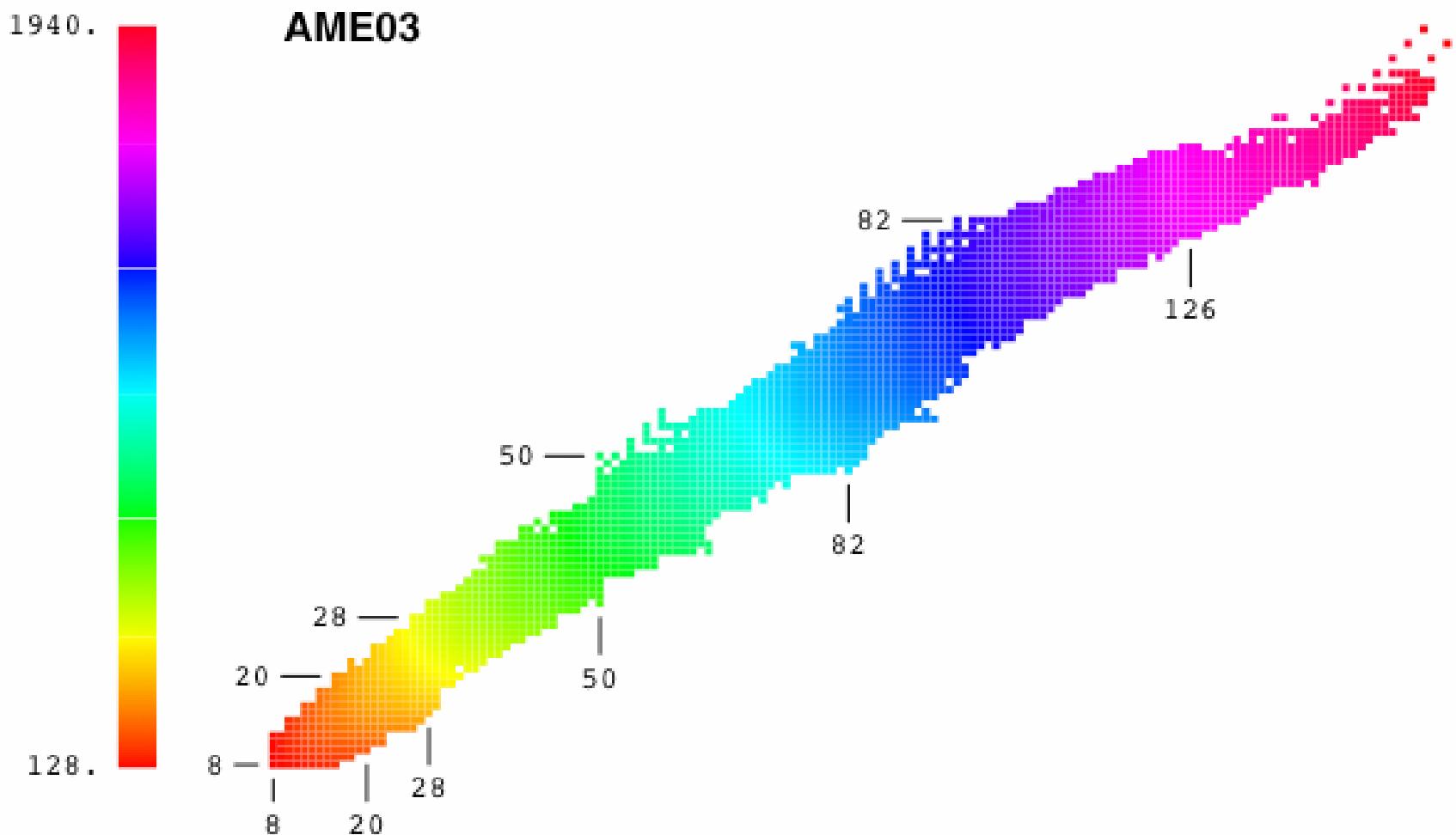
$$a_v \approx 16, a_s \approx 18, a_c \approx 0.71, a'_s \approx 23, a_p \approx 6$$

$$\Rightarrow \sigma_{\text{rms}} \approx 2.93 \text{ MeV.}$$

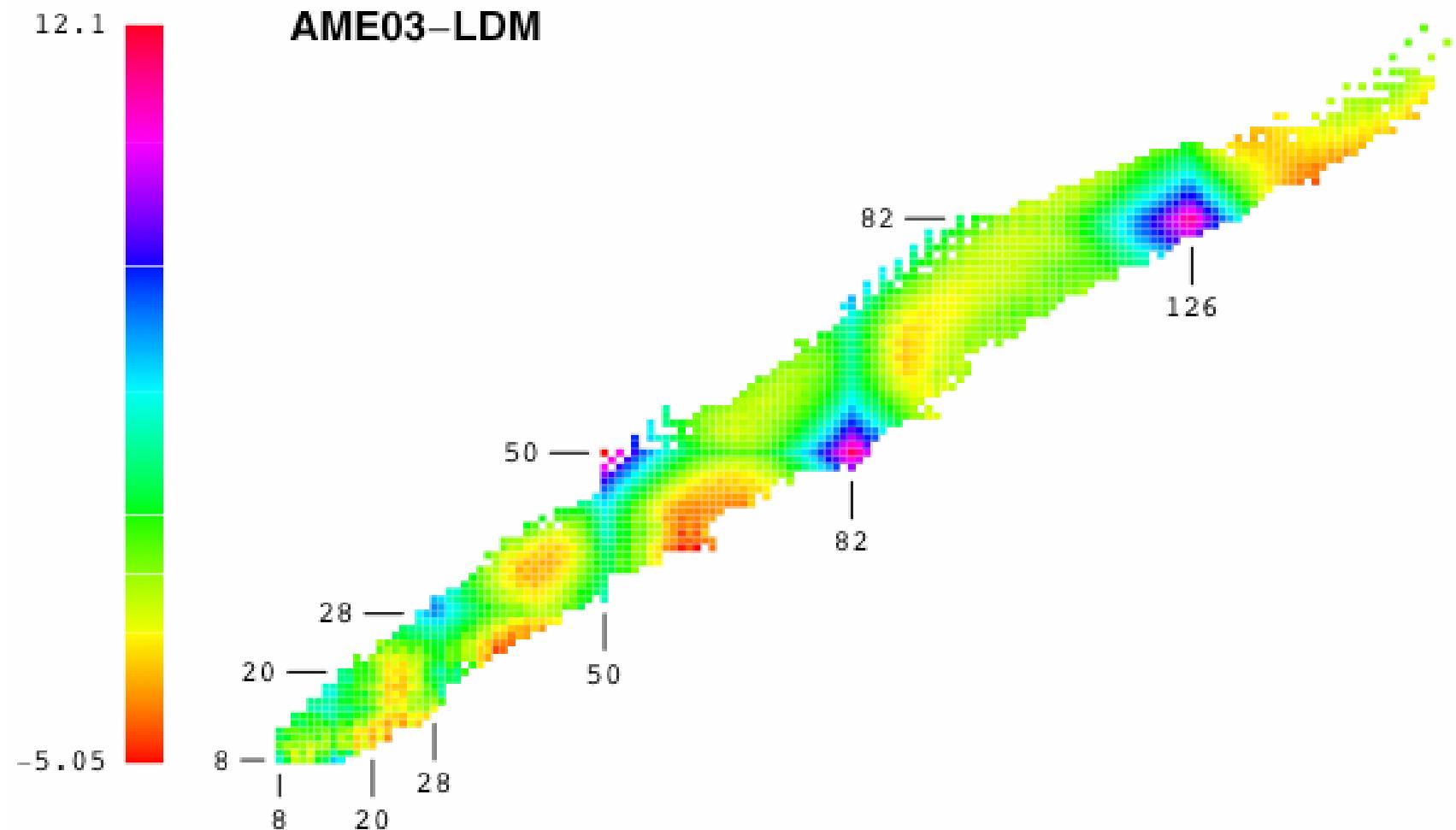
C.F. von Weizsäcker, Z. Phys. **96** (1935) 431

H.A. Bethe & R.F. Bacher, Rev. Mod. Phys. **8** (1936) 82

The nuclear mass surface



The ‘unfolding’ of the mass surface



Modified liquid-drop formula

- Add surface, Wigner and ‘shell’ corrections:

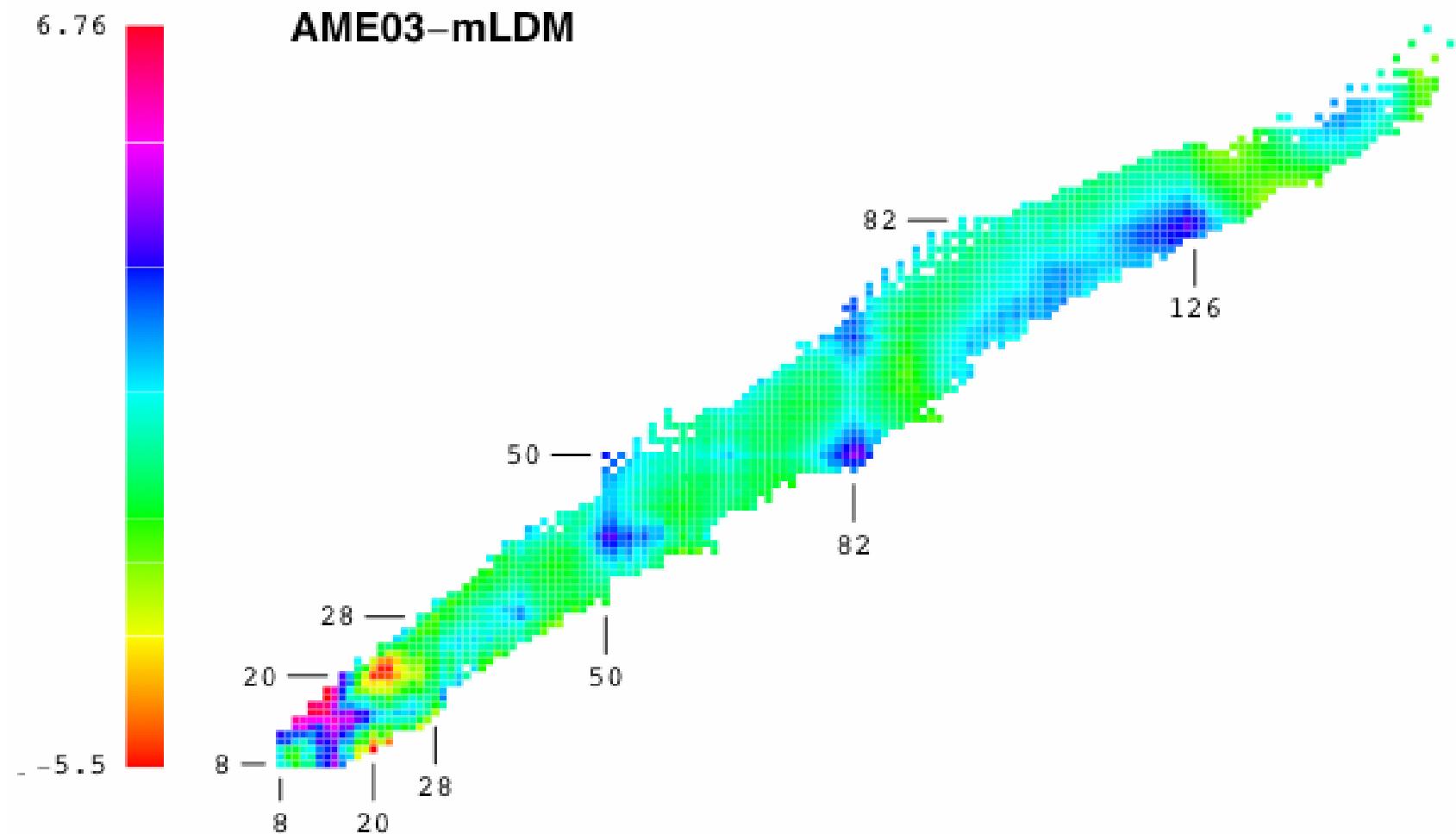
$$B(N,Z) = a_v A - a_s A^{2/3} - a_c \frac{Z(Z-1)}{A^{1/3}} + a_p \frac{\Delta(N,Z)}{A^{1/3}} - \frac{S_v}{1+y_s A^{-1/3}} \frac{4T(T+1)}{A} - a_f (n_\nu + n_\pi) + a_{ff} (n_\nu + n_\pi)^2$$

- For 2149 nuclei ($N, Z \geq 8$) in AME03:

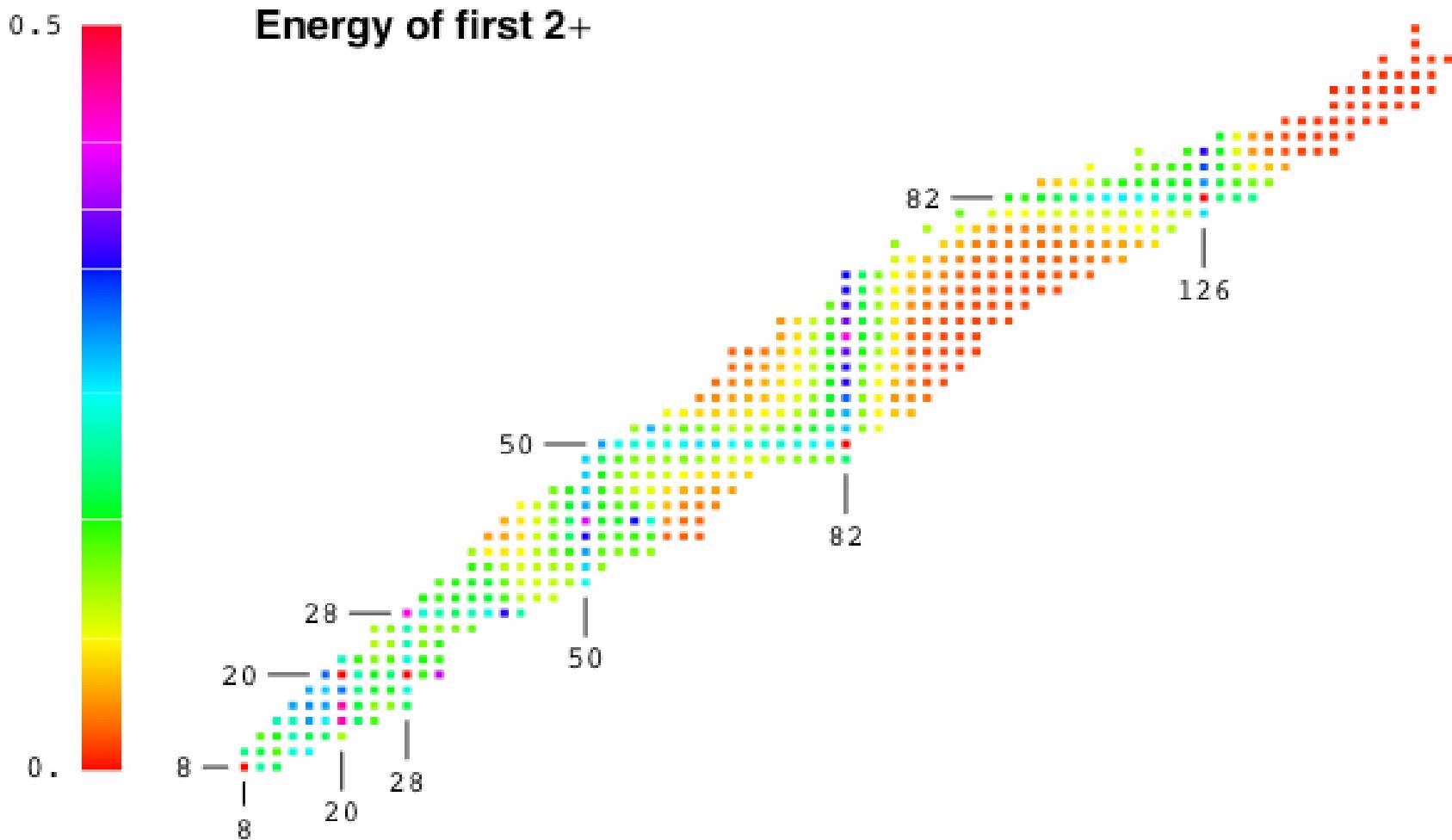
$$a_v \approx 16, a_s \approx 18, a_c \approx 0.71, S_v \approx 35, y_s \approx 2.9, a_p \approx 5.5, a_f \approx 0.85, a_{ff} \approx 0.016$$

$$\Rightarrow \sigma_{\text{rms}} \approx 1.16 \text{ MeV.}$$

Shell-corrected LDM



Shell structure from $E_x(2_1)$



Evidence for IP shell model

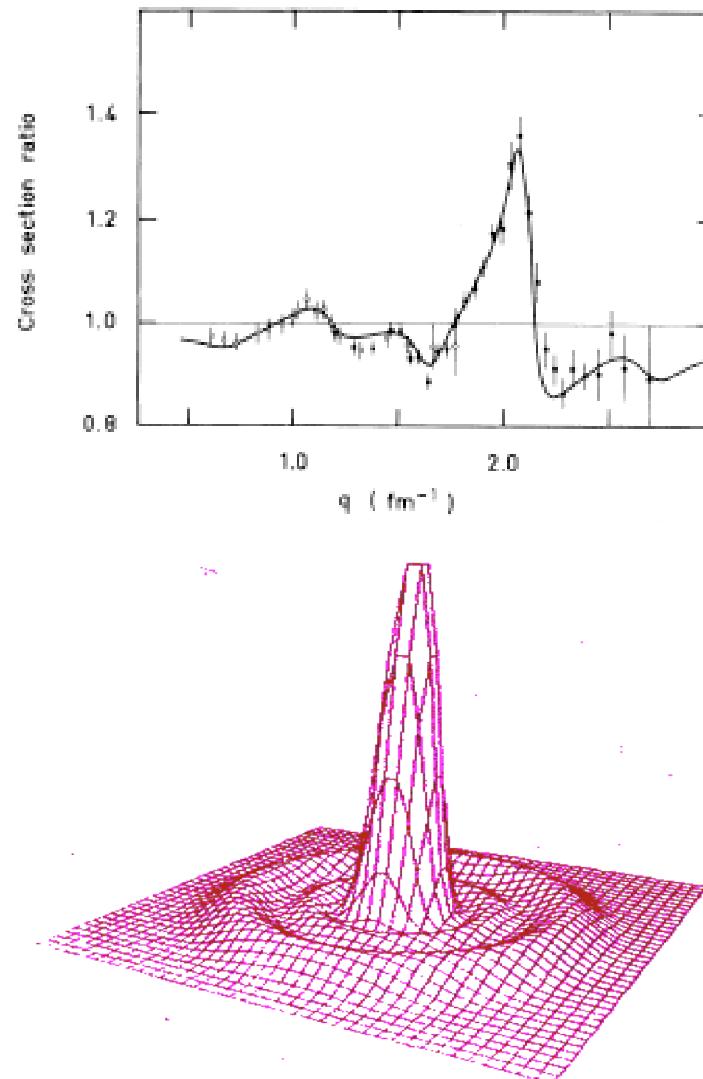
Z	Isotope	Observed J^π	Shell model nlj
3	^9Li	$(3/2^-)$	$1p_{3/2}$
5	^{13}B	$3/2^-$	$1p_{3/2}$
7	^{17}N	$1/2^-$	$1p_{1/2}$
9	^{21}F	$5/2^+$	$1d_{5/2}$
11	^{25}Na	$5/2^+$	$1d_{5/2}$
13	^{29}Al	$5/2^+$	$1d_{5/2}$
15	^{33}P	$1/2^+$	$2s_{1/2}$
17	^{37}Cl	$3/2^+$	$1d_{3/2}$
19	^{41}K	$3/2^+$	$1d_{3/2}$
21	^{45}Sc	$7/2^-$	$1f_{7/2}$
23	^{49}Va	$7/2^-$	$1f_{7/2}$
25	^{53}Mn	$7/2^-$	$1f_{7/2}$
27	^{57}Co	$7/2^-$	$1f_{7/2}$
29	^{61}Cu	$3/2^-$	$2p_{3/2}$
31	^{65}Ga	$3/2^-$	$2p_{3/2}$
33	^{69}As	$(5/2^-)$	$1f_{5/2}$
35	^{73}Br	$(3/2^-)$	$1f_{5/2}$

- Ground-state spins and parities of nuclei:

$$\left. \begin{array}{l} j \text{ in } \phi_{nljm_j} \Rightarrow J \\ l \text{ in } \phi_{nljm_j} \Rightarrow (-)^l = \pi \end{array} \right\} \Rightarrow J^\pi$$

Validity of SM wave functions

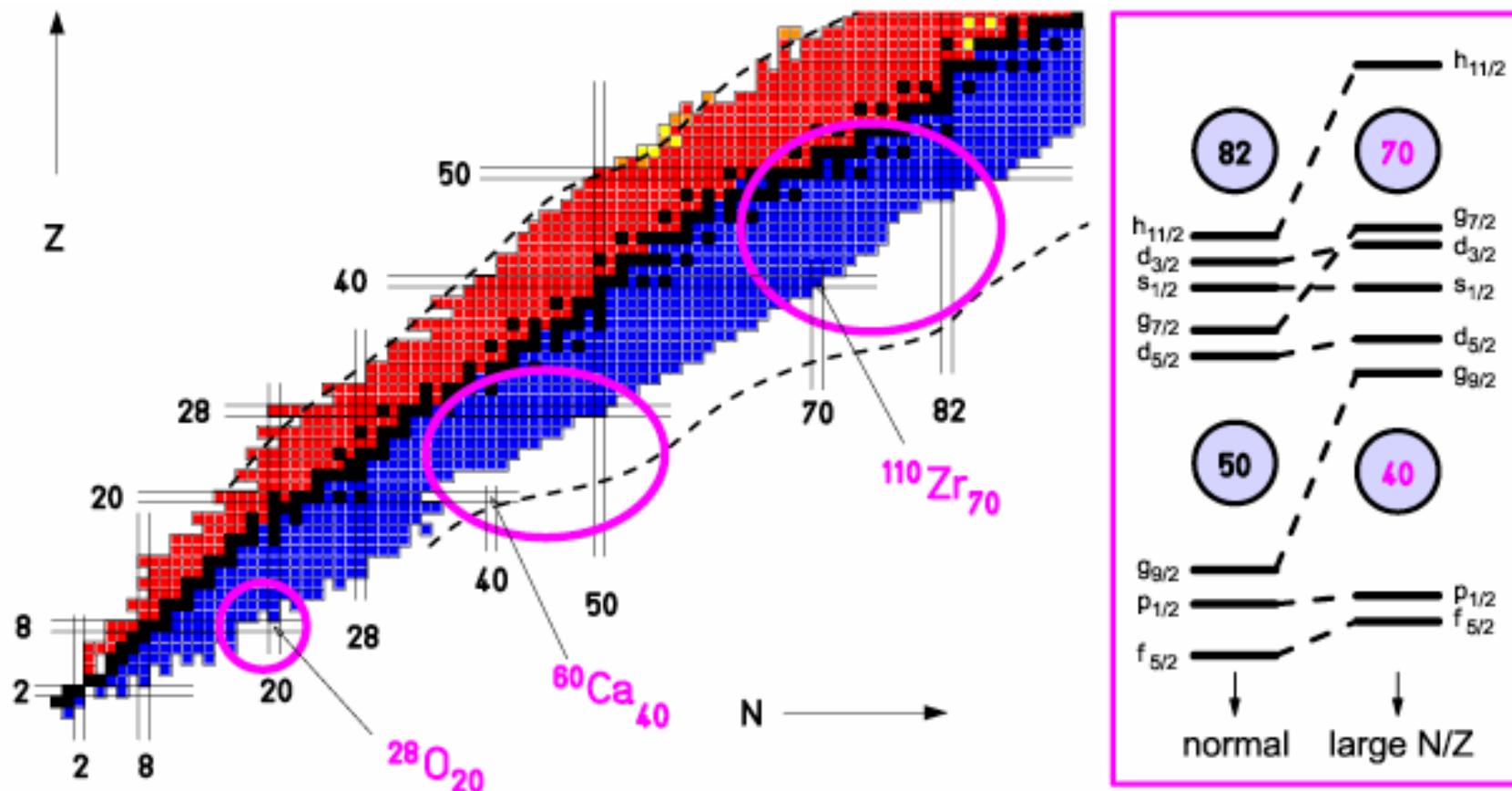
- Example: Elastic electron scattering on ^{206}Pb and ^{205}Tl , differing by a $3s$ proton.
- Measured ratio agrees with shell-model prediction for $3s$ orbit.



J.M. Cavedon *et al.*, Phys. Rev. Lett. **49** (1982) 978

NSDD Workshop, Trieste, April-May 2008

Variable shell structure



Beyond Hartree-Fock

- Hartree-Fock-Bogoliubov (HFB): Includes pairing correlations in mean-field treatment.
- Tamm-Dancoff approximation (TDA):
 - Ground state: closed-shell HF configuration
 - Excited states: mixed 1p-1h configurations
- Random-phase approximation (RPA): Correlations in the ground state by treating it on the same footing as 1p-1h excitations.

Nuclear shell model

- The full shell-model hamiltonian:

$$\hat{H} = \sum_{k=1}^A \left[\frac{\hat{p}_k^2}{2m} + \hat{V}(\mathbf{r}_k) \right] + \sum_{k < l} \hat{V}_{\text{RI}}(\mathbf{r}_k, \mathbf{r}_l)$$

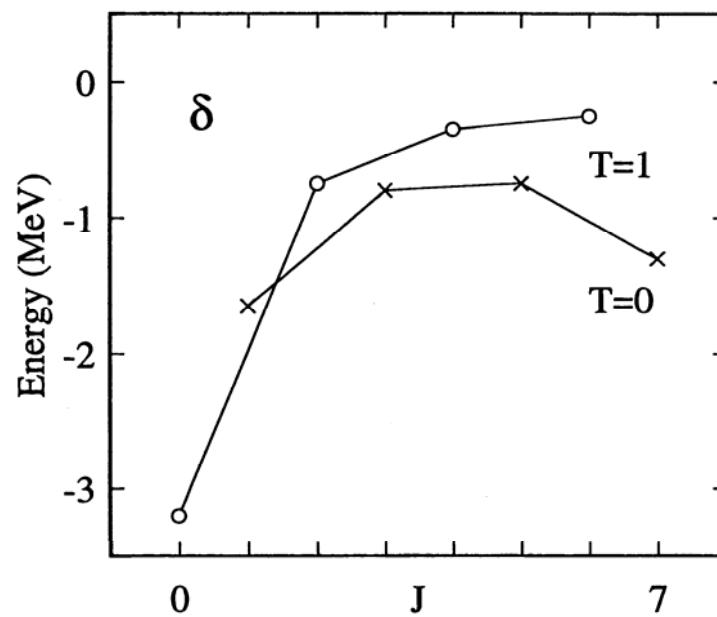
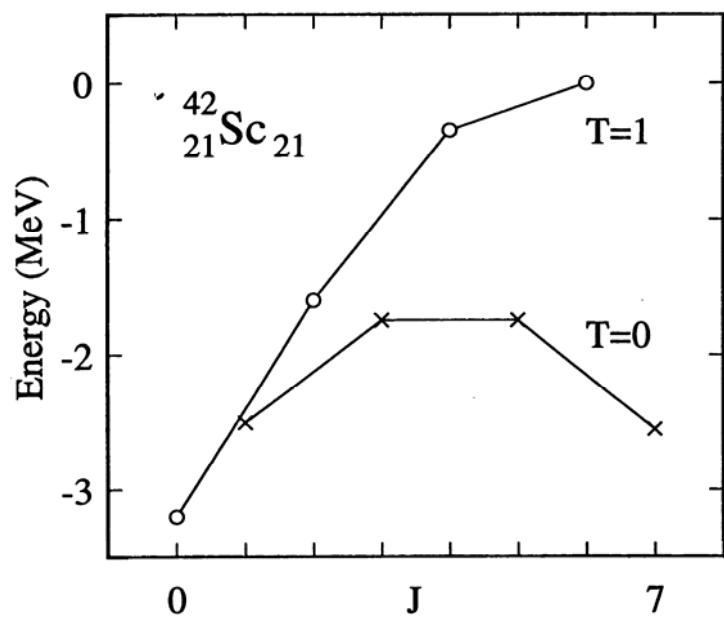
- Valence nucleons: Neutrons or protons that are in excess of the last, completely filled shell.
- Usual approximation: Consider the residual interaction V_{RI} among valence nucleons only.
- Sometimes: Include selected core excitations ('intruder' states).

Residual shell-model interaction

- Four approaches:
 - Effective: Derive from free nn interaction taking account of the nuclear medium.
 - Empirical: Adjust matrix elements of residual interaction to data. Examples: p , sd and pf shells.
 - Effective-empirical: Effective interaction with some adjusted (monopole) matrix elements.
 - Schematic: Assume a simple spatial form and calculate its matrix elements in a harmonic-oscillator basis. Example: δ interaction.

Schematic short-range interaction

- Delta interaction in harmonic-oscillator basis:
- Example of $^{42}\text{Sc}_{21}$ (1 neutron + 1 proton):



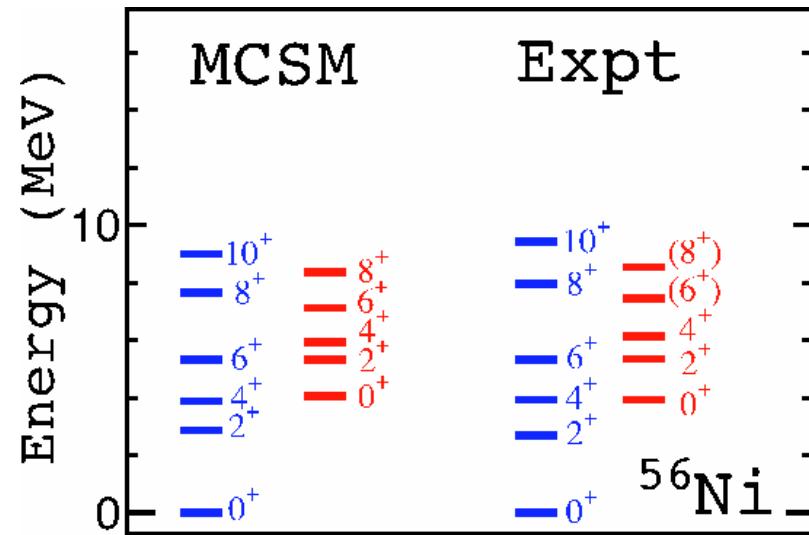
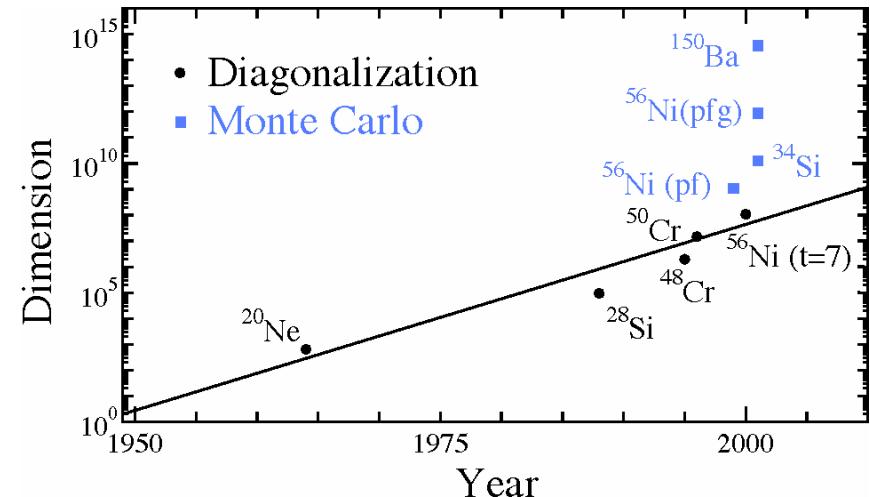
Large-scale shell model

- Large Hilbert spaces:

$$\left\langle \Psi_{i_1' i_2' \dots i_A'} \left| \sum_{k < l}^n \hat{V}_{\text{RI}}(\mathbf{r}_k, \mathbf{r}_l) \right| \Psi_{i_1 i_2 \dots i_A} \right\rangle$$

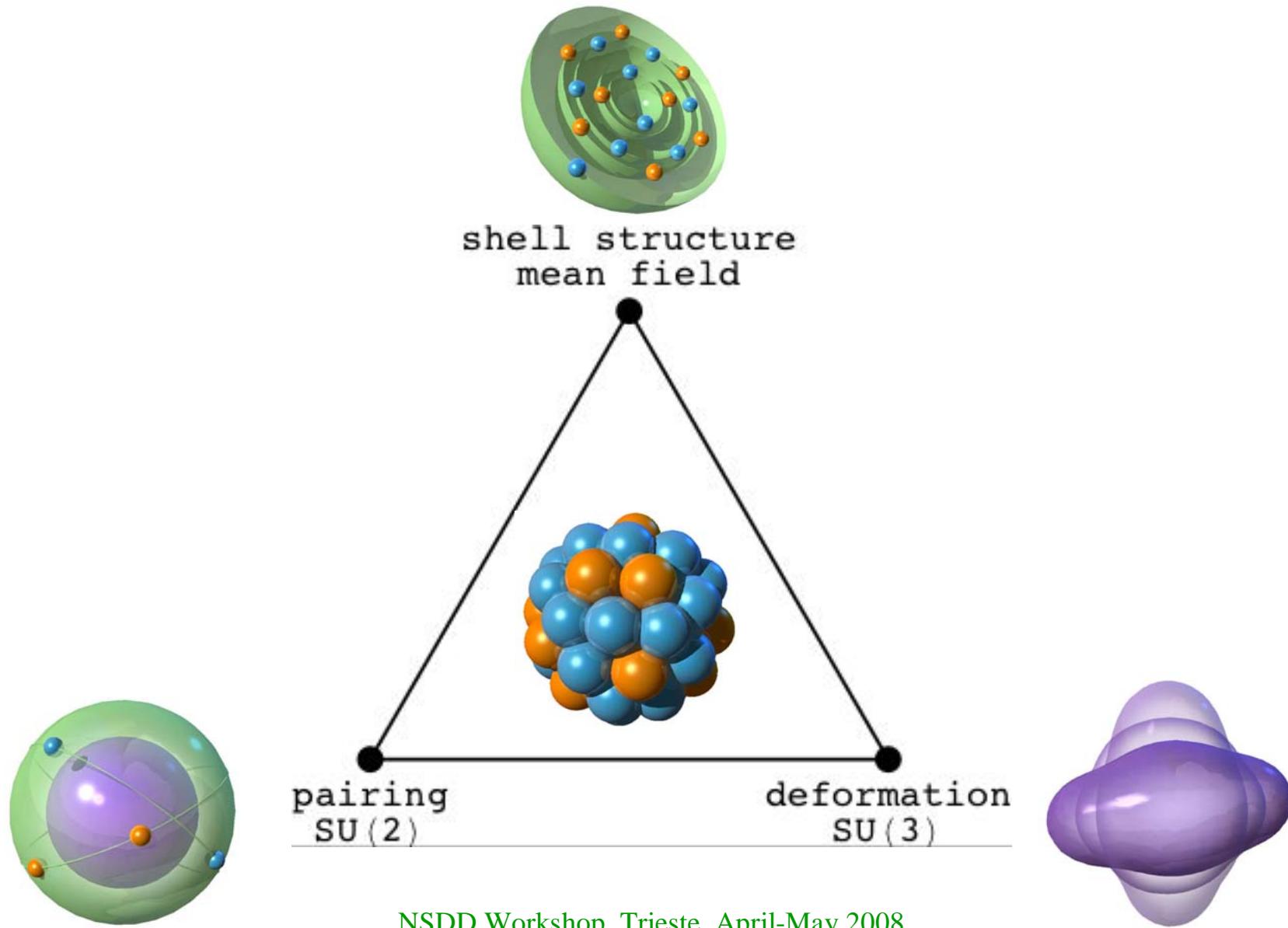
- Diagonalisation : $\sim 10^9$.
- Monte Carlo : $\sim 10^{15}$.

- Example : 8n + 8p in $pfg_{9/2}(^{56}\text{Ni})$.



M. Honma *et al.*, Phys. Rev. C **69** (2004) 034335

The three faces of the shell model

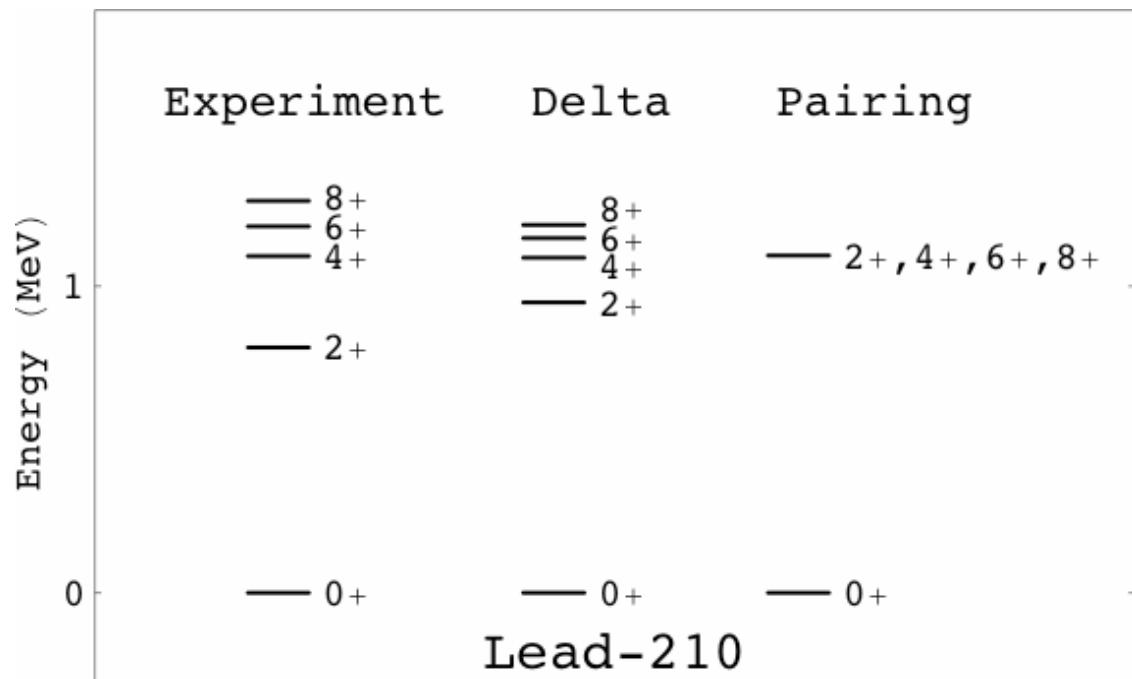


Racah's SU(2) pairing model

- Assume pairing interaction in a single- j shell:

$$\langle j^2 JM_J | \hat{V}_{\text{pairing}}(\mathbf{r}_1, \mathbf{r}_2) | j^2 JM_J \rangle = \begin{cases} -\frac{1}{2}(2j+1)g_0, & J=0 \\ 0, & J \neq 0 \end{cases}$$

- Spectrum ^{210}Pb :



Solution of the pairing hamiltonian

- Analytic solution of pairing hamiltonian for identical nucleons in a single- j shell:

$$\left\langle j^n \nu J \left| \sum_{1 \leq k < l}^n \hat{V}_{\text{pairing}}(\mathbf{r}_k, \mathbf{r}_l) \right| j^n \nu J \right\rangle = -g_0 \frac{1}{4} (n - \nu)(2j - n - \nu + 3)$$

- Seniority ν (number of nucleons not in pairs coupled to $J=0$) is a good quantum number.
- Correlated ground-state solution (*cf.* BCS).

G. Racah, Phys. Rev. **63** (1943) 367

NSDD Workshop, Trieste, April-May 2008

Nuclear superfluidity

- Ground states of pairing hamiltonian have the following *correlated* character:
 - Even-even nucleus ($\nu=0$): $(\hat{S}_+)^{n/2} |0\rangle$, $\hat{S}_+ = \sum_m \hat{a}_{m\downarrow}^+ \hat{a}_m^+ \gamma_\uparrow$
 - Odd-mass nucleus ($\nu=1$): $\hat{a}_{m\downarrow}^+ (\hat{S}_+)^{n/2} |0\rangle$
- Nuclear superfluidity leads to
 - Constant energy of first 2^+ in even-even nuclei.
 - Odd-even staggering in masses.
 - Smooth variation of two-nucleon separation energies with nucleon number.
 - Two-particle (2n or 2p) transfer enhancement.

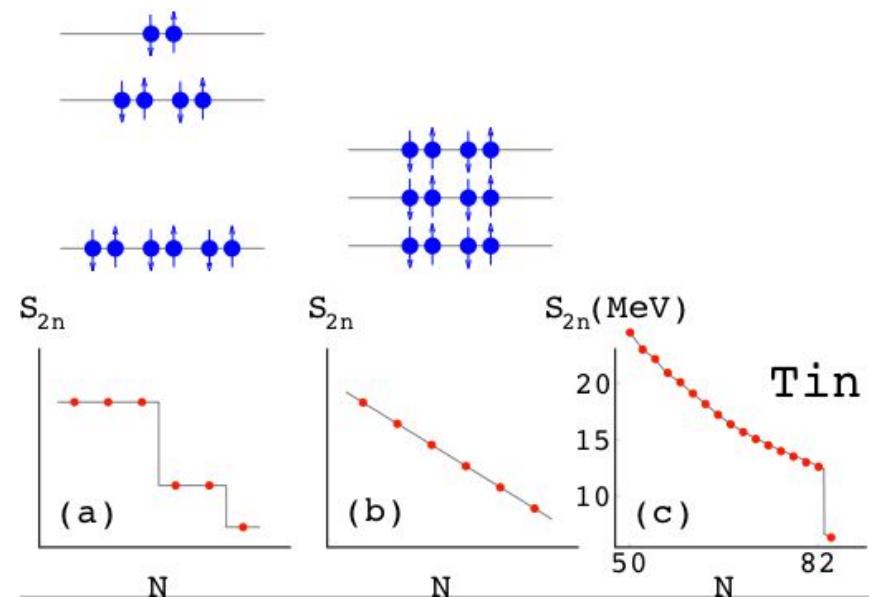
Two-nucleon separation energies

- Two-nucleon separation energies S_{2n} :

(a) Shell splitting dominates over interaction.

(b) Interaction dominates over shell splitting.

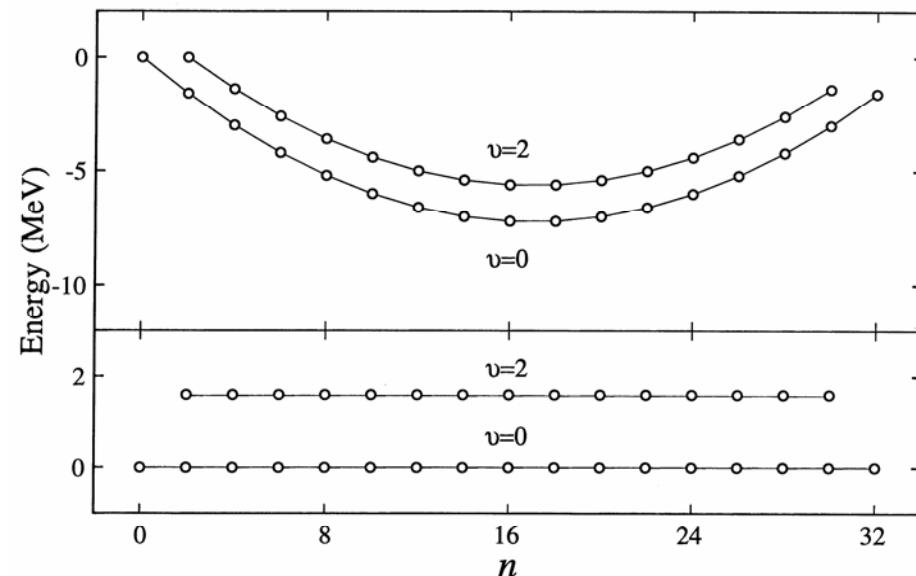
(c) S_{2n} in tin isotopes.



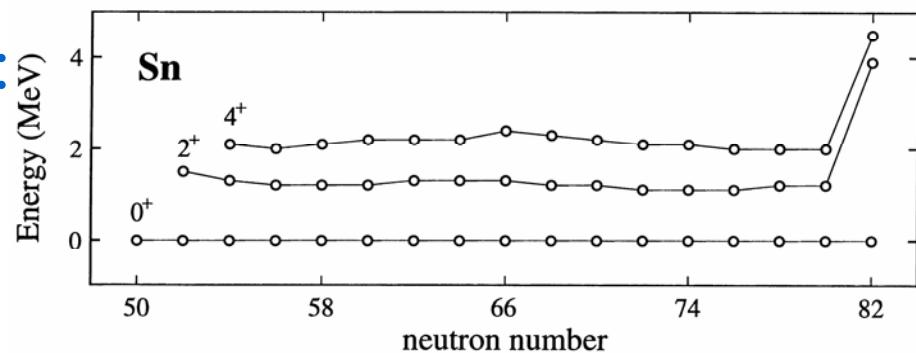
Pairing gap in semi-magic nuclei

- Even-even nuclei:
 - Ground state: $v=0$.
 - First-excited state: $v=2$.
 - Pairing produces constant energy gap:

$$E_x(2_1^+) = \frac{1}{2}(2j+1)G$$



- Example of Sn isotopes:



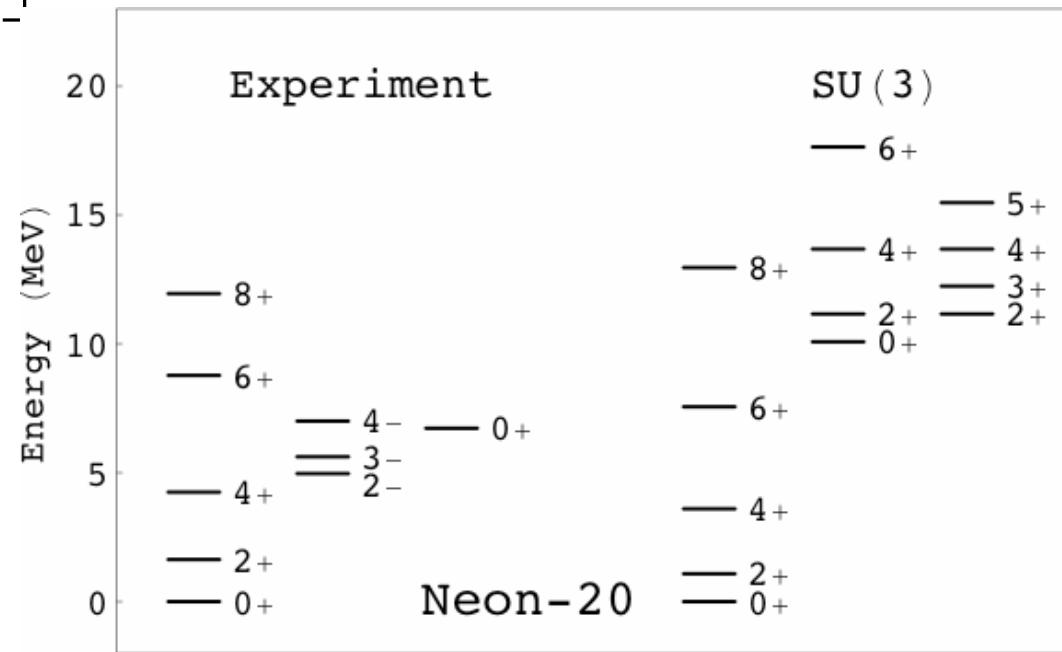
Elliott's SU(3) model of rotation

- Harmonic oscillator mean field (*no* spin-orbit) with residual interaction of quadrupole type:

$$\hat{H} = \sum_{k=1}^A \left| \frac{p_k^2}{2m} + \frac{1}{2} m \omega^2 r_k^2 \right| - g_2 \hat{Q} \cdot \hat{Q},$$

$$\hat{Q}_\mu \propto \sum_{k=1}^A r_k^2 Y_{2\mu}(\hat{\mathbf{r}}_k)$$

$$+ \sum_{k=1}^A p_k^2 Y_{2\mu}(\hat{\mathbf{p}}_k)$$



J.P. Elliott, Proc. Roy. Soc. A **245** (1958) 128; 562