Nuclear structure theory

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Lecture 2: Ab-initio methods (brief)

Traditional shell model

RIA 2006 Summer School at Oak Ridge

Solving the ab-initio quantum many-body problem

Exact or virtually exact solutions available for:

- A=3: solution of Faddeev equation.
- A=4: solvable via Faddeev-Yakubowski approach.
- Light nuclei (up to A=12 at present): Green's function Monte Carlo (GFMC); virtually exact; limited to certain forms of interactions.

Highly accurate approximate solutions available for:

- Light nuclei (up to A=16 at present): No-core Shell model (NCSM); truncation in model space.
- Light and medium mass region (A=4, 16, 40 at present): Coupled cluster theory; truncation in model space and correlations.

Green's Function Monte Carlo

Idea:

1. Determine accurate approximate wave function via variation of the energy (The high-dimensional integrals are done via Monte Carlo integration).

$$E = \frac{\langle \Psi_{\text{trial}} | \hat{H} | \Psi_{\text{trial}} \rangle}{\langle \Psi_{\text{trial}} | \Psi_{\text{trial}} \rangle}$$

2. Refine wave function and energy via projection with Green's function

$$|\Psi\rangle = \lim_{\tau \to \infty} e^{-\tau(\hat{H}-E)} |\Psi_{\text{trial}}\rangle$$

☺ Virtually exact method.

☹ Limited to certain forms of Hamiltonians; computationally expensive.

Working in a finite model space

NCSM and Coupled-cluster theory solve the Schroedinger equation in a model space with a *finite* (albeit large) number of configurations or basis states.

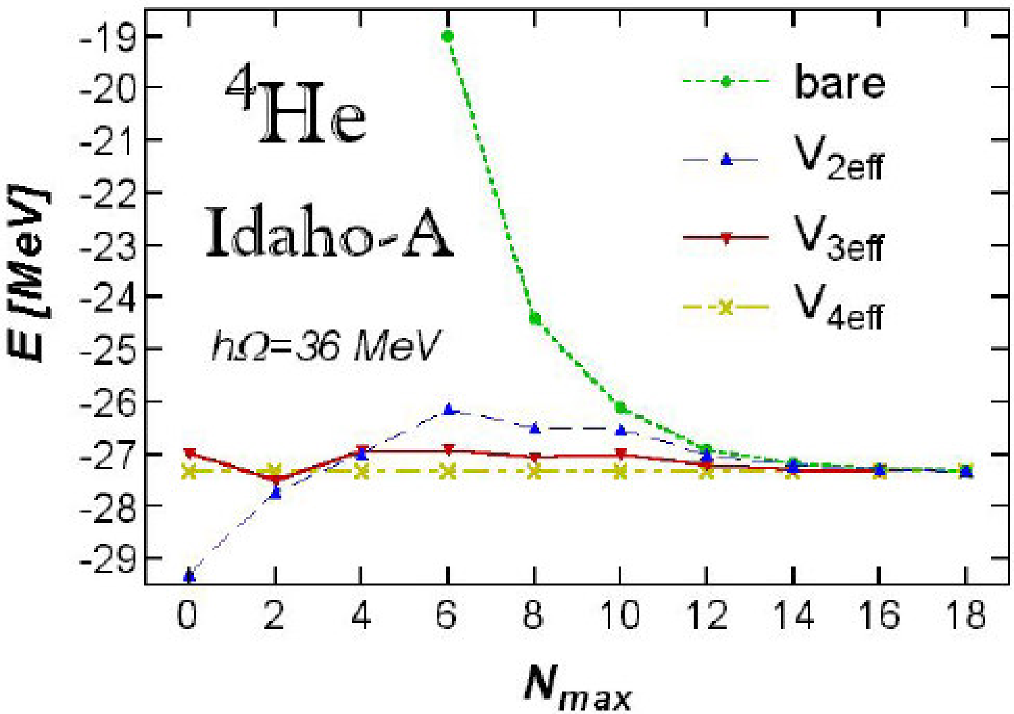
Problem: High-momentum components of high-precision NN interactions require enormously large spaces.

Solution: Get rid of the high-momentum modes via a renormalization procedure. (Lee-Suzuki approach)

Price tag:

Generation of 3, 4, …, A-body forces unavoidable.

Observables other than the energy also need to be transformed.



E. Ormand
http://www.phy.ornl.gov/npss03/ormand2.ppt

No-core shell model

Idea: Solve the A-body problem in a harmonic oscillator basis.

1. Take K single particle orbitals
2. Construct a basis of Slater determinants
3. Express Hamiltonian in this basis
4. Find low-lying states via diagonalization

☺ Get eigenstates and energies

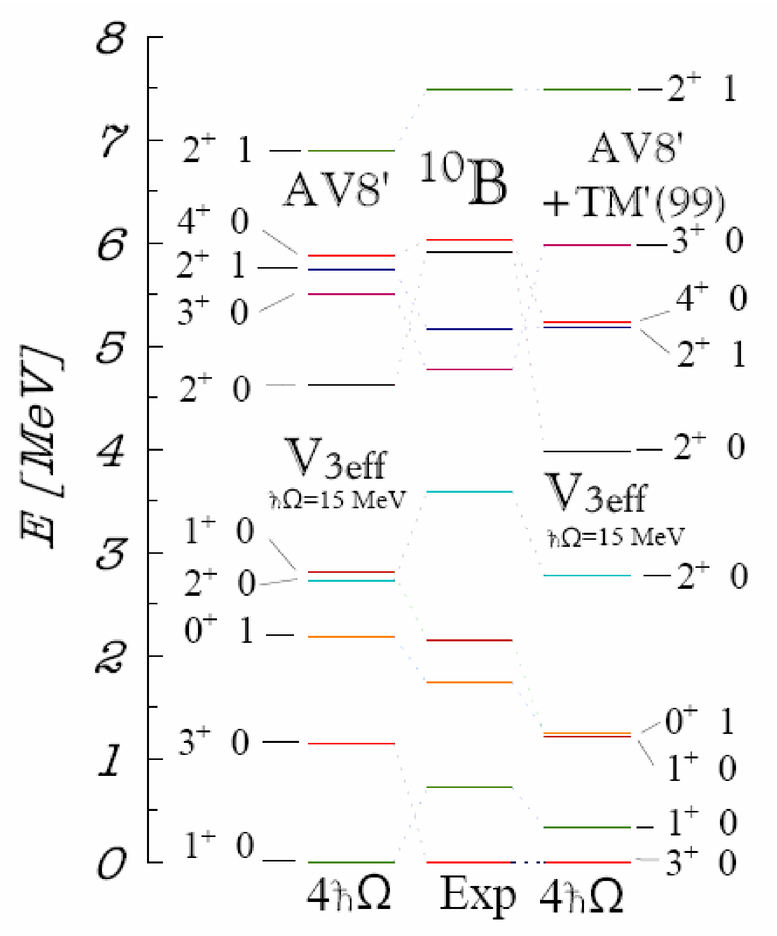
☺ No restrictions regarding Hamiltonian

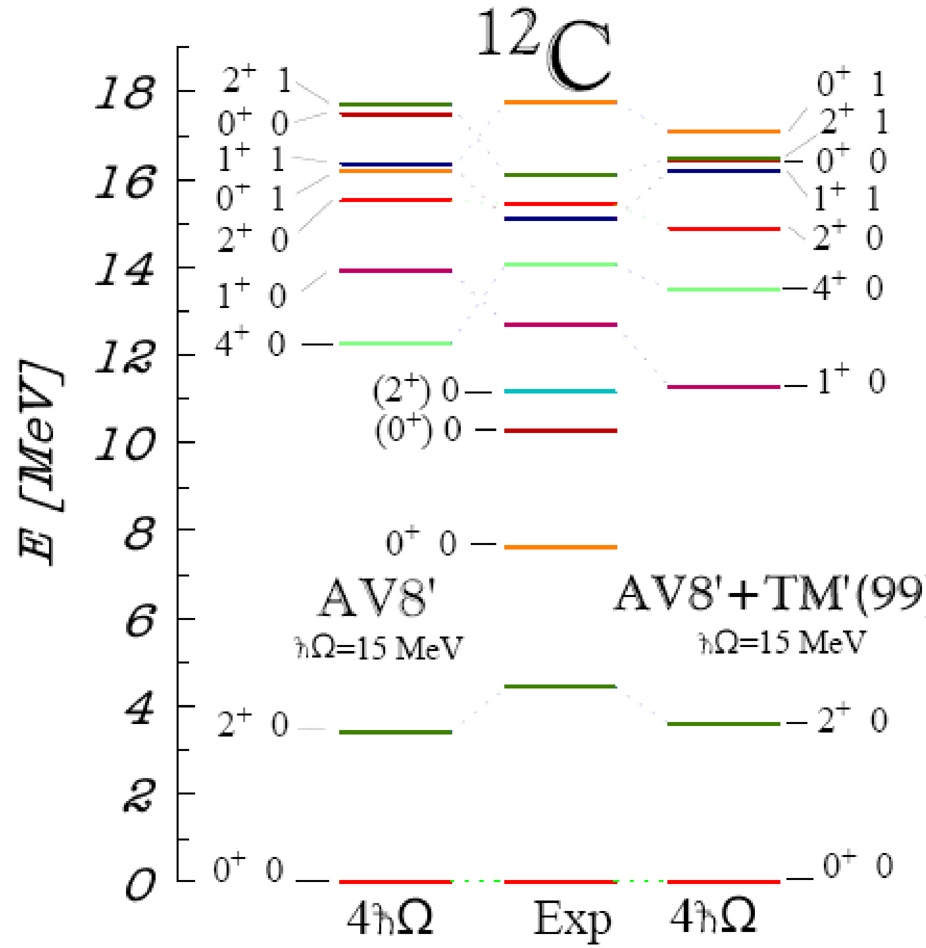
☹ Number of configurations and resulting matrix very large: There are

$$\binom{K}{A} = \frac{K!}{(K-A)!A!}$$

ways to distribute A nucleons over K single-particle orbitals.

No-core Shell Model results for ^{10}B and ^{12}C





P. Navratil and W. E. Ormand, Phys. Rev. C68 (2003) 034305

Coupled-cluster theory

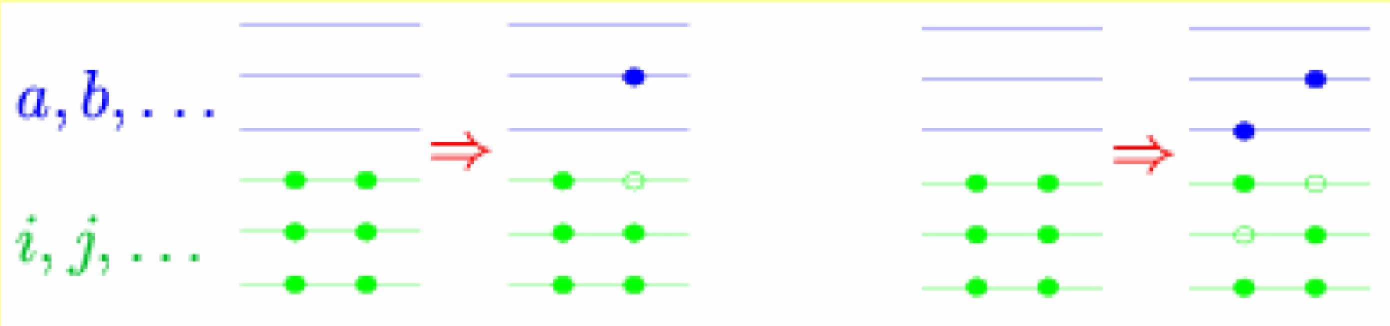
Ansatz:

$$
\begin{aligned}
|\Psi\rangle &= e^{T}|\Phi\rangle \\
T &= 1 + T_1 + T_2 + \ldots \\
T_1 &= \sum_{ia} t_i^a a_a^\dagger a_i \\
T_2 &= \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

☺ Scales gently (polynomial, not exponential) with increasing problem size.

☹ Open-shell systems require much more work.

Correlations are exponentiated 1p-1h and 2p-2h excitations. Part of np-nh excitations included!



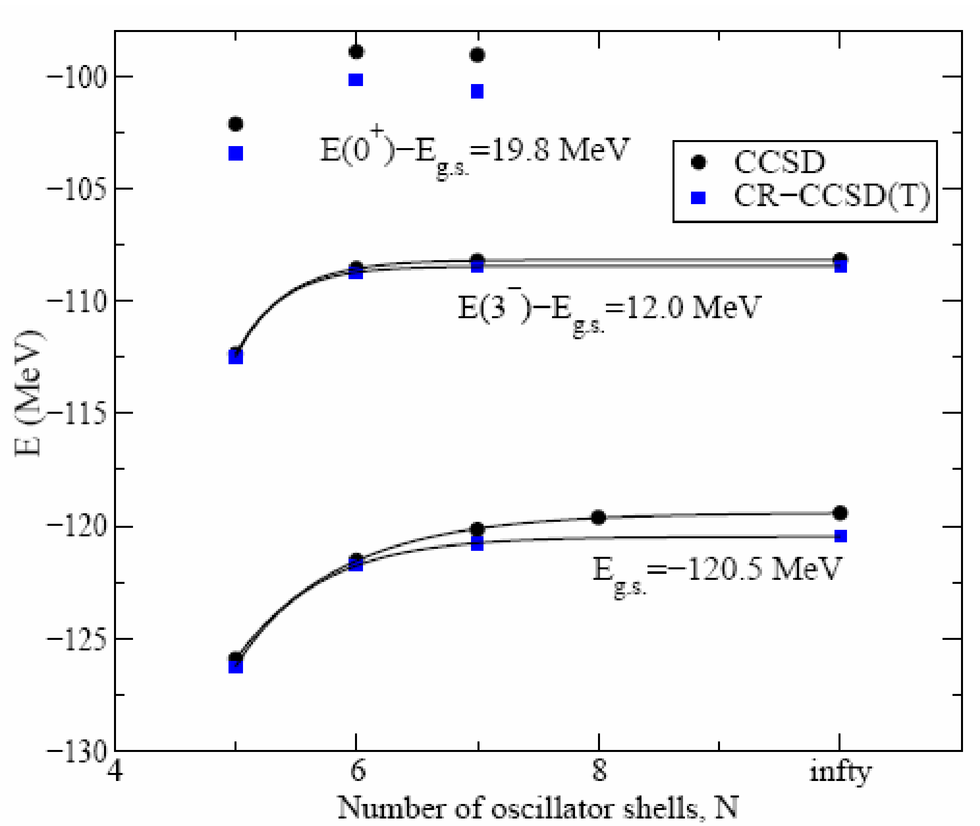
Coupled cluster equations

$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle \\
\overline{H} &\equiv e^{-T}He^{T} = \left(He^{T}\right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \ldots\right)_c
\end{aligned}
$$

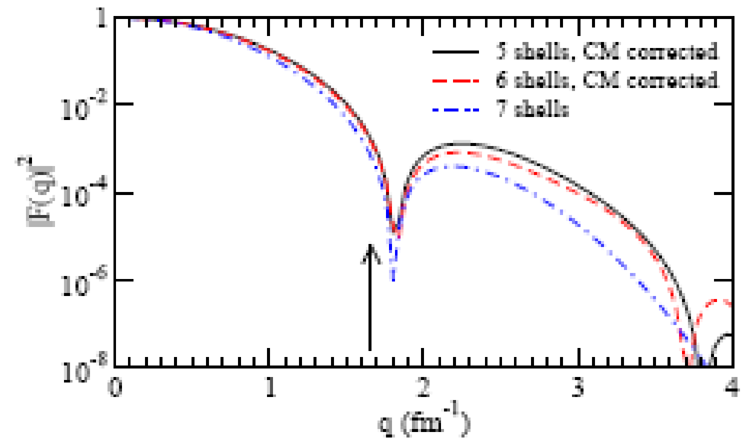
Coupled-cluster calculation for ^{16}O

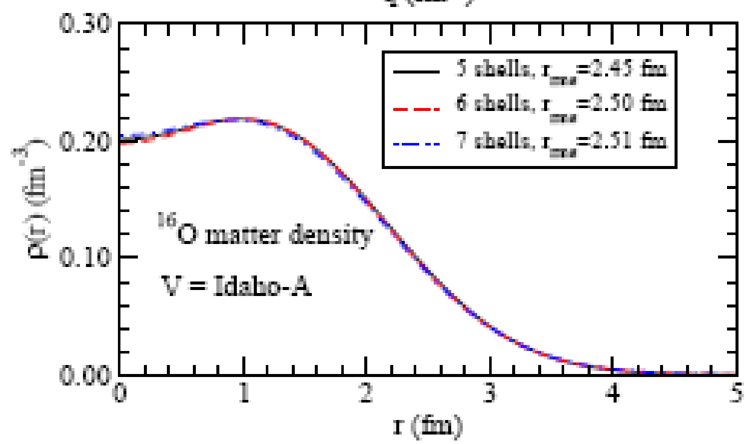
Interaction: Idaho-A based G-matrix

Model space: Up to 8 oscillator shells



M. Wloch et al, Phys. Rev. Lett. 94, 212501 (2005).



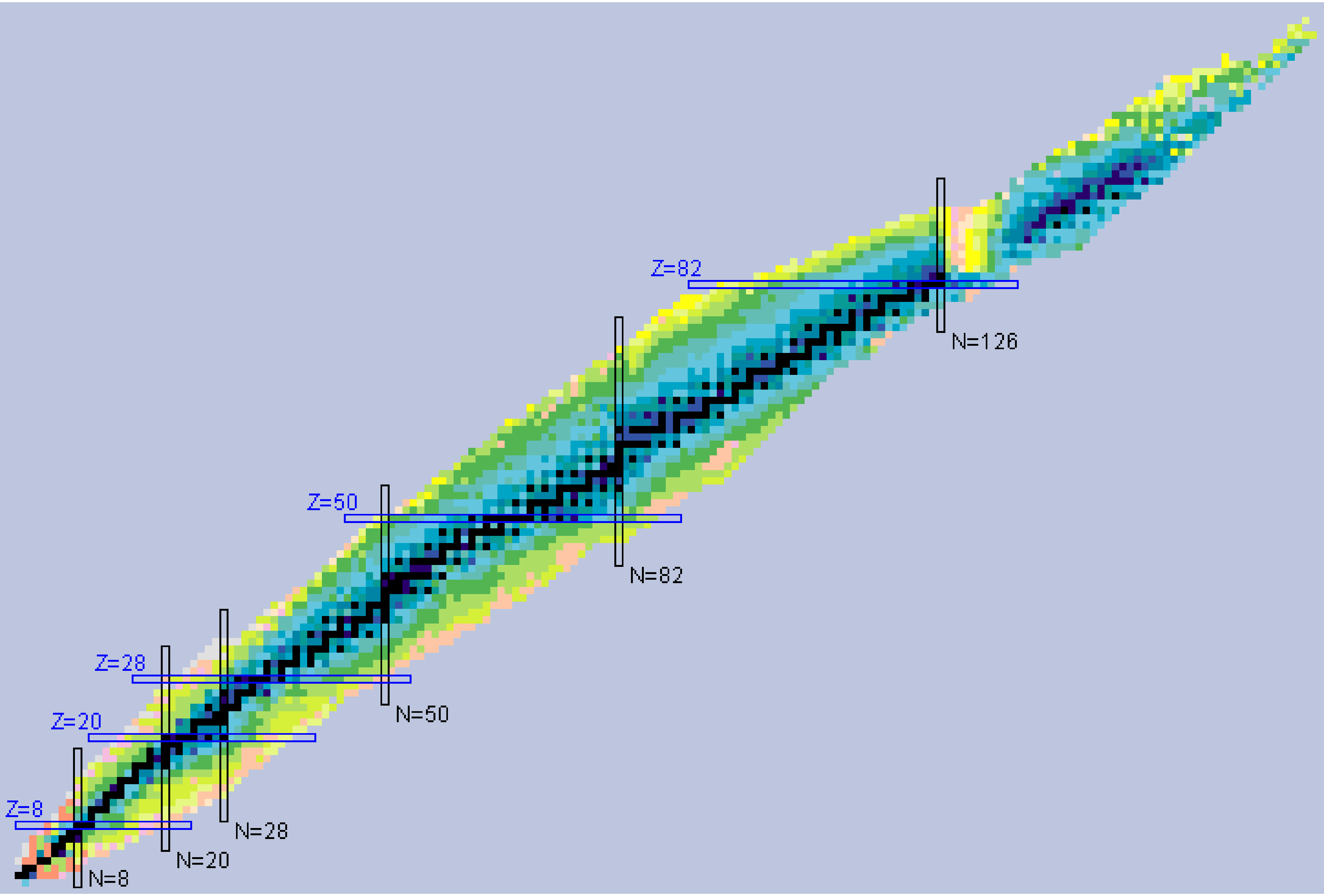


Results converged w.r.t size of model space

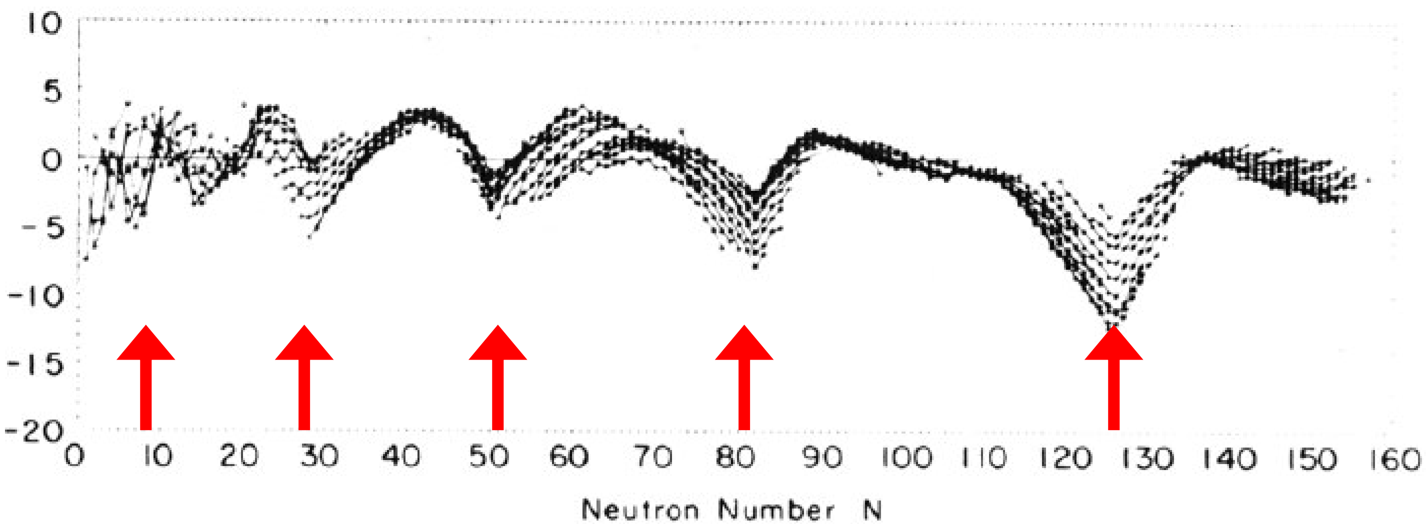
Excited 3^- state: 1p-1h, about 6MeV to high

Some deficiencies in form factor.

Three-nucleon force missing.

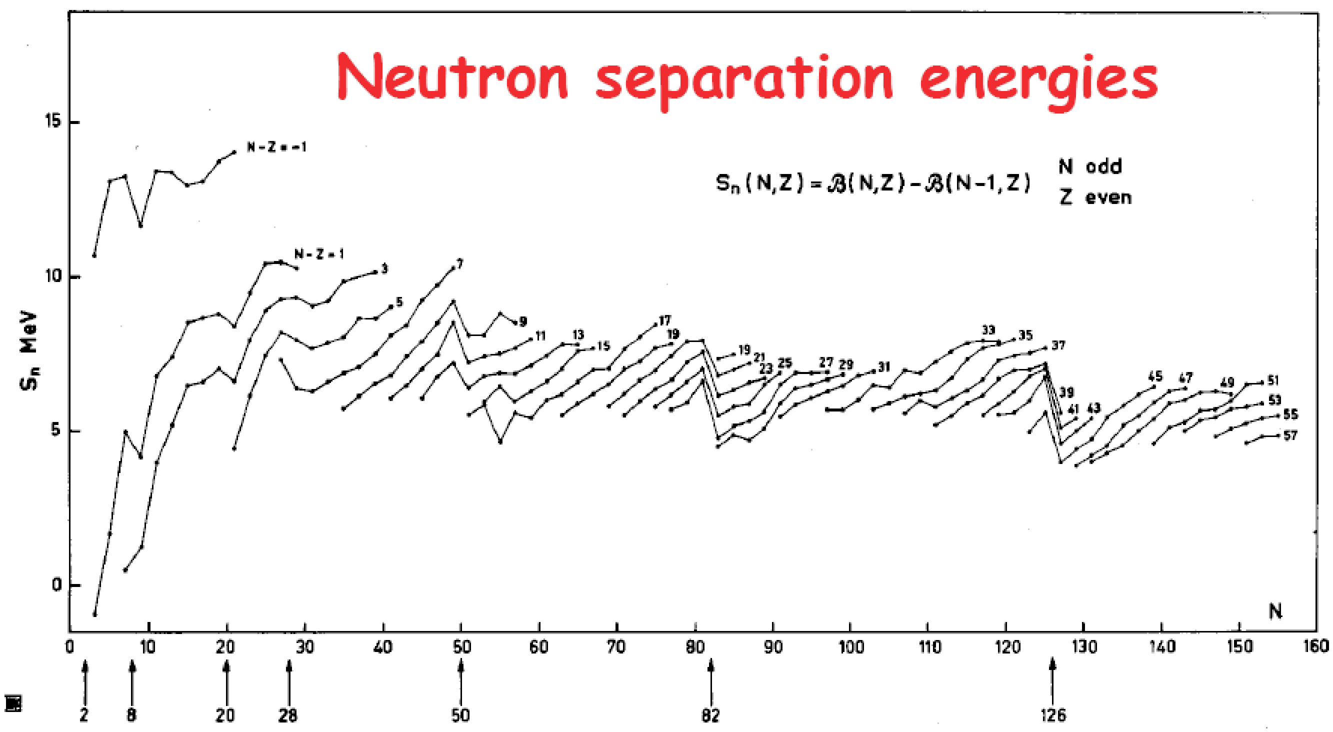

Z=82
N=126
N=82
Z=50
N=50
Z=28
Z=20
N=28
Z=8
N=20
N=8

Shell structure in nuclei



From W.D. Meyers and W.J. Swiatecki, Nucl. Phys. 81, 1 (1966).

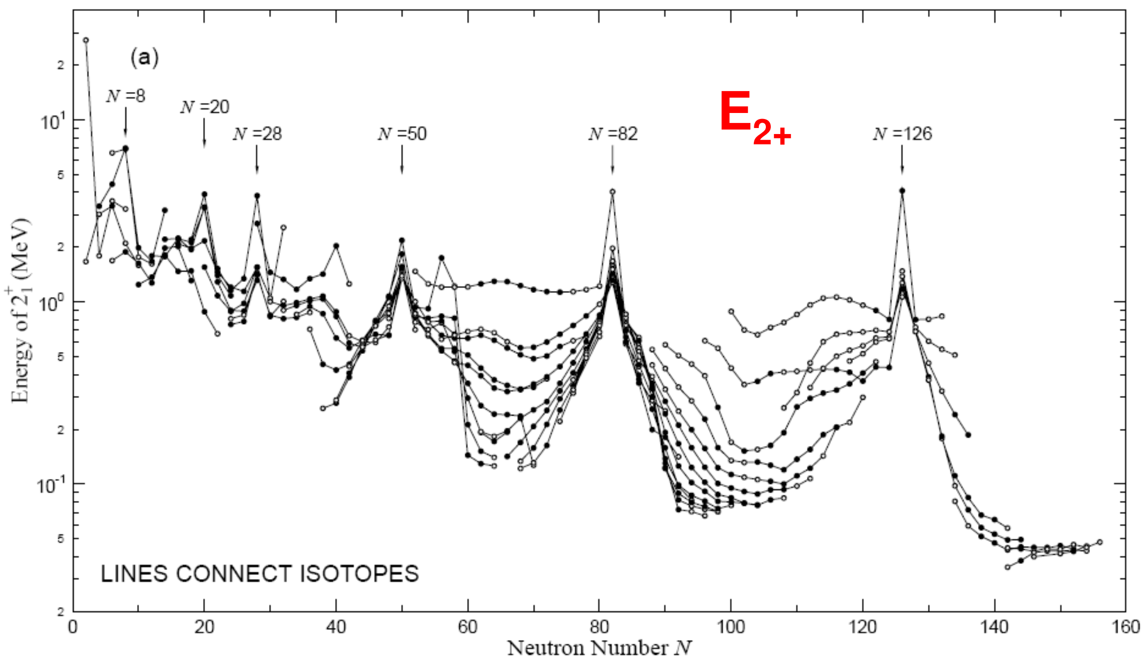
Mass differences: Liquid drop – experiment. Minima at closed shells.

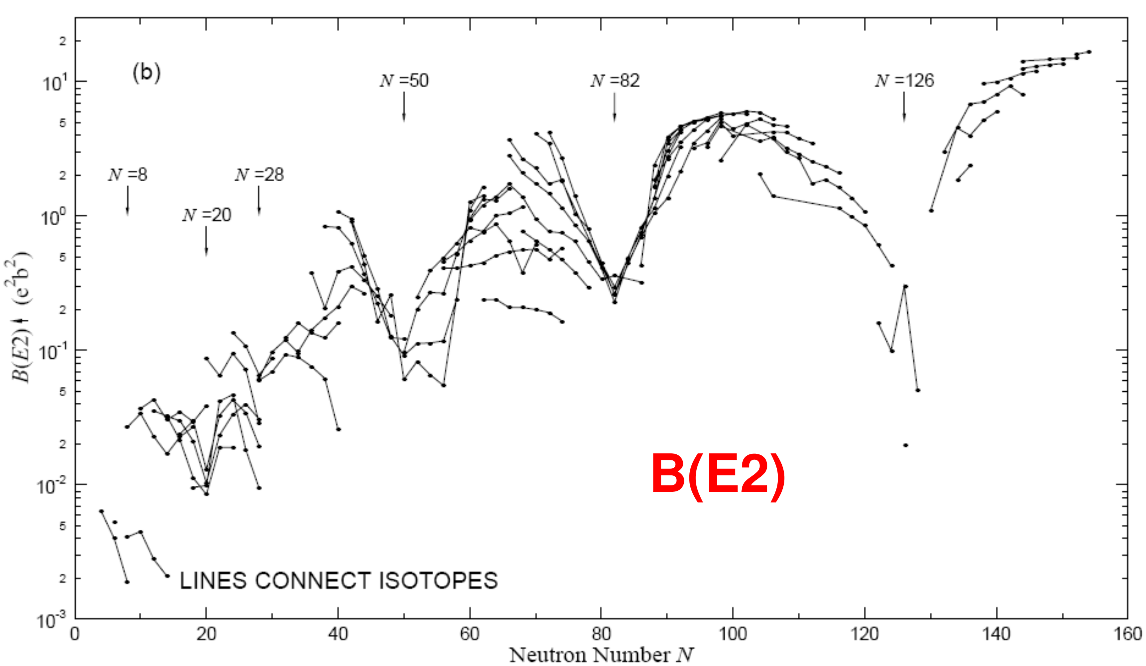


Relatively expensive to remove a neutron form a closed neutron shell.

Bohr & Mottelson, Nuclear Structure.

Shell structure cont'd





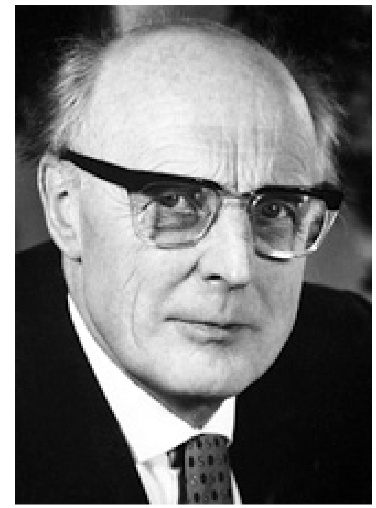
Nuclei with magic N

- Relatively high-lying first 2^+ exited state
- Relatively low B(E2) transition strength

S. Raman et al, Atomic Data and Nuclear Data Tables 78 (2001) 1.

1963 Nobel Prize in Physics

Maria Goeppert-Mayer

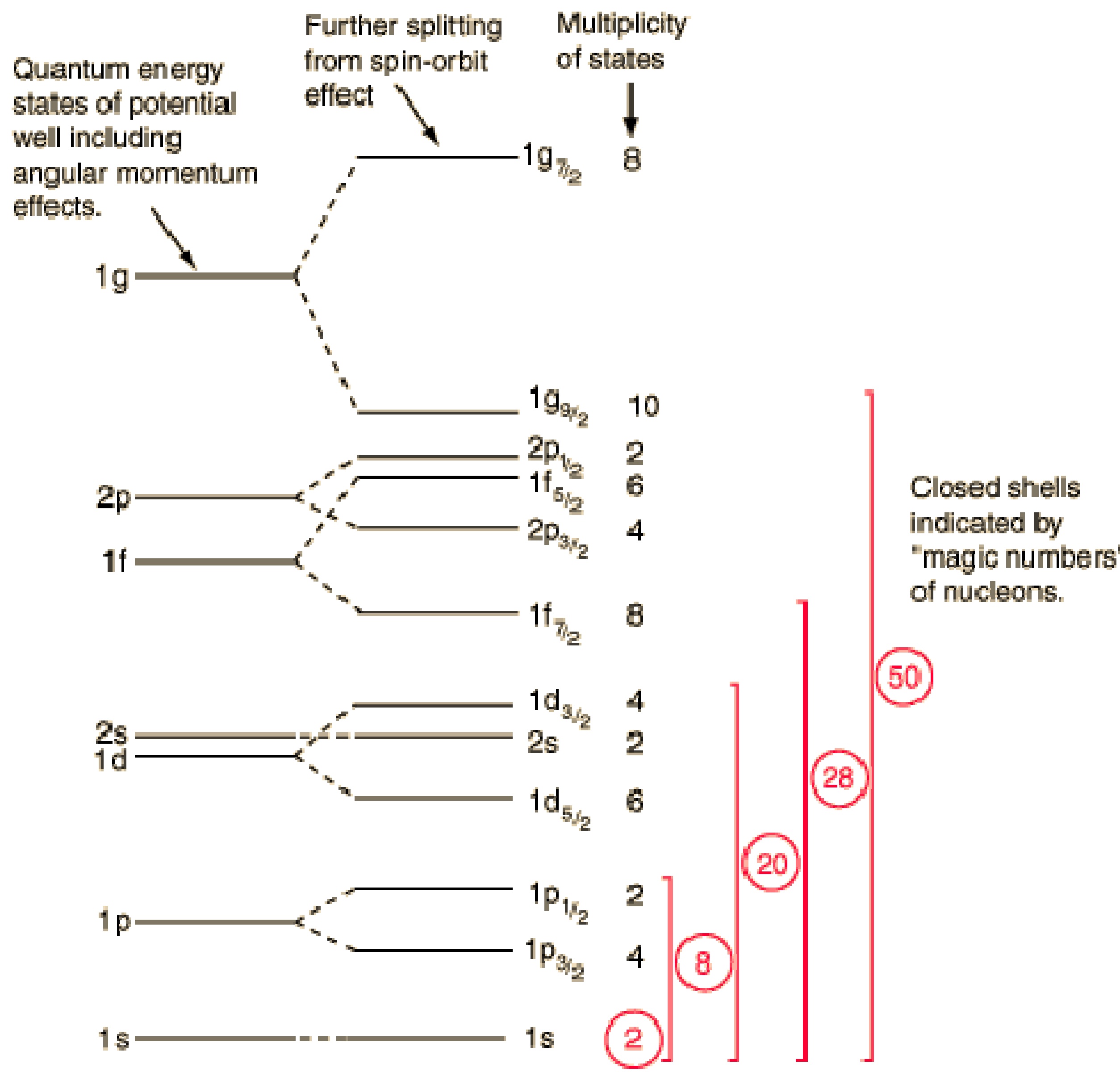


J. Hans D. Jensen

“for their discoveries concerning nuclear shell structure”

Magic numbers

Need spin-orbit force to explain magic numbers beyond 20.



http://hyperphysics.phy-astr.gsu.edu/hbase/nuclear/shell.html

Modification of shell structure at the drip lines!

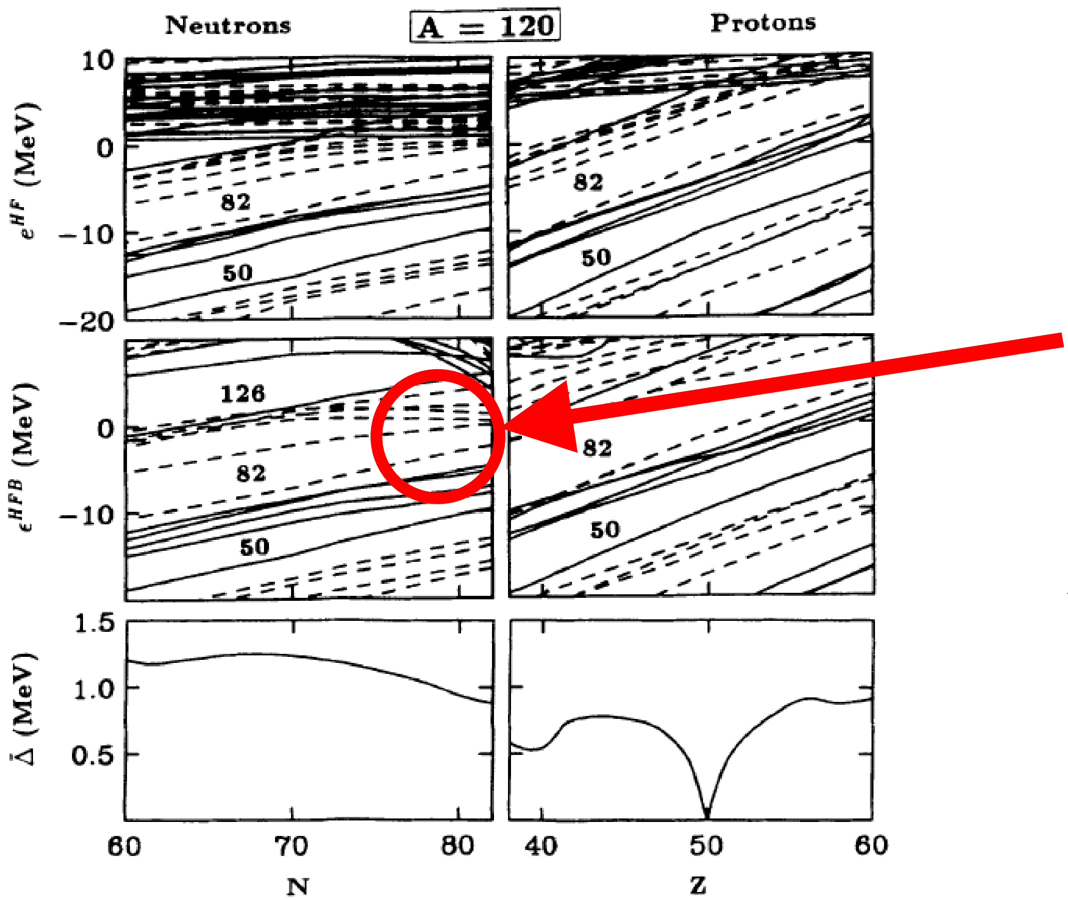


FIG. 3. Spherical single-particle levels for the A=120 isobars calculated in the SkP HF model (top) and SkP HFB model (middle) as a function of neutron number. The single-particle canonical HFB energies are given by $\epsilon_k = \langle \Psi_k | h | \Psi_k \rangle$. Solid (dashed) lines represent the orbitals with positive (negative) parity. The bottom portion shows the average neutron and proton gaps defined by $\bar{\Delta} = \int \Delta(\boldsymbol{r})\rho(\boldsymbol{r})d^3r / \int \rho(\boldsymbol{r})d^3r$.

J. Dobaczewski et al, PRL 72 (1994) 981.

Quenching of 82 shell gap when neutron drip line is approached.

Also observed in lighter nuclei

Caution: Shell structure seen in many observables.

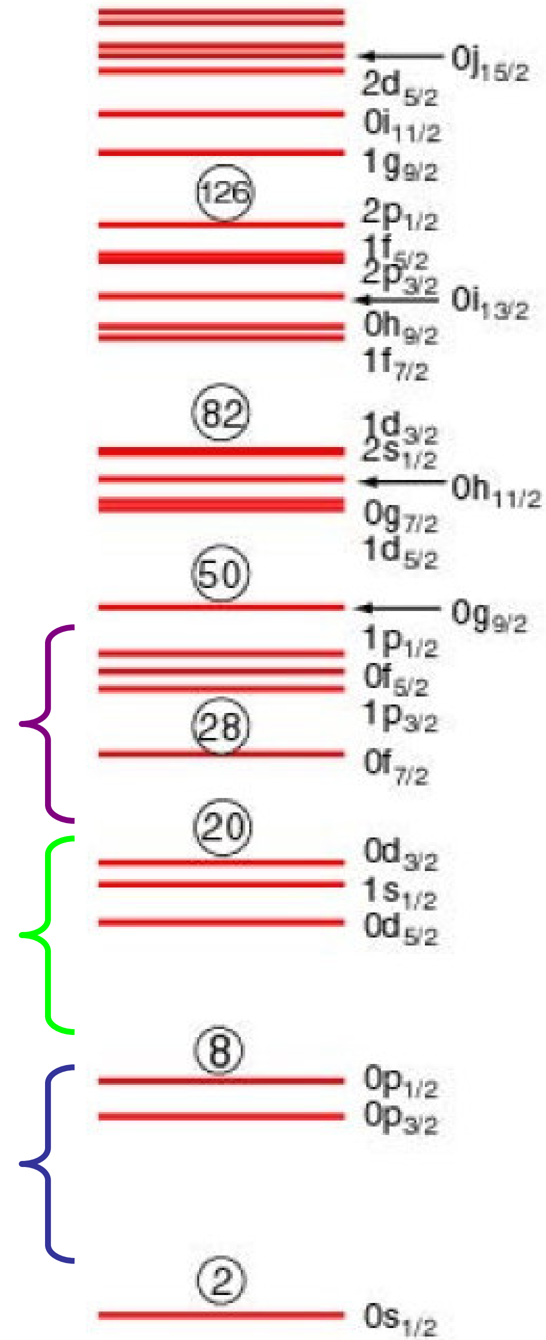
Traditional shell model

Main idea: Use shell gaps as a truncation of the model space.

- Nucleus (N,Z) = Double magic nucleus (N^*, Z^*)
  + valence nucleons ($N-N^*$, $Z-Z^*$)

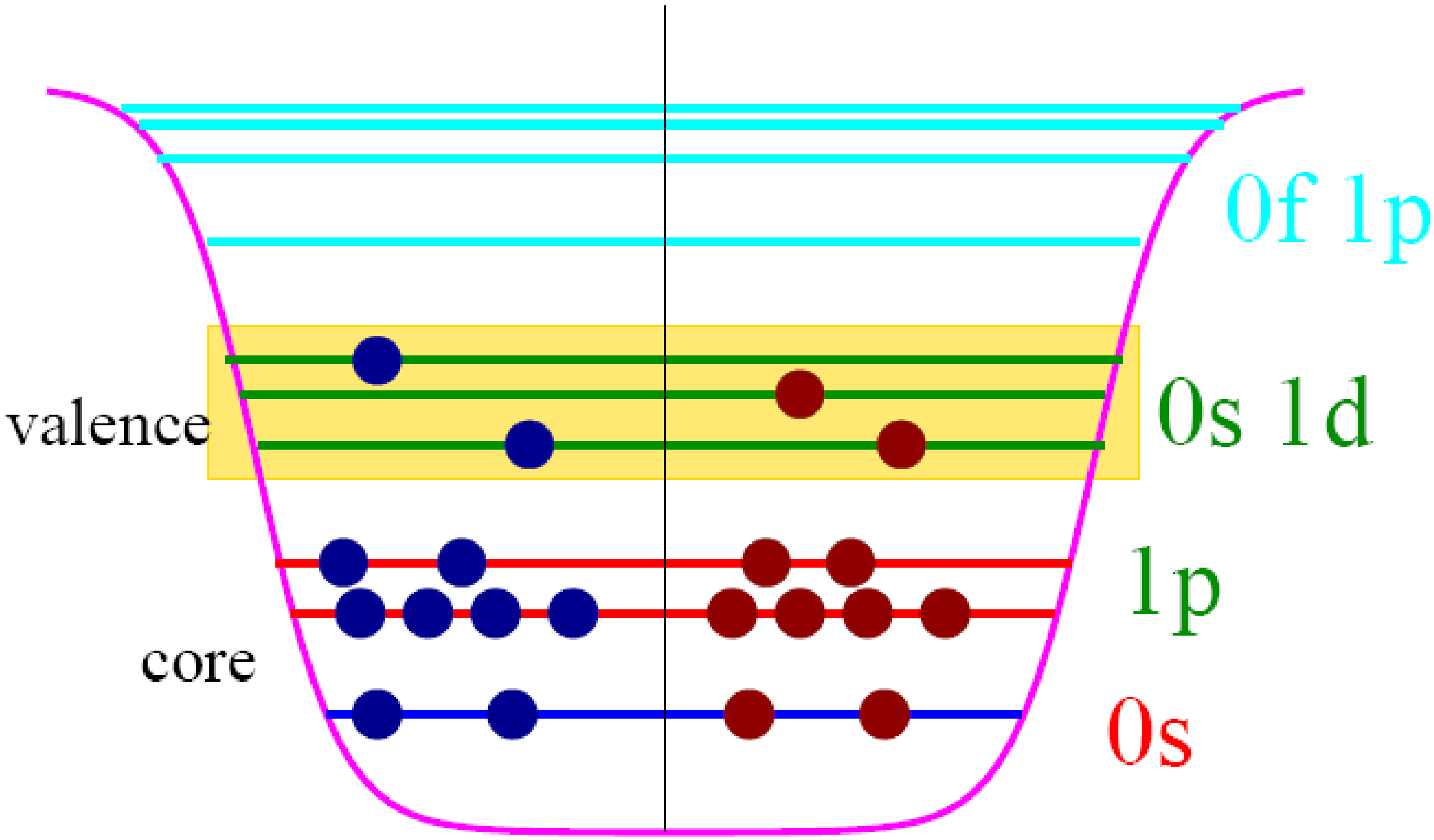
- Restrict excitation of valence nuclons to one oscillator shell.
  – Problematic: Intruder states and core excitations not contained in model space.

- Examples:
  - pf-shell nuclei: ^{40}Ca is doubly magic
  - sd-shell nuclei: ^{16}O is doubly magic
  - p-shell nuclei: ^{4}He is doubly magic



Shell model

Example: ^{20}Ne



Shell-model Hamiltonian

Hamiltonian governs dynamics of valence nucleons; consists of one-body part and two-body interaction:

$$\hat{H} = \sum_j \varepsilon_j \hat{a}_j^\dagger \hat{a}_j + \sum_{JTj_1j_2j_1'j_2'} \langle j_1 j_2 | \hat{V} | j_1' j_2' \rangle_{JT} \hat{A}^\dagger_{JT;j_1j_2} \hat{A}_{JT;j_1'j_2'}$$

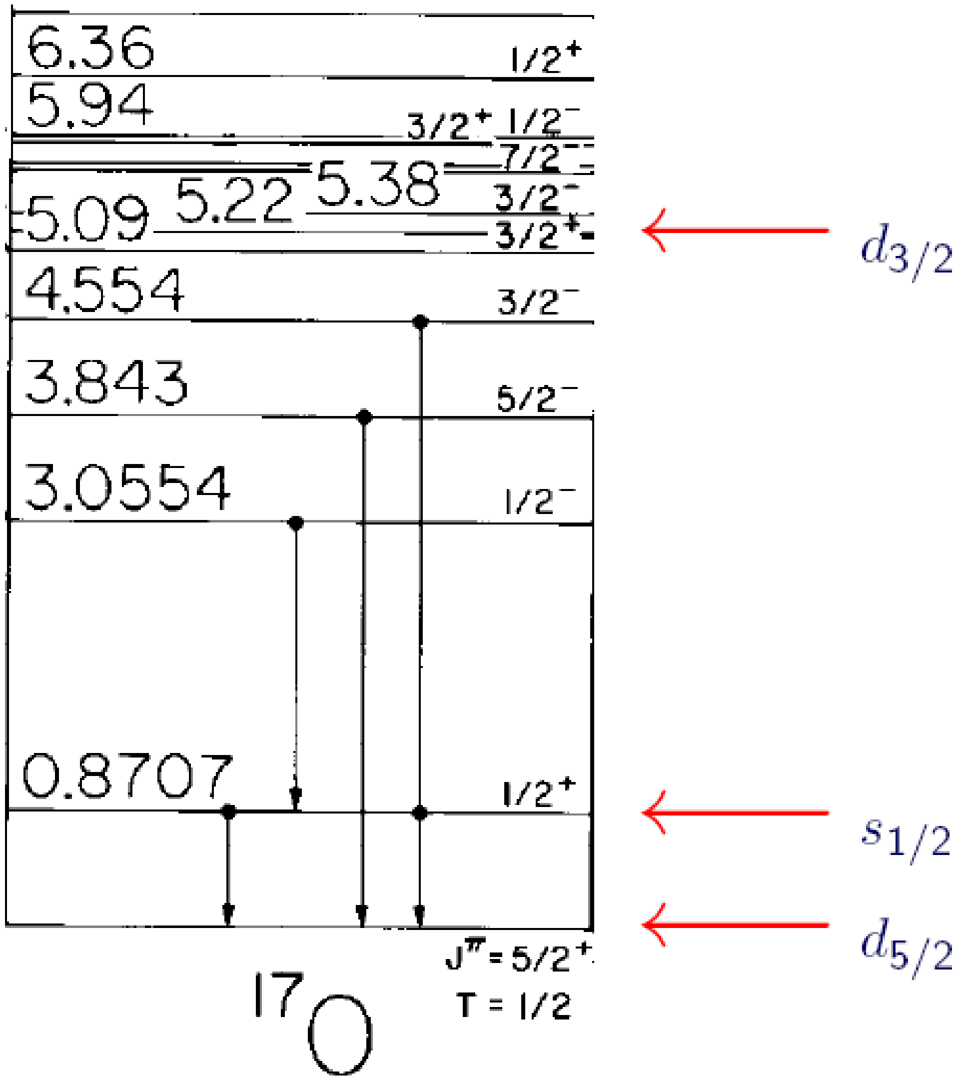
Single-particle energies (SPE)

Two-body matrix elements (TBME) coupled to good spin and isospin

Annihilates pair of fermions

Q: How does one determine the SPE and the TBME?

Empirical determination of SPE and TBME



- Determine SPE from neighbors of closed shell nuclei having mass

  A = closed core +1

- Determine TBME from nuclei with mass

  A = closed core + 2.

- The results of such Hamiltonians become inaccurate for nuclei with a larger number of valence nucleons.
- Thus: More theory needed.

Effective shell-model interaction: G-matrix

- Start from a microscopic high-precision two-body potential
- Include in-medium effects in G-matrix
- Bethe-Goldstone equation

Pauli operator blocks occupied states (core)

$$G = V + V \frac{Q_P}{E - H_0} G$$

microscopic bare interaction

Single-particle Hamiltonian

- Formal solution:

$$G = \frac{V}{1 - V Q_P / (E - H_0)}$$

- Properties: in-medium effects renormalize hard core.
- But: The results of computations still disagree with experiment.

See, e.g. M. Hjorth-Jensen et al, Phys. Rep.261 (1995) 125.

Further empirical adjustments are necessary

Two main strategies

1. Make minimal adjustments only. Focus on monopole TBME:

$$V_{T;j_1,j_2} \propto \sum_J (2J+1) \langle j_1 j_2 | V | j_1 j_2 \rangle_{JT}$$

- Rationale:
  - Monopole operators are diagonal in TBME.
  - Set scale of nuclear binding.
  - Sum up effects of neglected three-nucleon forces.

2. Make adjustments to all linear combinations of TBME that are sensitive to empirical data (spectra, transition rates); keep remaining linear combinations of TBME from G-matrix.

- Rationale:
  - Need adjustments in any case.
  - Might as well do best possible tuning.

Two-body G-matrix + monopole corrections

G-matrix and monopole adjustments compared to experiment.

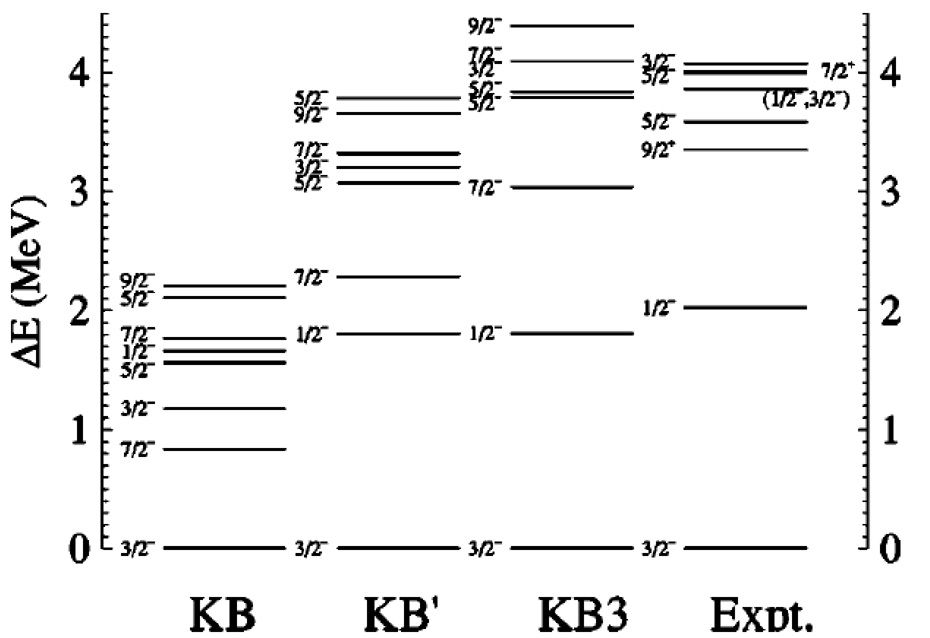


FIG. 18. The level scheme of ^{49}Ca obtained with the interactions KB, KB′, and KB3, compared to the experimental result.

Martinez-Pinedo et al, PRC 55 (1997) 187.

Monopole corrections capture neglected three-body physics.

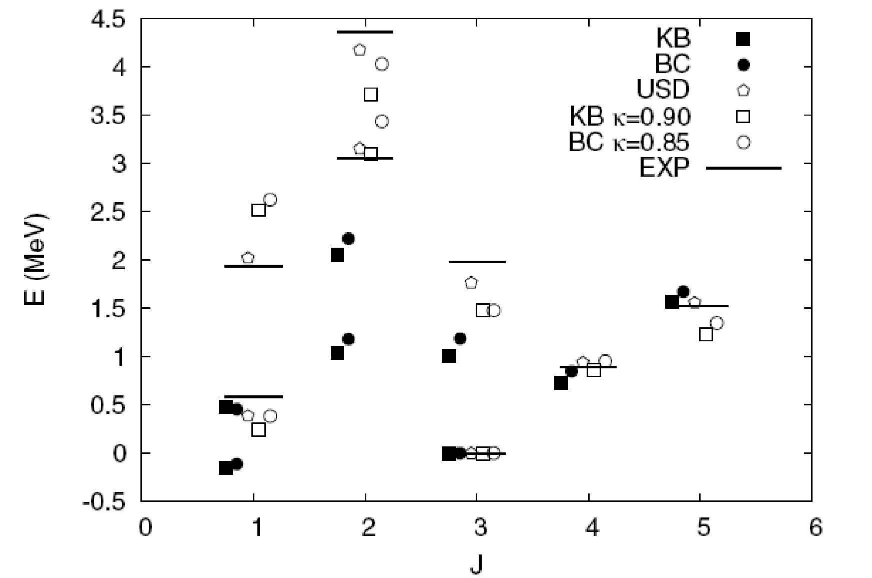


FIG. 2. Excitation energies for ^{22}Na referred to the $J = 3$ lowest state. See text.

A. P. Zuker, PRL 90 (2003) 42502.

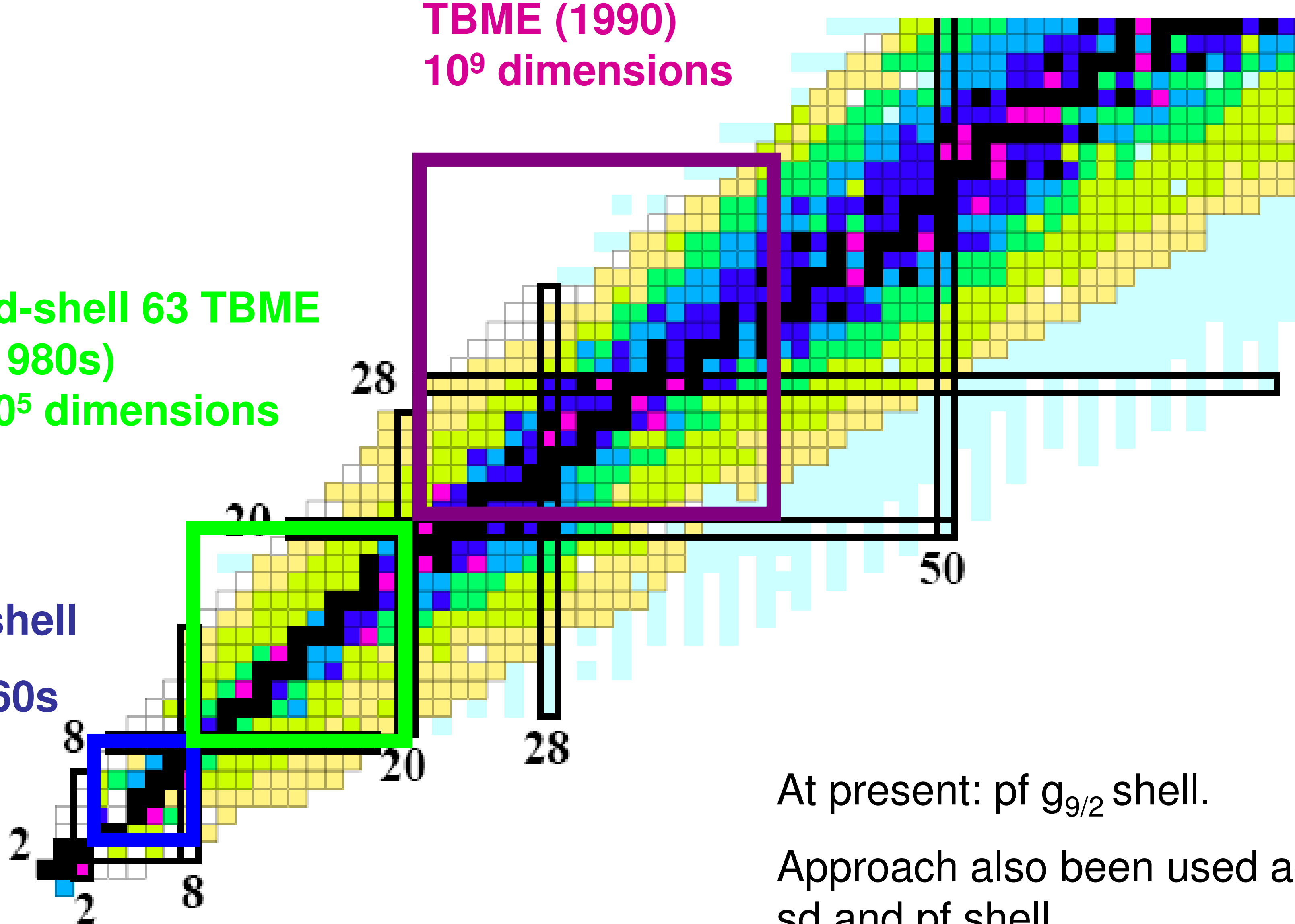
Semi-empirical interactions for the nuclear shell model

pf-shell ~200 TBME (1990)
10^9 dimensions

sd-shell 63 TBME (1980s)
10^5 dimensions

p-shell

1960s



At present: pf $g_{9/2}$ shell.

Approach also been used across sd and pf shell.

Shell-model computations

1. Construct Hamiltonian matrix
2. Use Lanczos algorithm to compute a few low-lying states.
3. Problem: rapidly increasing matrix dimensions

Publicly available programs

- Oxbash (MSU)
- Antoine (Strasbourg)

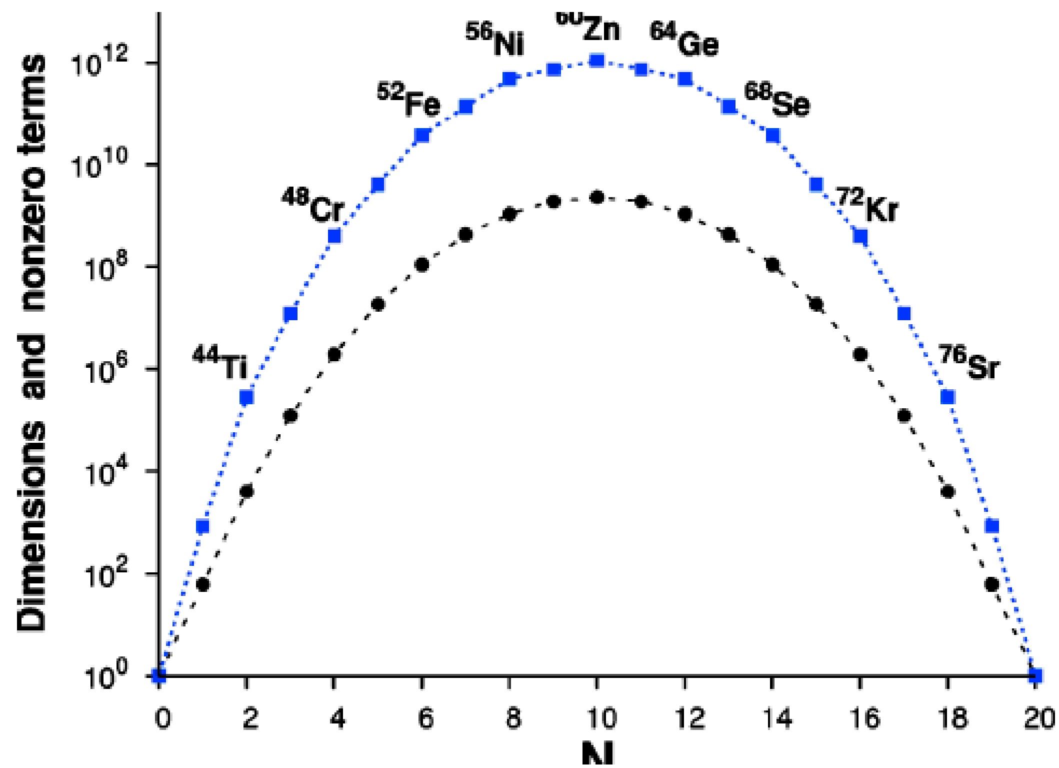
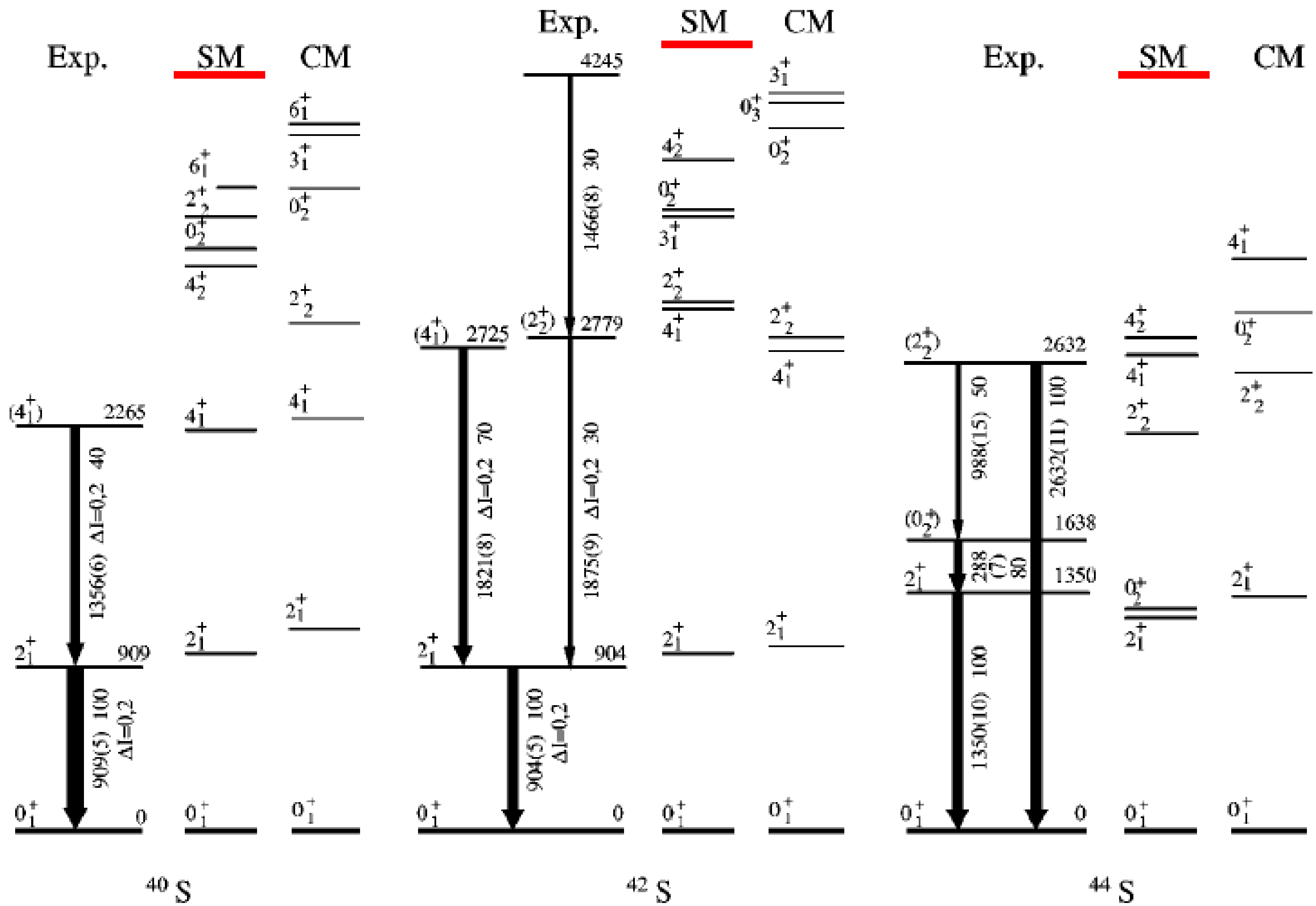


FIG. 7. (Color in online edition) m-scheme dimensions (circles) and total number of nonzero matrix elements (squares) in the pf shell for nuclei with $M=T_z=0$ as a function of neutron number N. The dotted and dashed lines serve as guides for the eye.

Caurier et al, Rev. Mod. Phys. 77 (2005) 427.

Results of shell-model calculations



Spectra and transition strengths suggests that N=28 Nucleus ^{44}S exhibits shape mixing in low excited states → erosion of N=28 shell gap.

Sohler et al, PRC 66 (2002) 054302.

Shell-model results for neutron-rich pf-shell nuclei.

Subshell closure at neutron number N=32 in neutron rich pf-shell nuclei (enhanced energy of excited 2^+ state).

No new N=34 subshell.

S. N. Liddick et al, PRL 92 (2004) 072502.

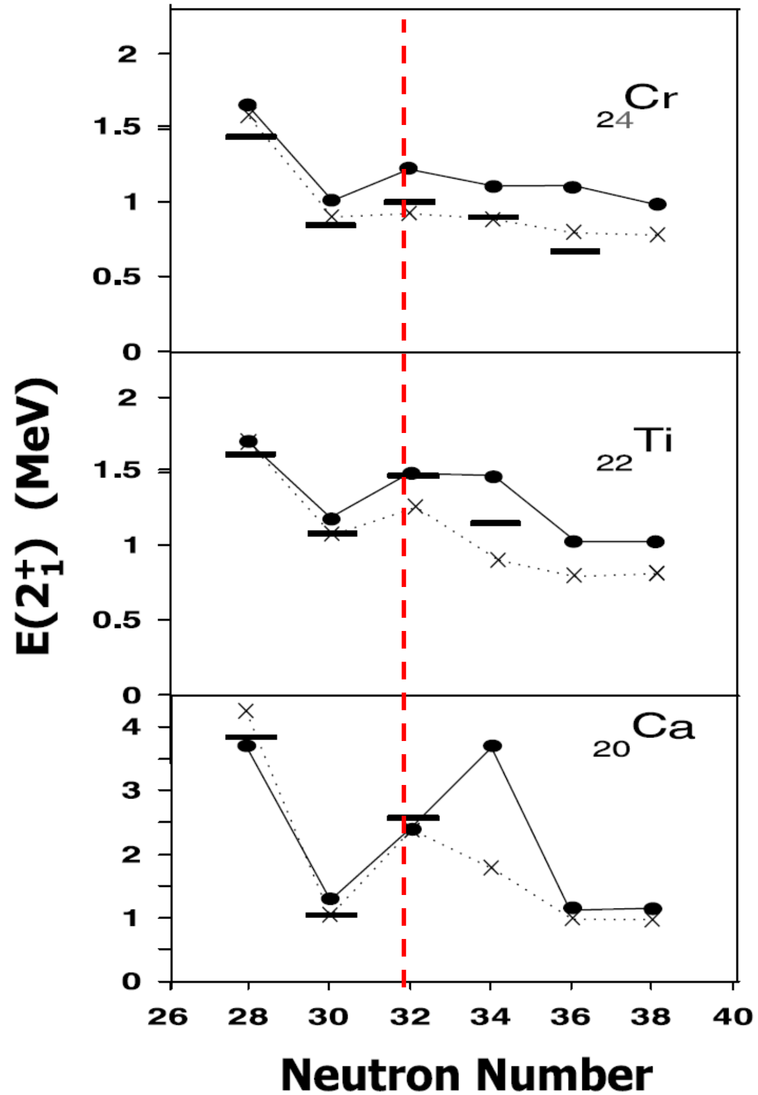


FIG. 3. $E(2_1^+)$ values versus neutron number for the even-even $_{24}$Cr, $_{22}$Ti, and $_{20}$Ca isotopes. Experimental values are denoted by dashes. Shell model calculations using the GXPF1 [14] and KB3G [22] interactions are shown as filled circles and crosses, respectively.

Summary

- Shell model a powerful tool for understanding of nuclear structure.
- Shell quenching / erosion of shell structure observed when drip lines are approached.
- Shell model calculations based on microscopic interactions
  - Adjustments are needed
  - Due to neglected three body forces (?!)
- Effective interactions have reached maturity to make predictions, and to help understanding experimental data.