Workshop for young scientists with research interests focused on physics at FAIR
14-19 February 2016
Garmisch-Partenkirchen

Large-scale configuration interaction description

of the structure of heavy nuclei around ^{100}Sn and ^{208}Pb

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Thanks to
R. Liotta, R. Wyss, T. Bäck, A. Johnson, B. Cederwall (KTH)
Liyuan Jia, Guanjian Fu (Shanghai)

Modeling the Atomic Nucleus

The nucleus as a self-organized (not so) many-body system

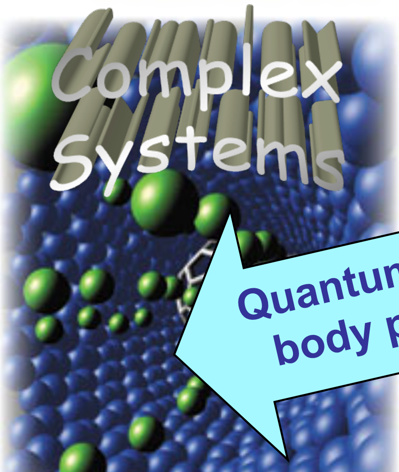
How does it organize itself and what phenomena emerge?

The limit of its existence?

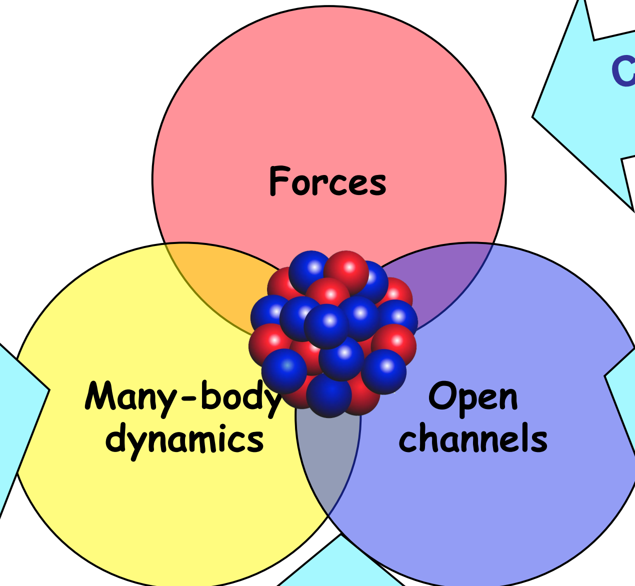
Pflops..

Computational physics

nano…

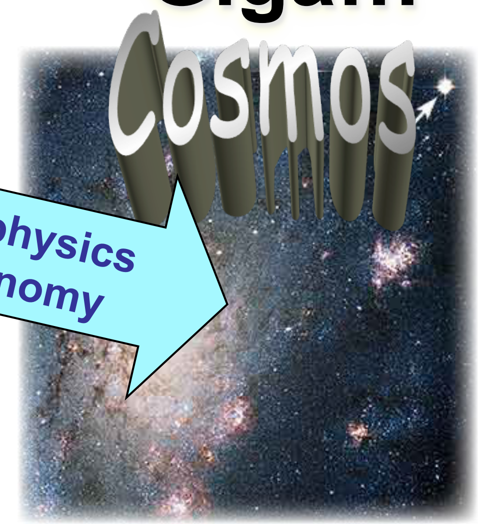


Quantum many-body physics

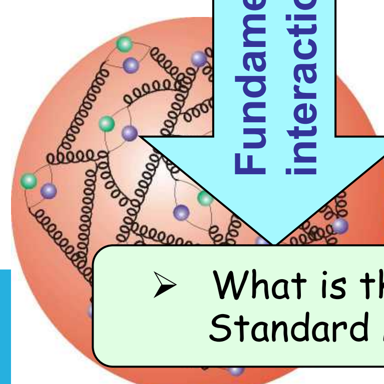


Astrophysics Astronomy

Giga…



Fundamental interactions



- How do collective phenomena **emerge** from simple constituents?
- How can complex systems display astonishing simplicities?
- What are unique properties of **open** systems?

- What is the New Standard Model?

- How do nuclei shape the physical universe?
- What is the origin of the elements?

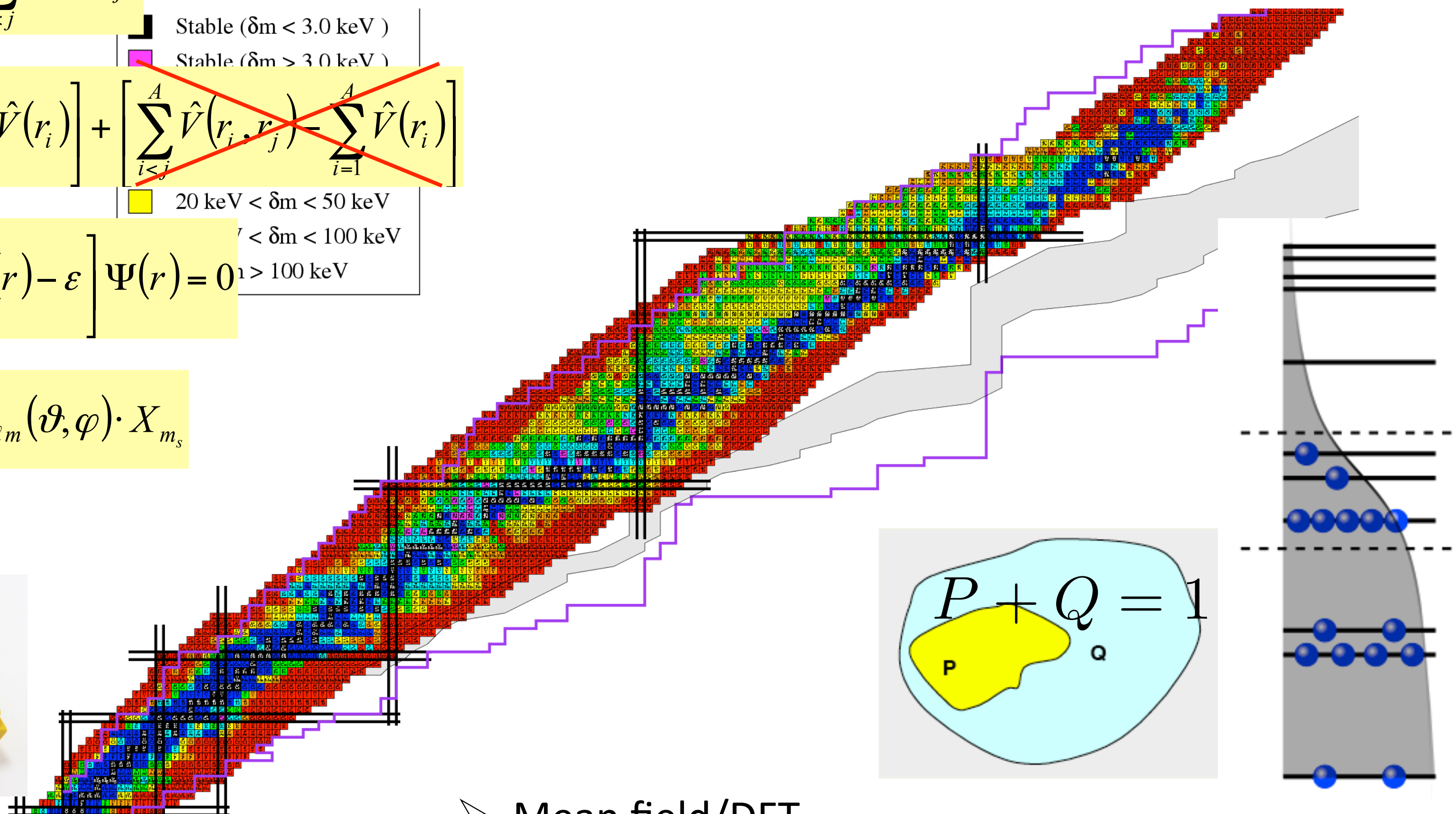
Nuclear theory: guiding principles
The quest for the mean field

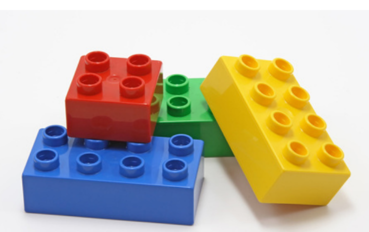
$$\hat{H} = \sum_{i=1}^{A} \frac{\hat{p}_i^2}{2m_i} + \sum_{i<j}^{A} \hat{V}(r_i, r_j)$$

$$\hat{H} = \sum_{i=1}^{A} \left[\frac{\hat{p}_i^2}{2m_i} + \hat{V}(r_i) \right] + \left[\cancel{\sum_{i<j}^{A} \hat{V}(r_i, r_j) - \sum_{i=1}^{A} \hat{V}(r_i)} \right]$$

$$\left[-\frac{\hbar^2}{2 \cdot m} \nabla^2 + V(r) - \varepsilon \right] \Psi(r) = 0$$

$$\Psi(r) = \frac{u_\ell(r)}{r} \cdot Y_{\ell m}(\vartheta, \varphi) \cdot X_{m_s}$$





CAUTION:
Building blocks are neutron and protons

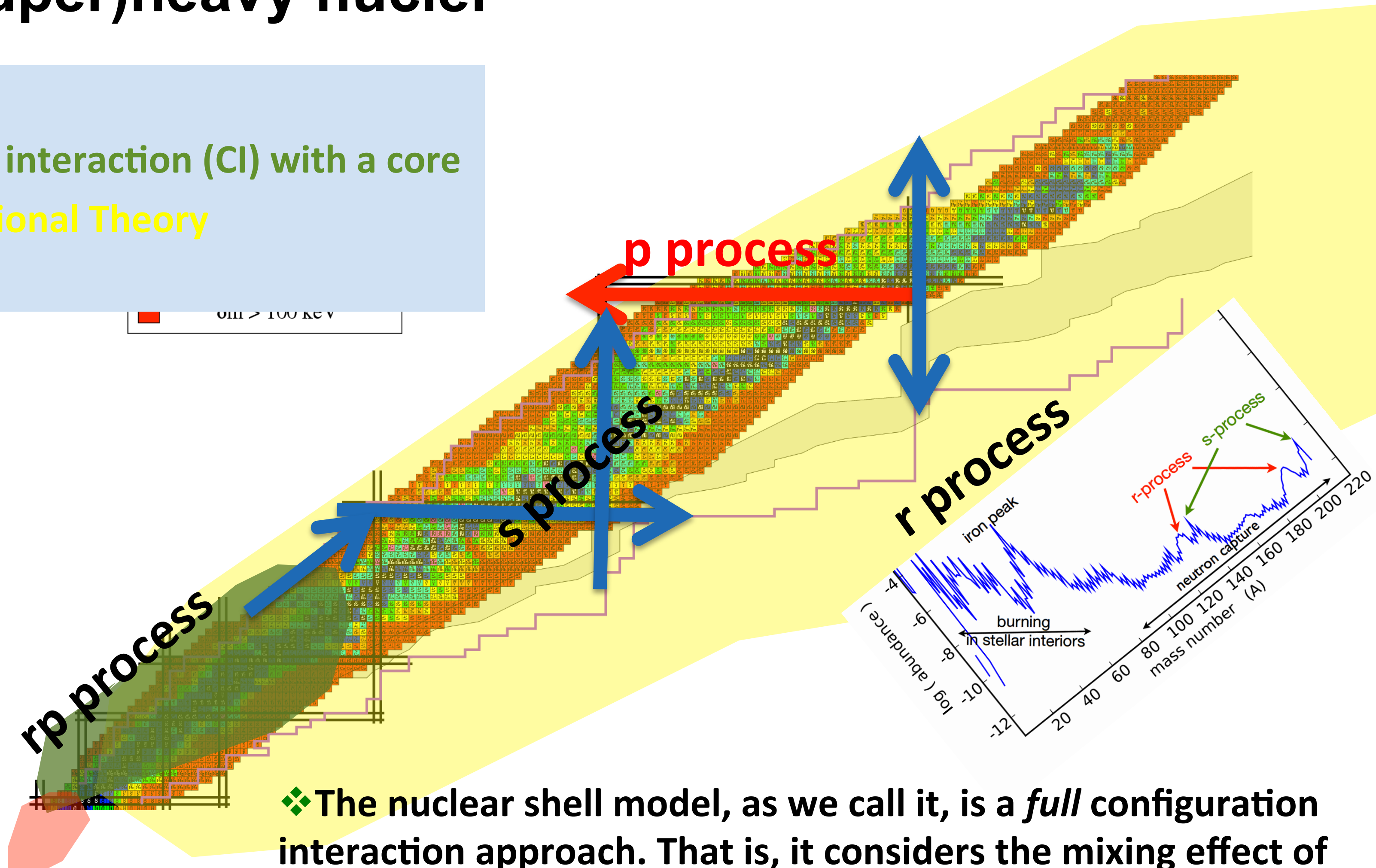
- Mean field/DFT
  plus pairing (BCS, HFB, EP)
- Shell model
  SPE+Monpole+Correlation (Pairing, QQ correlation)
- Ab initio approaches

Motivation
microscopic shell-model description of (super)heavy nuclei

Ab initio

Configuration interaction (CI) with a core

Density Functional Theory



- The nuclear shell model, as we call it, is a *full* configuration interaction approach. That is, it considers the mixing effect of all possible configurations within a given model space.
- The most accurate and precise theory on the market. But there is a price to pay

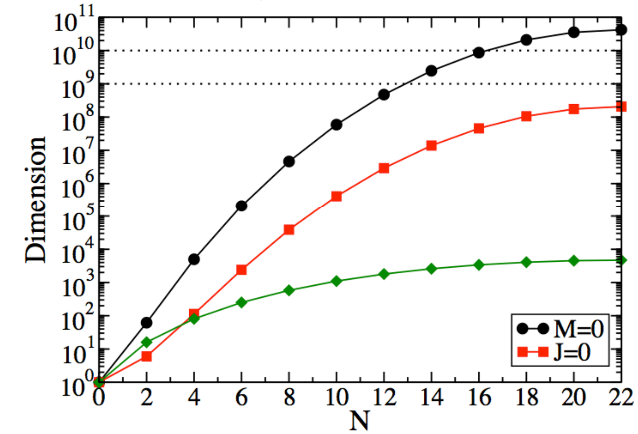
Conjugate Gradient Solver for Lattice QCD

$$Ax=b$$

Lanczos approach for CI

$$Ax=\lambda x$$

Pb isotopes below N=126



Usually the Lanczos iteration approach is used for the diagonalization since we only need the lowest a few eigenstates

- H operation enhances low-lying components.

$$|\psi_0\rangle, H|\psi_0\rangle, H^2|\psi_0\rangle, H^3|\psi_0\rangle, \cdots$$

$$|\psi_k\rangle \equiv \frac{1}{N_k} H^k |\psi_0\rangle$$

$$|\psi_0\rangle, |\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, \cdots$$

- We diagonalize the hamiltonian by these basis vectors.
- As these vectors are non-orthgonal, we orthogonalize them.
- These vectors are called Lanczos vectors.

- Lanczos method can covert original matrix to tridiagonal one, which is easily diagonalized.

$$H \longrightarrow \begin{pmatrix} \alpha_1 & \beta_1 & & & & \\ \beta_1 & \alpha_2 & \beta_2 & & & \\ & \beta_2 & \alpha_3 & \beta_3 & & \\ & & \beta_3 & \alpha_4 & \beta_4 & \\ & & & \beta_4 & \alpha_5 & \beta_5 \\ & & & & \beta_5 & \alpha_6 \end{pmatrix}$$

$$|\phi_{L+1}\rangle = H|\phi_L\rangle - \alpha_L|\phi_L\rangle - \beta_L|\phi_{L-1}\rangle$$

$$\alpha_L = \langle \phi_L | H | \phi_L \rangle$$

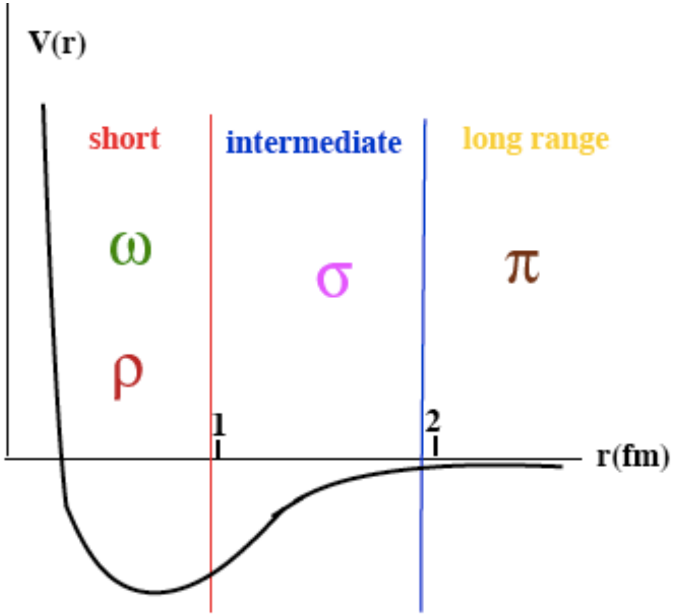
$$\beta_L = \langle \phi_{L-1} | H | \phi_L \rangle$$

$$E_1>E_2>E_3>E_4>E_5>E_6$$

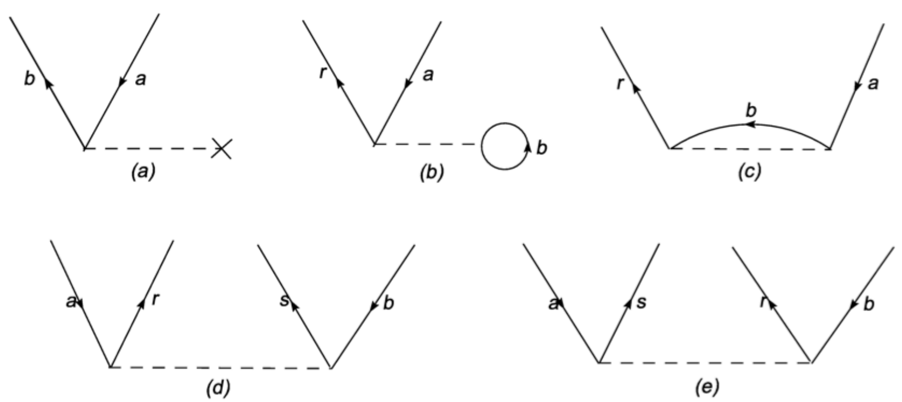
- Ground state energy can be obtained by L Lanczos vectors. We consider convergence of ground state energy as a function of L.

“Bare” Nucleon-Nucleon Potentia

- Argonne V18: PRC 56, 1720 (1997)
- CD-Bonn 2000: PRC 63, 024001 (2000)
- *N³LO: PRC 68, 041001 (2003)*
- *INOY: PRC 69, 054001 (2004)*



Perturbation treatment



and many others.
Usually we stop at the second or third order

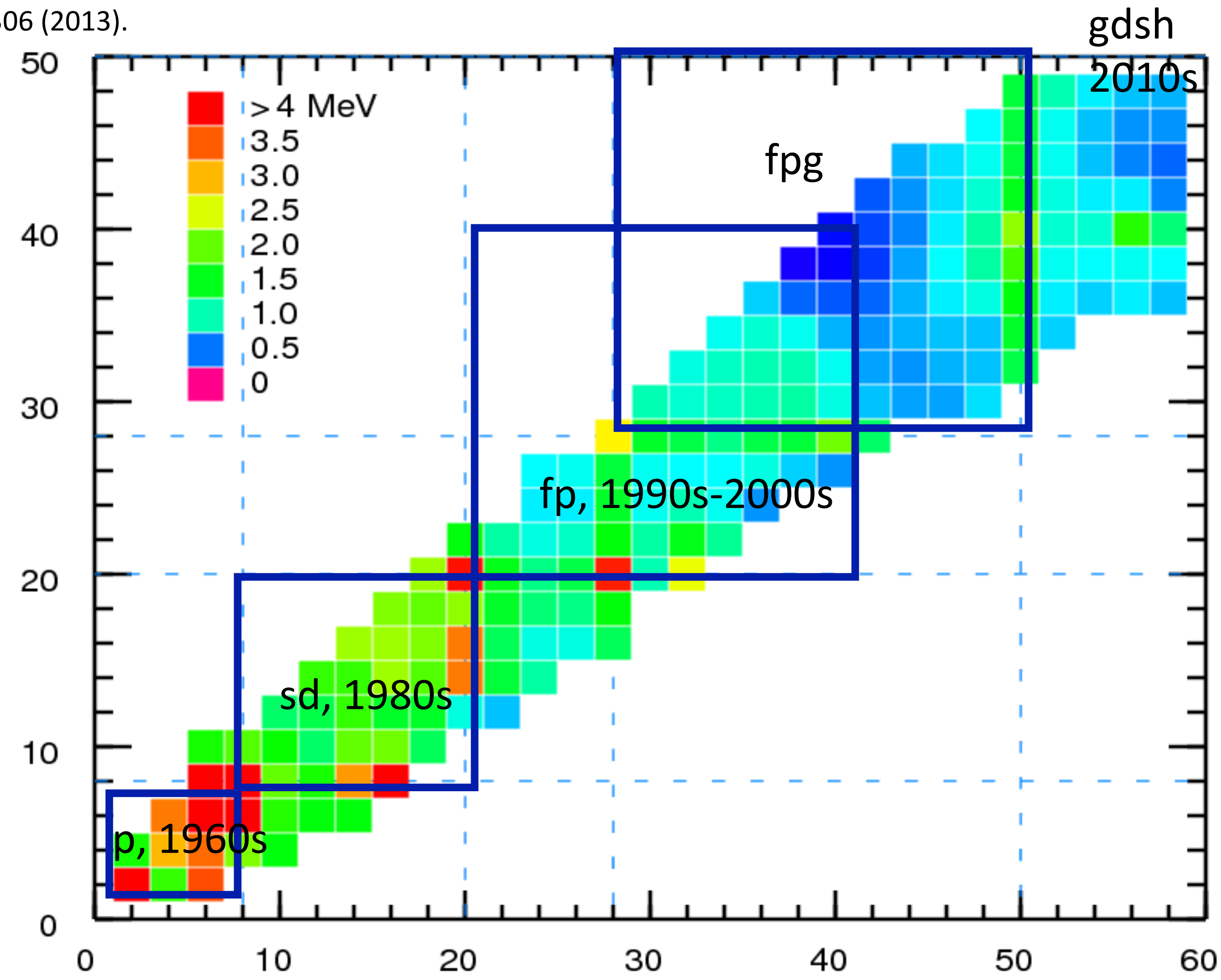
Quest of the effective interaction

◆Empirical effective interaction

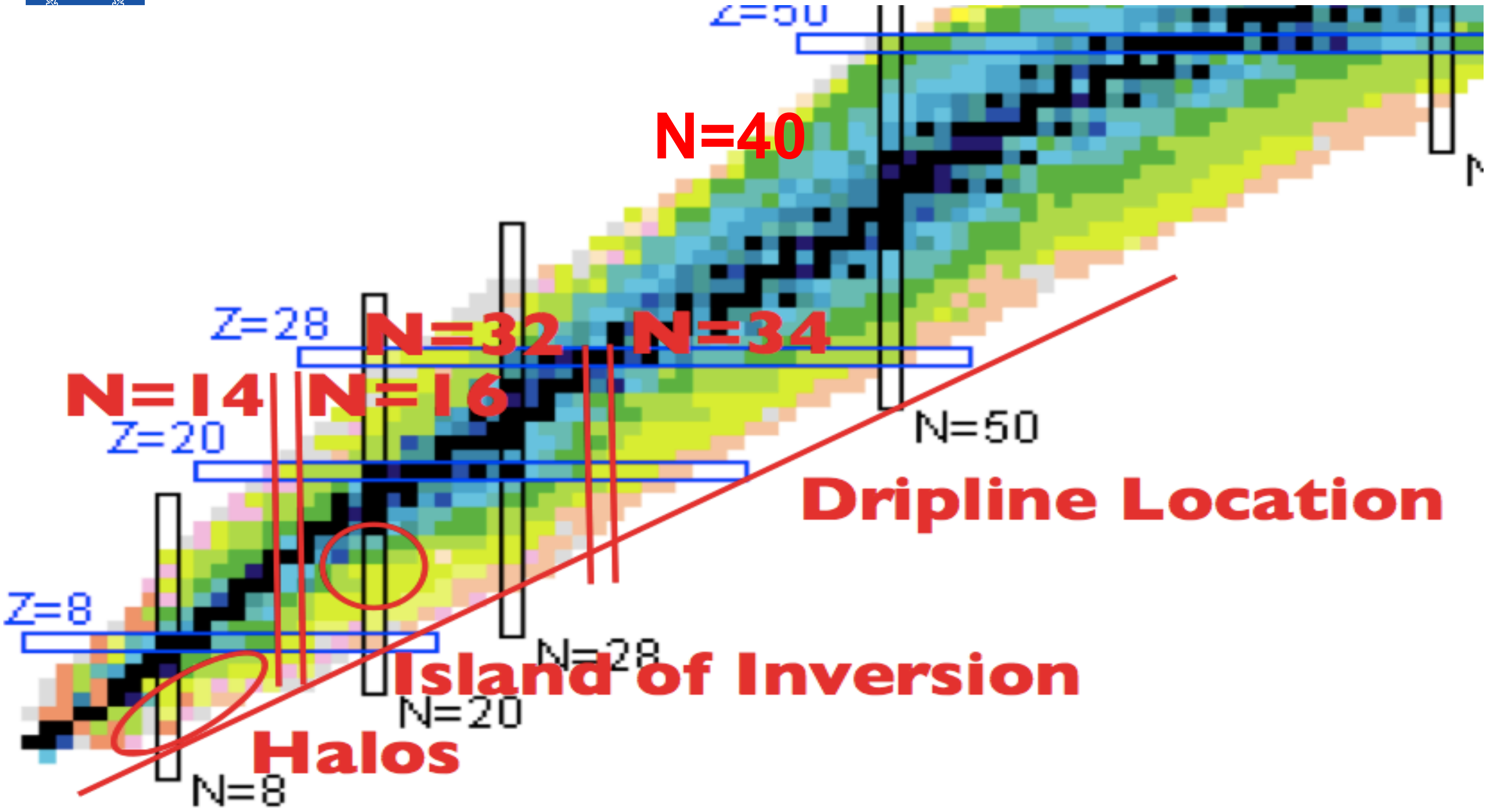
❖USD, B. A. Brown and W. A. Richter, Phys. Rev. C 74, 034315 (2006).
❖fp (KB3, gxpf), 1990s
❖fpg, M. Honma et al., Phys. Rev. C 80, 064323 (2009)
❖**gdsh, CQ, Z. Xu, Phys. Rev. C 86, 044323 (2012)**
❖**Cross-shell fpg+gdsh to understand the effect of the N=50 shell**
T. Bäck, CQ et al.PRC 87, 031306 (2013).

One has to consider:

- The core polarization effects induced by the assumed inert core
- Optimization of the monopole interaction due to the neglect of three-body and other effects



1D to 2D shell structure
Shell evolution at drip lines

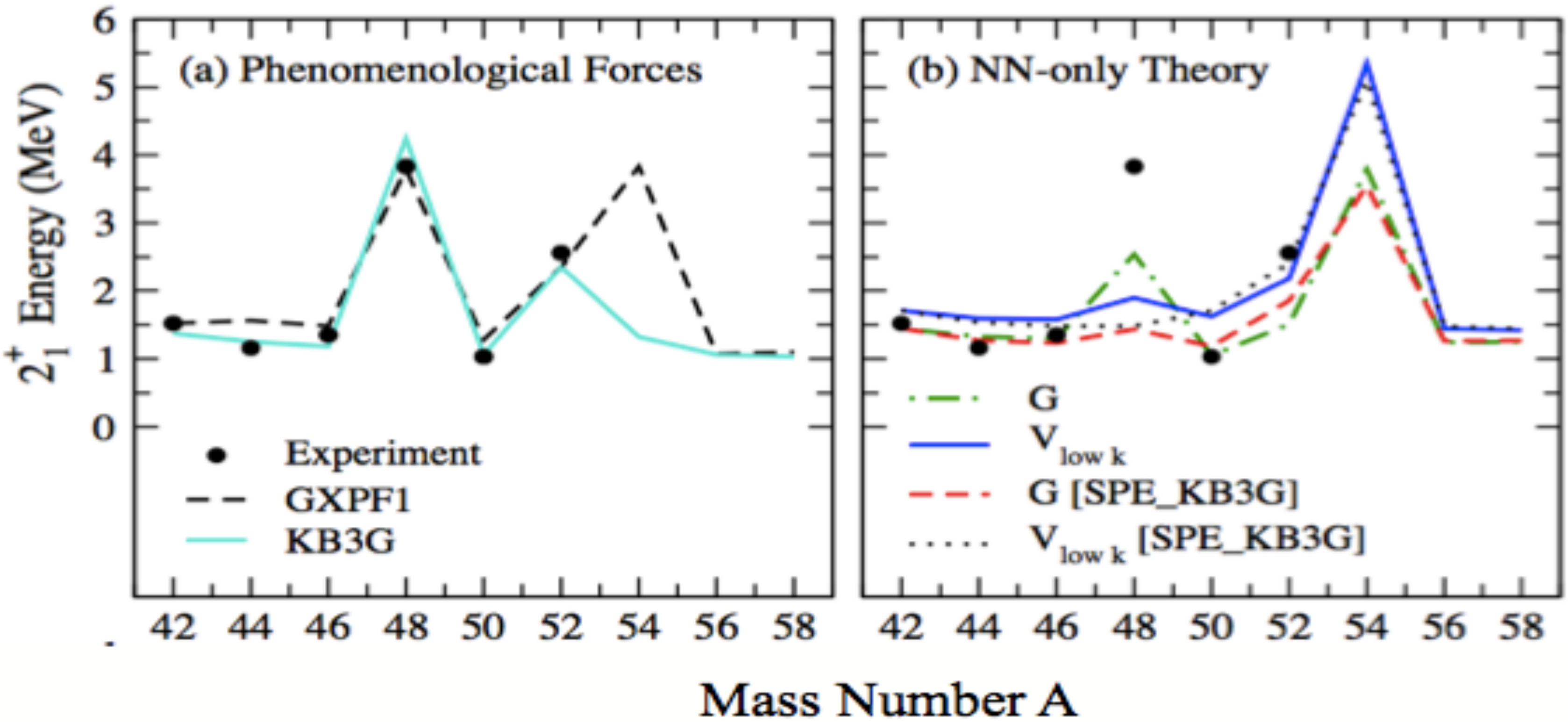


O. Sorlin, M.-G. Porquet, Prog. Part. Nucl. Phys. 61, 602 (2008).

Z. Xu, CQ, Phys. Lett. B (2013)

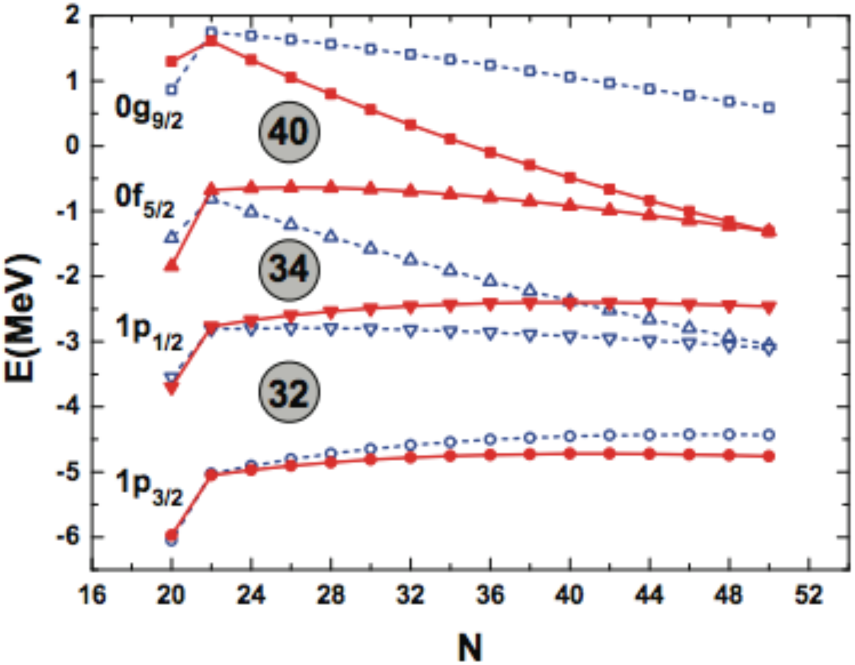
Shell model predictions for the 2+ energies,

which are one of the key quantities for determining the shell gap



With four parameters I can fit an elephant, and with five I can make him wiggle his trunk.
--John von Neumann

Single-particle structure of Ca isotopes



Binding energy

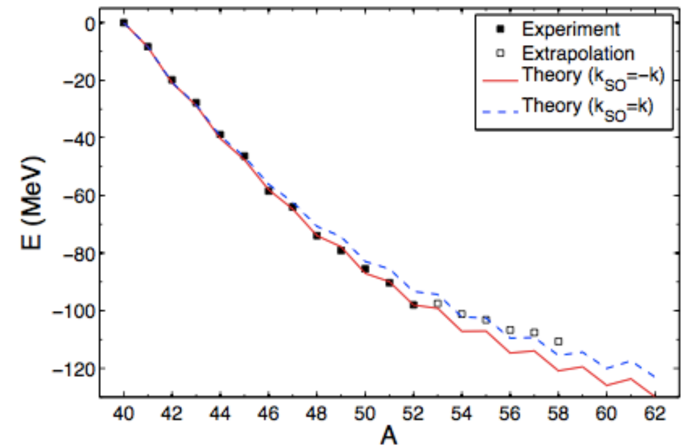


FIG. 6. (Color online) Experimental [34, 37] and calculated ground-state energies of Ca isotopes, relative to that of ^{40}Ca, as a function of mass number A.

Simple rules of shell evolution

- HO magic numbers like N=8, 20 disappear;
- New SO magic numbers like N = 6, 14, 16, 32 and 34 will appear;
- The traditional SO magic numbers N = 28 and 50 and the magic number N = 14 will be eroded somehow but are more robust than the HO magic numbers;
- Pseudospin symmetry breaks, resulting in new shell closures like N = 56 and 90;
- HO shell closures like N = 40 and 70 will not emerge.

Z. Xu, C. Qi, Phys. Lett. B 724, 247 (2013)

Monopole Hamiltonian

Determines average energy of eigenstates in a given configuration.

- Important for binding energies, shell gaps

$$H_m = \sum_a \varepsilon_a n_a + \sum_{a \le b} \frac{1}{1+\delta_{ab}} \left[\frac{3V_{ab}^1 + V_{ab}^0}{4} n_a (n_a - \delta_{ab}) + (V_{ab}^1 - V_{ab}^0)(T_a \cdot T_b - \frac{3}{4} n_a \delta_{ab}) \right]$$

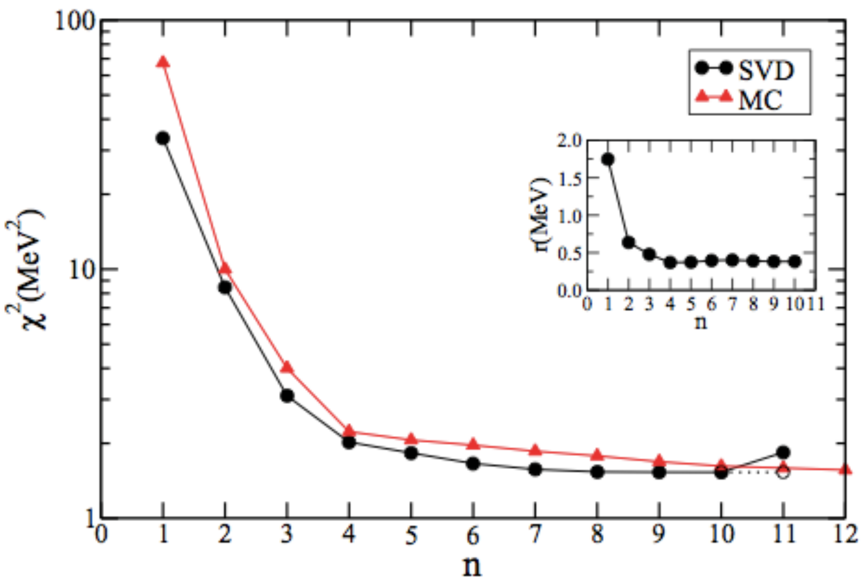
n_a, T_a … number, isospin operators of orbit *a*

Monopole centroids

- Angular-momentum averaged effects of two-body interaction
- **The monopole interaction itself does not induce mixing between different configurations.**
- **Strong mixture of the wave function is mainly induced by the residual J=0 *pairing* and *QQ* np interaction**

$$V_{ab}^T = \frac{\sum_J (2J+1) V_{abab}^{JT}}{\sum_J (2J+1)}$$

Optimization of the monopole interaction for Sn isotopes



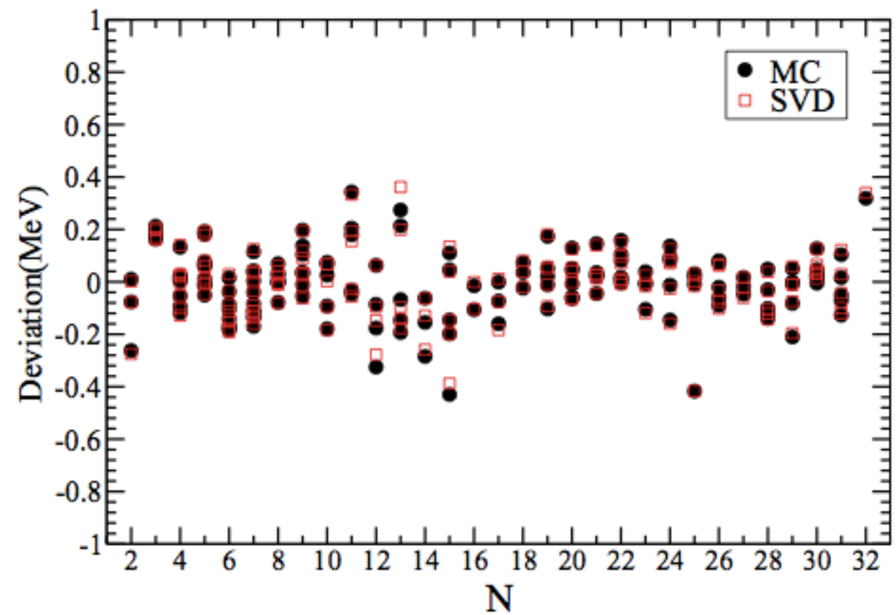
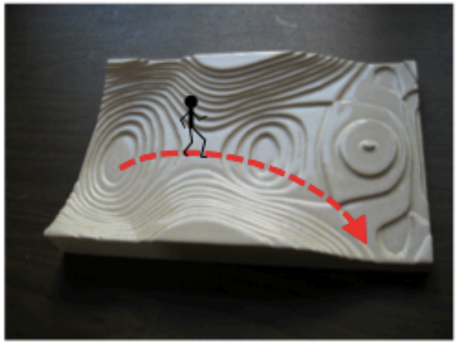


FIG. 4. (Color online) Differences between experimental and calculated binding energies $E^{\mathrm{Expt.}} - E^{\mathrm{Cal.}}$ as a function of valence neutron number.

The ground and yrast excited states in Sn isotopes can be reproduced within an average deviation of about 130 keV.



Random walk (Metropolis)

CQ, Z. Xu, Phys. Rev. C 86, 044323 (2012)

Binding energy and odd-even staggering in Pb isotopes

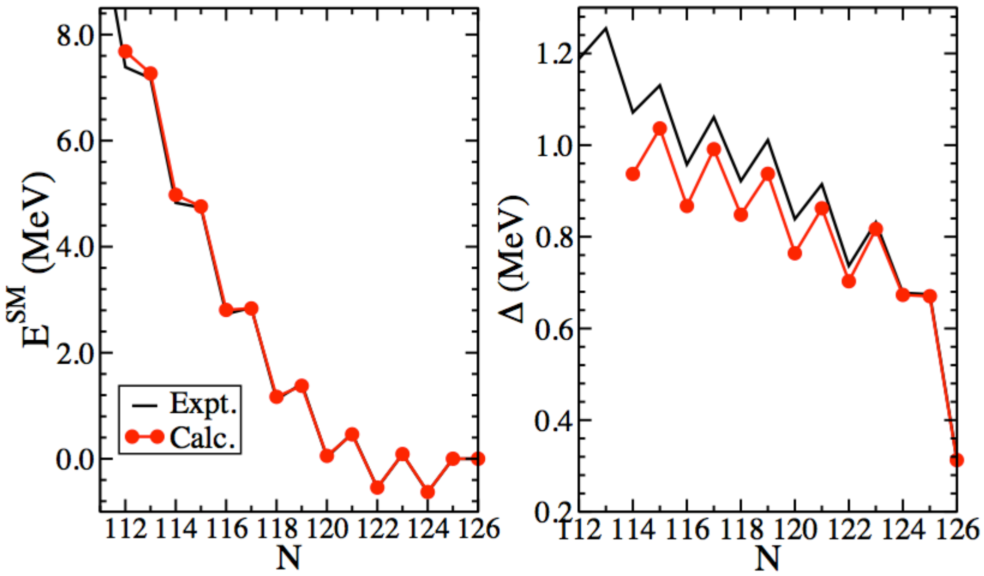
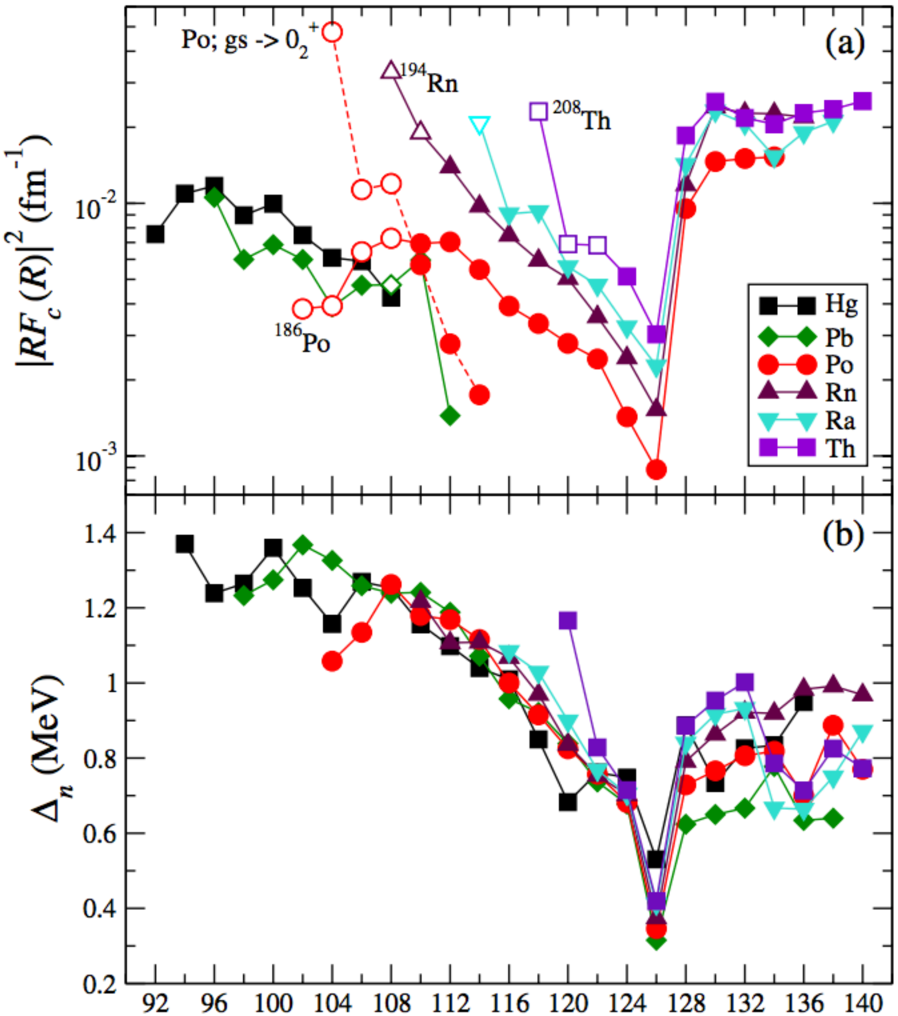


FIG. 9. (color online) Left: Experimental [80] and calculated shell-model correlation energies as a function of neutron number; Right: The empirical pairing gaps as extracted according to Eq. (5).

$$E_i^{\mathrm{cal}} = C + N\varepsilon_0 + \frac{N(N-1)}{2}V_m + \langle \Psi_I | H | \Psi_I \rangle,$$

Pairing gap and clustering

Larger pairing energy => Enhanced two-particle clustering at the nuclear surface



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

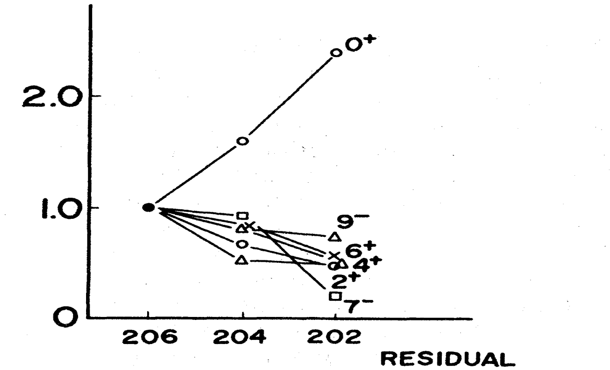
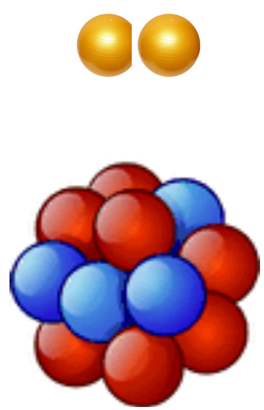


FIG. 13. Isotope dependence of triton strengths leading to the lowest state of $J^\pi = 0^+, 2^+, 4^+, 6^+, 7^-$, and 9^-.

M. Takahashi, PRC27,1454(1983)



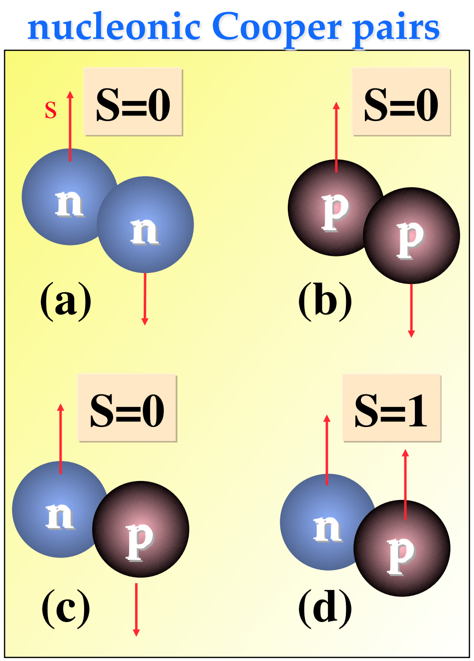
$$\Delta = G \sum_i u_i v_i,$$

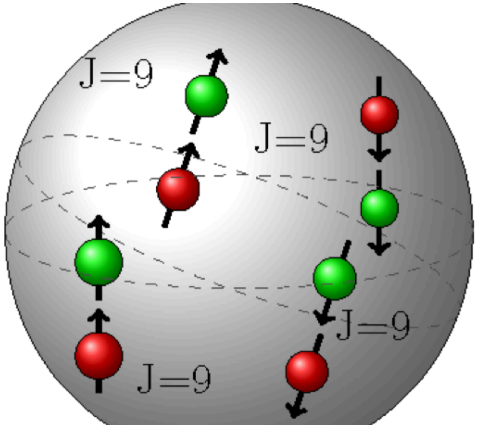
'Strong' pairing

A.N. Andreyev CQ et al., PhysRevLett.110.242502 (2013).

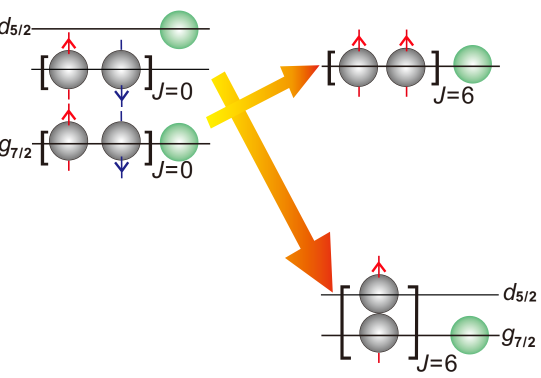
CQ, et al Phys. Lett. B 734, 203 (2014)

Long quest for np pair correlation

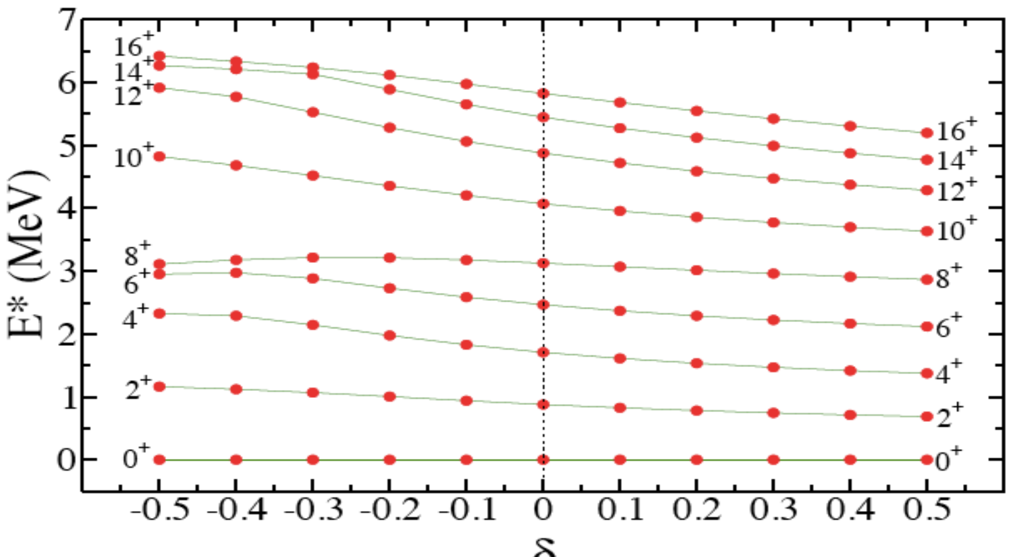




Spin flip in ^{101,103}Sn



CQ, Z. Xu, Phys. Rev. C 86, 044323 (2012)

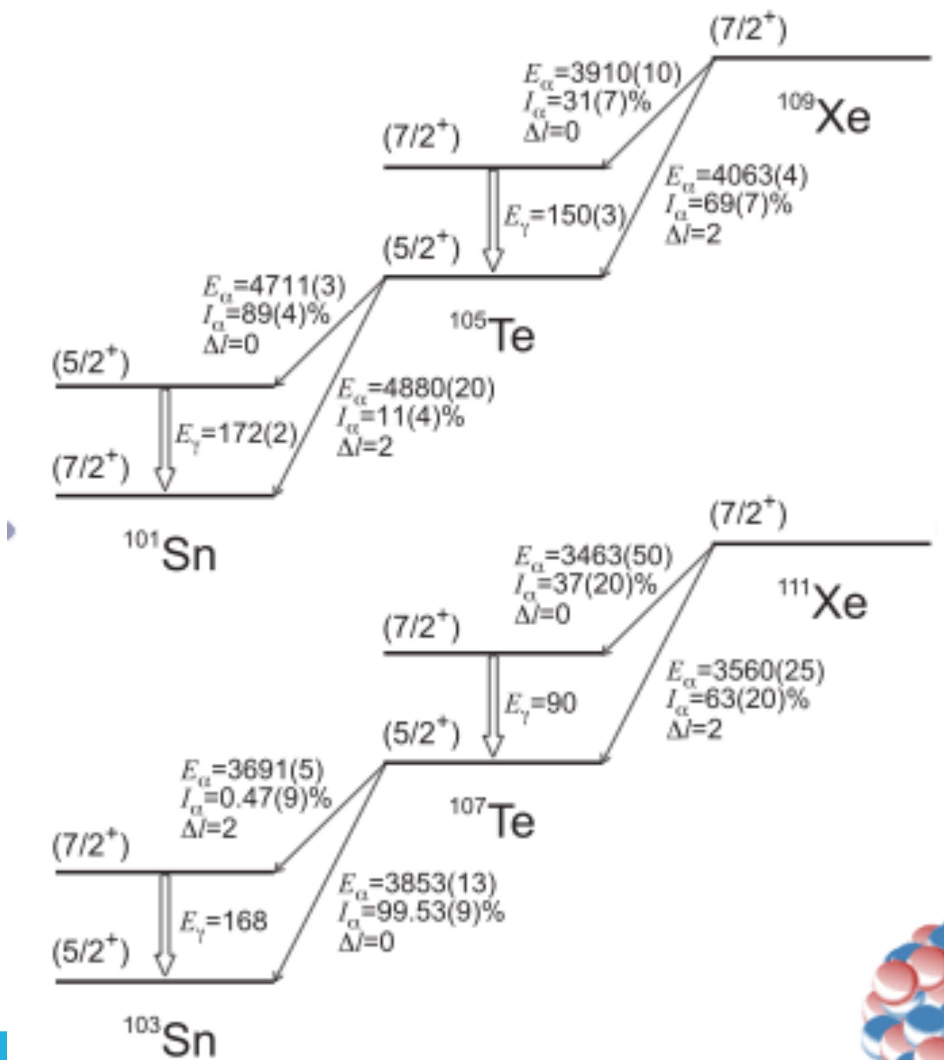


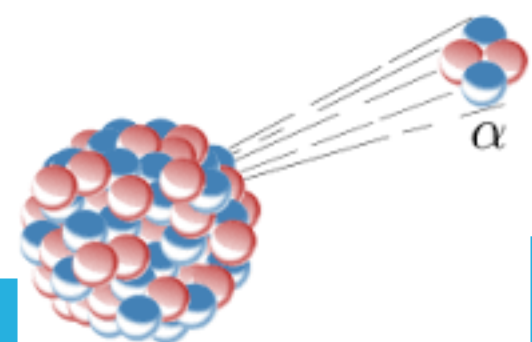
B. Cederwall,.., CQ et al., Nature 469, 68 (2011)
CQ, PRC 81, 034318 (2010)
CQ et al., PRC 84, 021301 (2011)
Z. Xu, CQ et al, Nucl. Phys. A 877, 51 (2012).

Seniority-like

Equidistant pat

Superallowed alpha decay





J. G. Darby et al. Phys. Rev. Lett. 105, 162502 (2010)

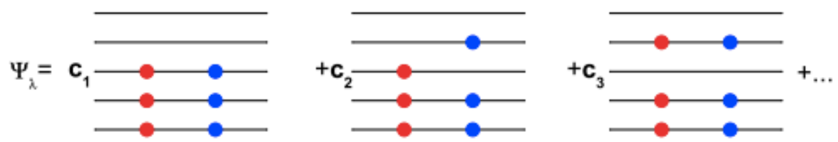
$$H = H_m + H_M$$

$$E^{\mathrm{SM}} = \langle\Psi_I|H|\Psi_I\rangle$$

$$\boxed{= \sum_{\alpha} \varepsilon_\alpha < \hat{N}_\alpha > + \sum_{\alpha\le\beta} V_{m;\alpha\beta} \left\langle \frac{\hat{N}_\alpha(\hat{N}_\beta - \delta_{\alpha\beta})}{1+\delta_{\alpha\beta}} \right\rangle}$$

$$+\langle\Psi_I|H_M|\Psi_I\rangle, \tag{4}$$

‘Monopole’ truncation

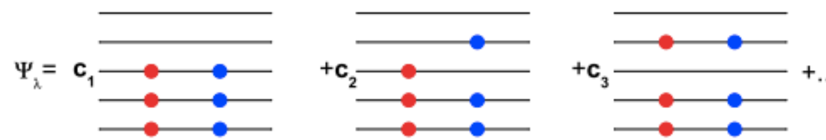


- The idea behind is that the Hamiltonian is dominated by the diagonal monopole channel. The monopole interaction can change significantly the (effective) mean field and drive the evolution of the shell structure.
- Easy to implement and keeps the simplicity of the M-scheme algorithm
- Possibility to include certain intruder configurations

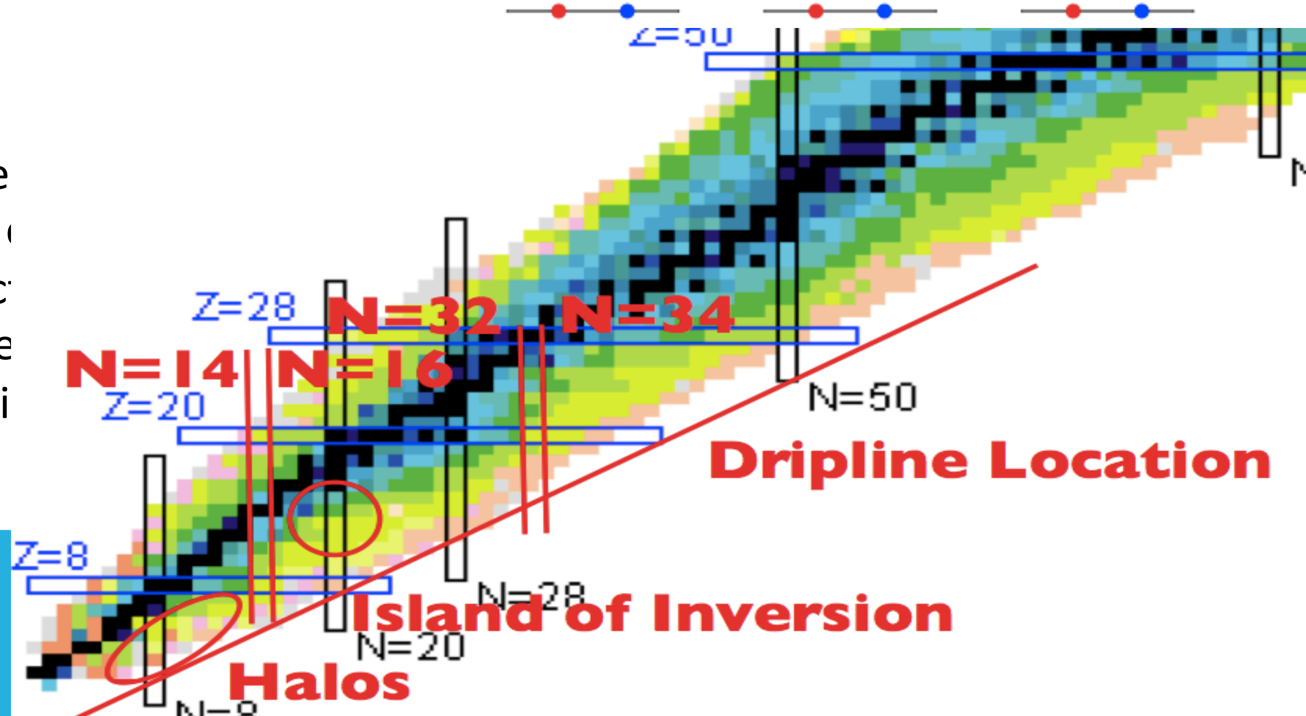
$$H = H_m + H_M$$

$$E^{\mathrm{SM}} = \langle \Psi_I | H | \Psi_I \rangle$$
$$\boxed{= \sum_{\alpha} \varepsilon_\alpha < \hat{N}_\alpha > + \sum_{\alpha \le \beta} V_{m;\alpha\beta} \left\langle \frac{\hat{N}_\alpha (\hat{N}_\beta - \delta_{\alpha\beta})}{1 + \delta_{\alpha\beta}} \right\rangle}$$
$$+ \langle \Psi_I | H_M | \Psi_I \rangle, \qquad (4)$$

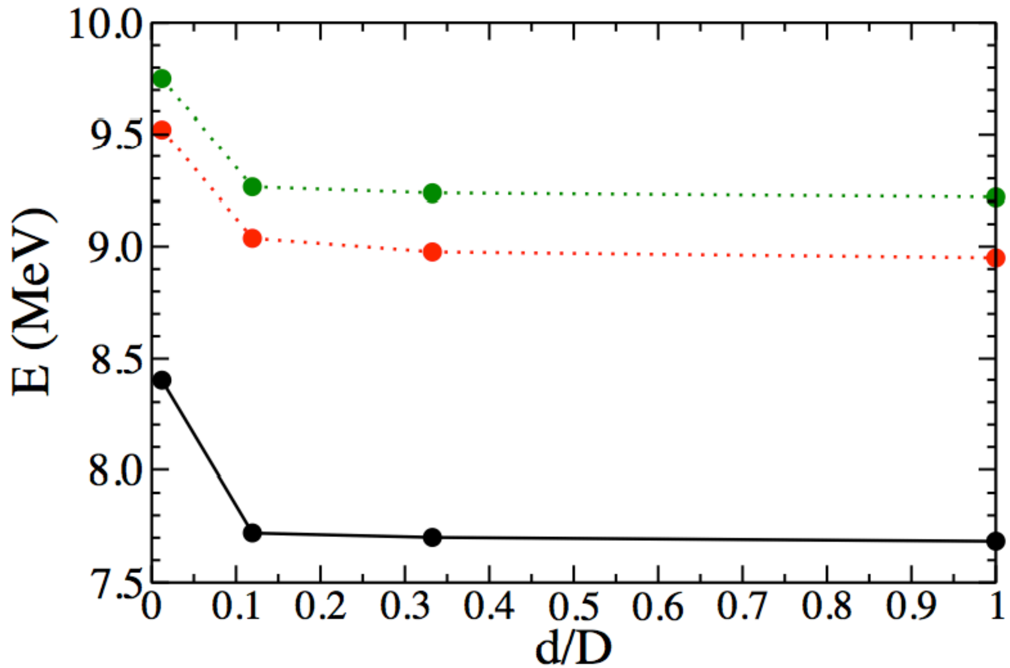
‘Monopole’ truncation



- The idea behind is that the
  The monopole interaction
  evolution of the shell struc
- Easy to implement and kee
- Possibility to include certai



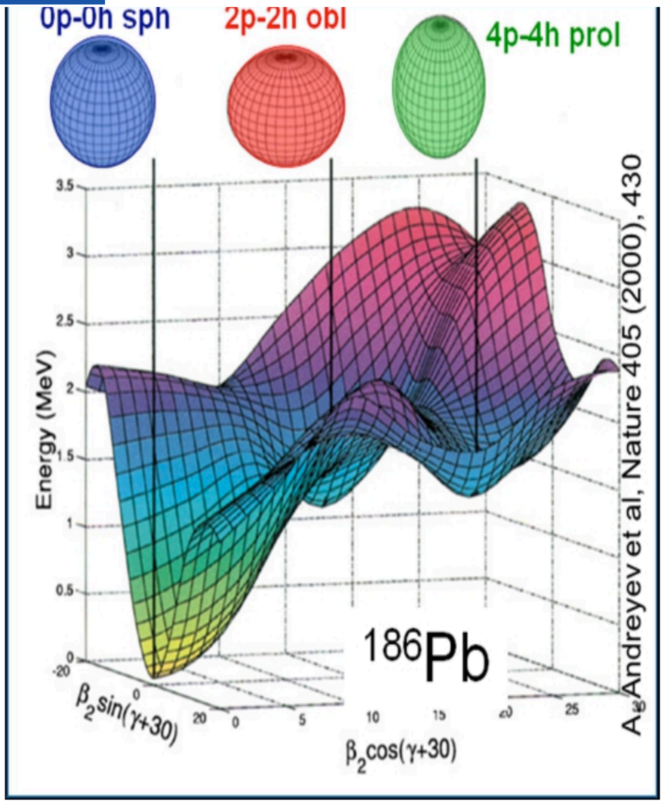
Convergence for ^{194}Pb



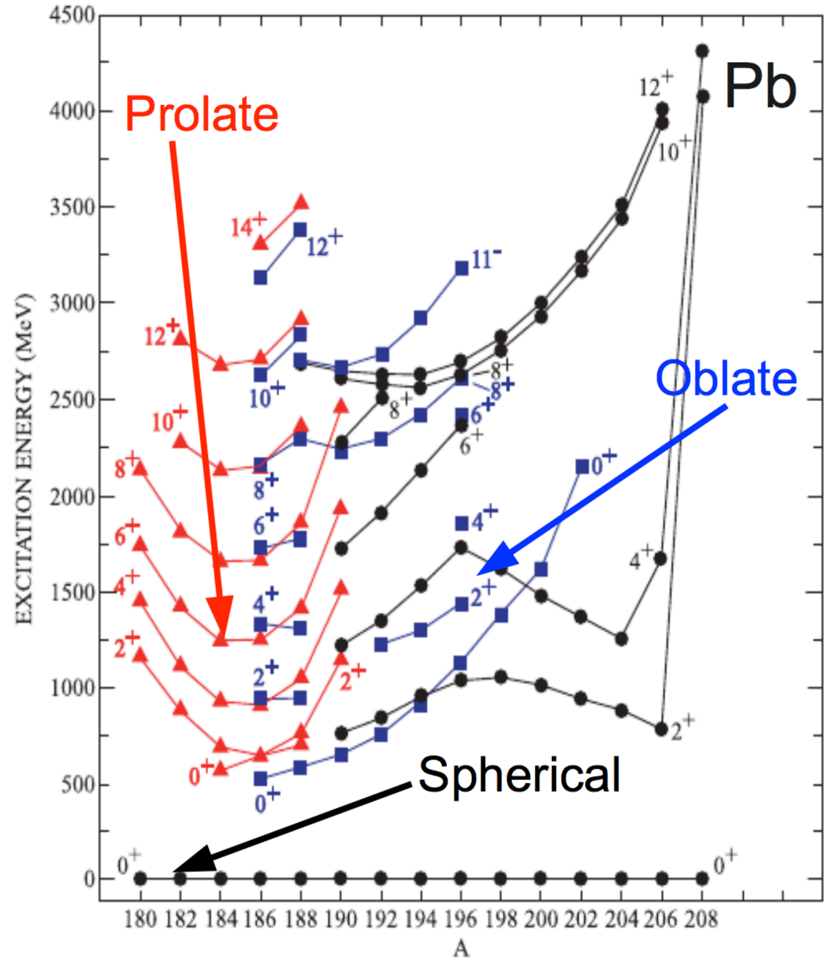
$$
\begin{aligned}
E^{\mathrm{SM}} &= \langle \Psi_I | H | \Psi_I \rangle \\
&= \sum_{\alpha} \varepsilon_\alpha < \hat{N}_\alpha > + \sum_{\alpha \le \beta} V_{m;\alpha\beta} \left\langle \frac{\hat{N}_\alpha (\hat{N}_\beta - \delta_{\alpha\beta})}{1 + \delta_{\alpha\beta}} \right\rangle \\
&\quad + \langle \Psi_I | H_M | \Psi_I \rangle, \qquad (4)
\end{aligned}
$$

CQ, LY Jia, GJ Fu, to be published

Why lead isotopes



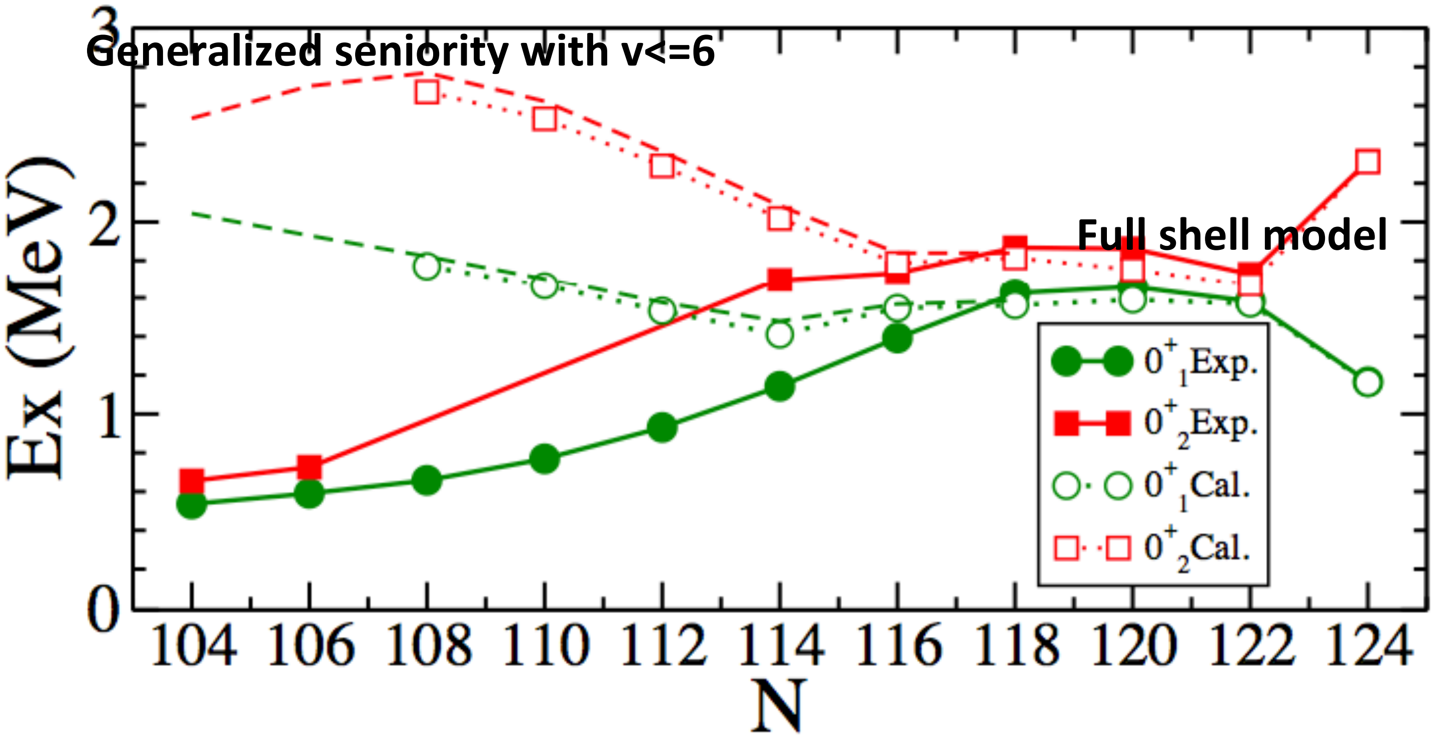
A. N. Andreyev et al., Nature 405, 430 (2000).



Shell-model calculations of Pb may provide

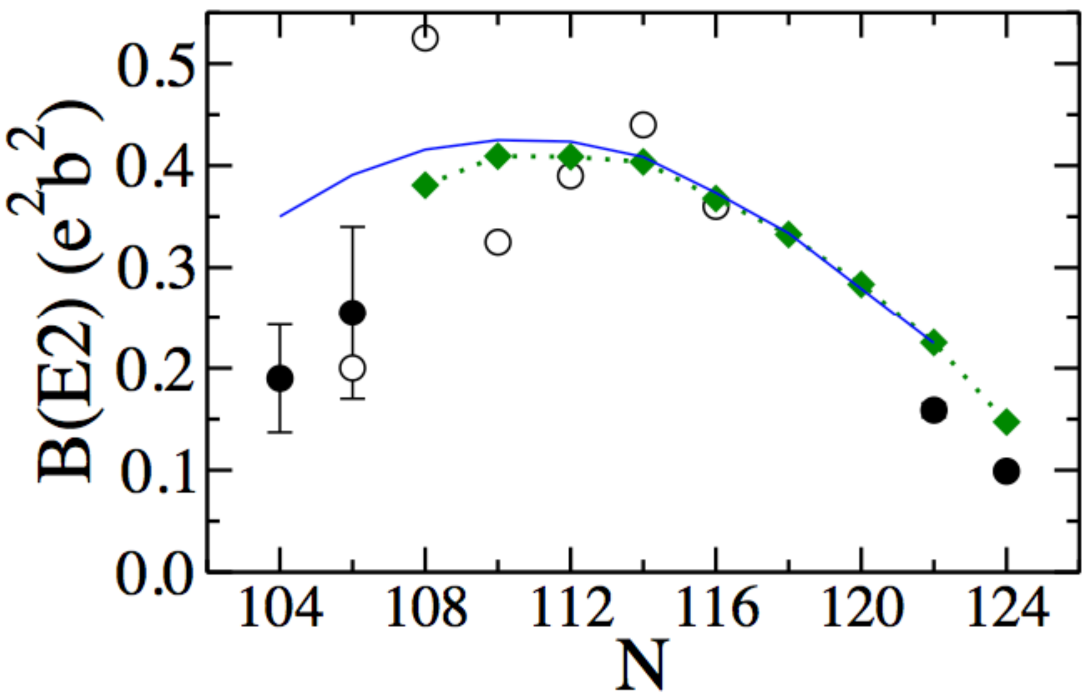
- Better description of the (spherical) low-lying levels which may be beyond the scope of symmetry truncated models like IBM
- Critical test of the effective interaction
- Benchmarks for approximation/truncation methods
- Further constraint on the role of (coexisting) deformed shapes

The excited 0^+ states

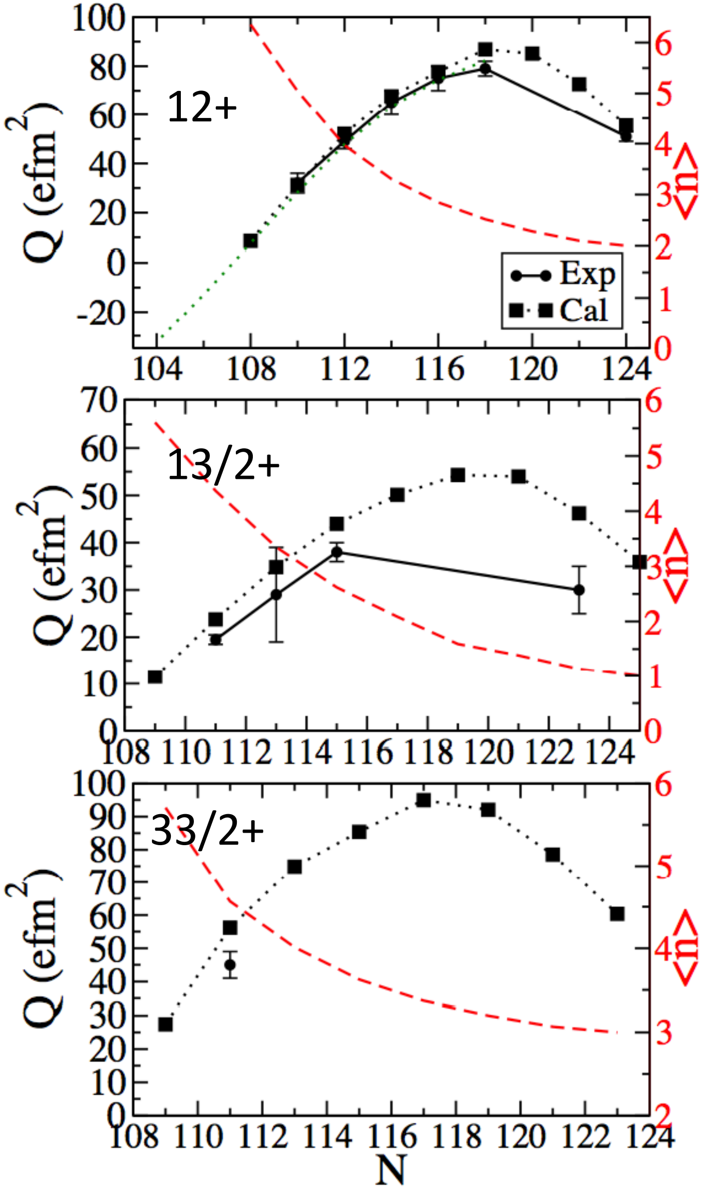


To how much extent those spherical components contribute to the observed excited 0+ states?

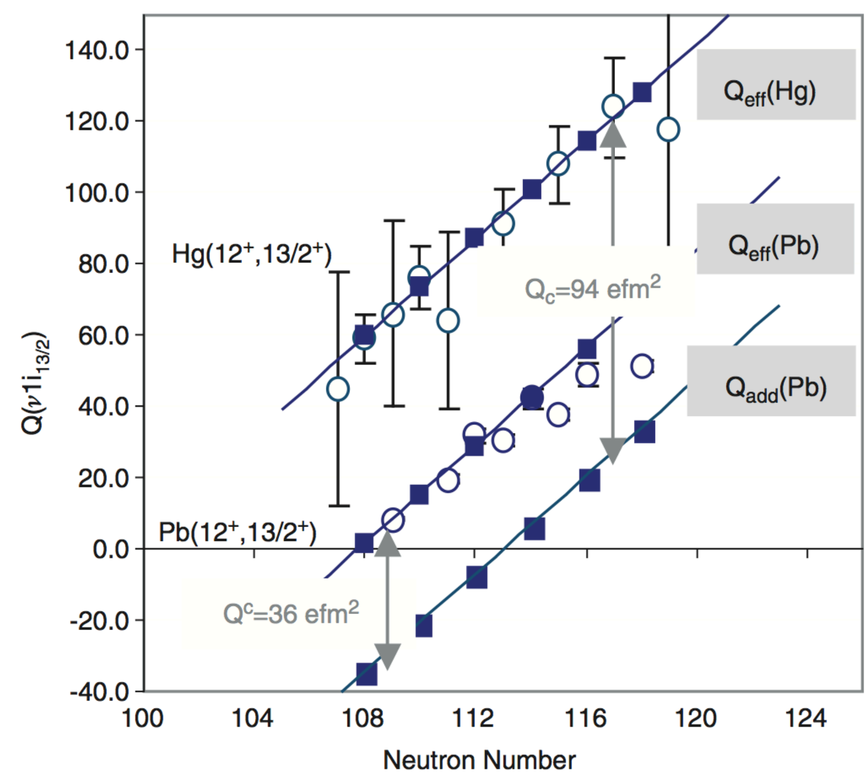
B(E2; 0^+->2^+) in Pb isotopes



The isomeric states in Pb isotopes



$$\left\langle j^n; vJ \left\| \sum_{i=1}^{n} Q_z(i) \right\| j^n; vJ \right\rangle = \frac{2j+1-2n}{2j+1-2v} \left\langle j^2; vJ \left\| \sum_{i=1}^{2} Q_z(i) \right\| j^2; vJ \right\rangle$$



G. Neyens, Rep. Prog. Phys. 66 (2003) 633

The coupling of 1,2,3 particles in $i_{13/2}$.

Cd isotopes

PRL **110**, 192501 (2013) PHYSICAL REV

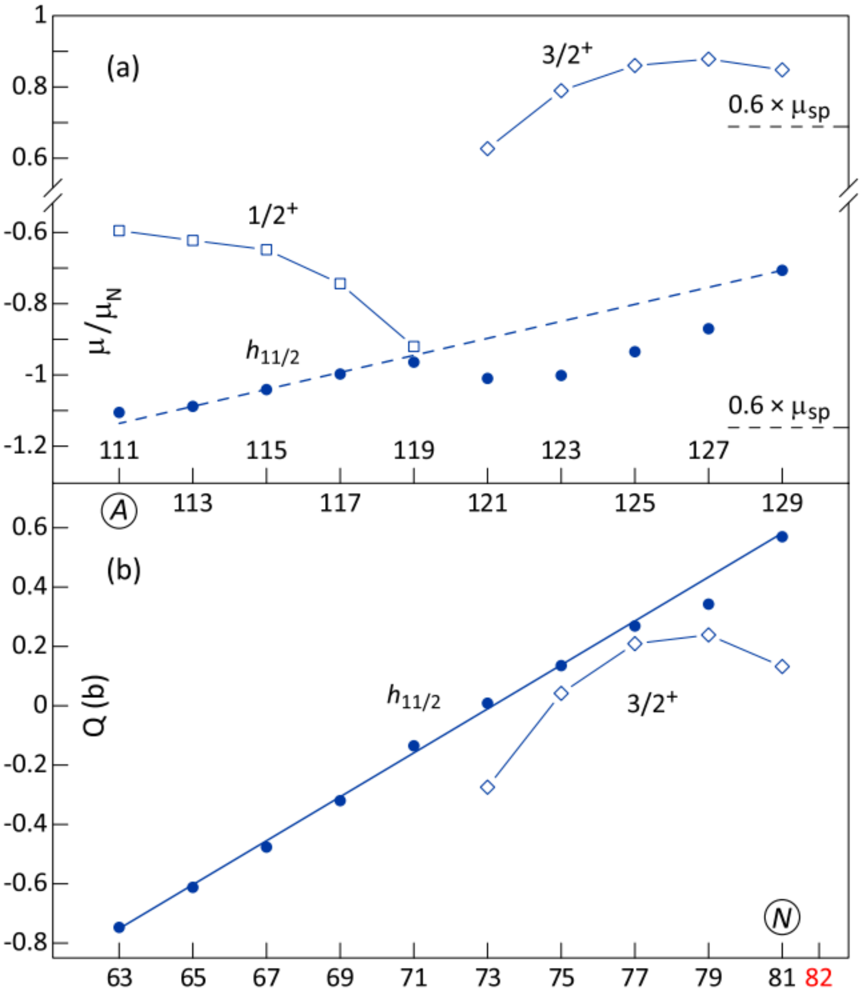


FIG. 2 (color online). Magnetic (a) and quadrupole (b) moments of $^{111-129}$Cd from this work. The experimental error bars are smaller than the markers. A straight line is fitted through the $h_{11/2}$ quadrupole moments, consistent with Eq. (2). The dashed line indicates the effect of core polarization.

Sn isotopes

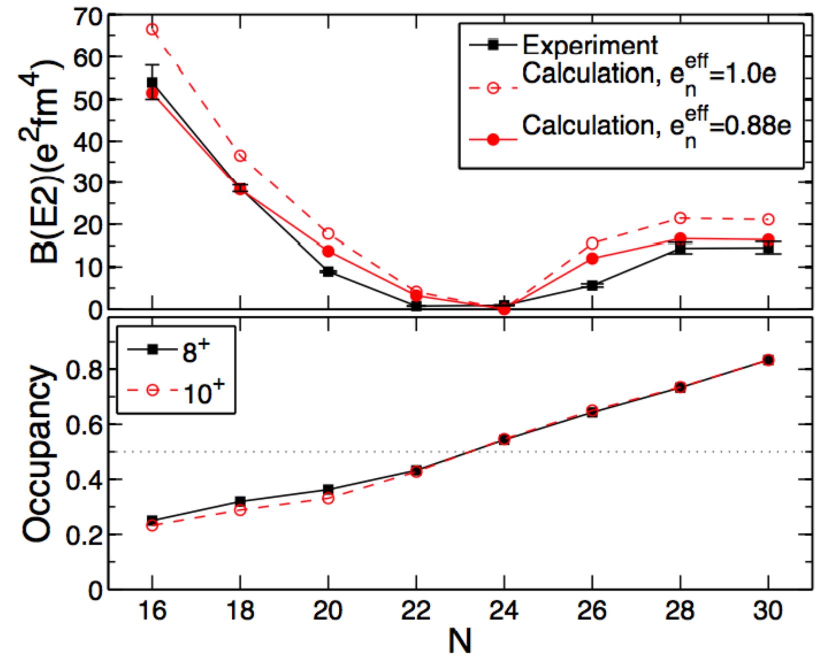


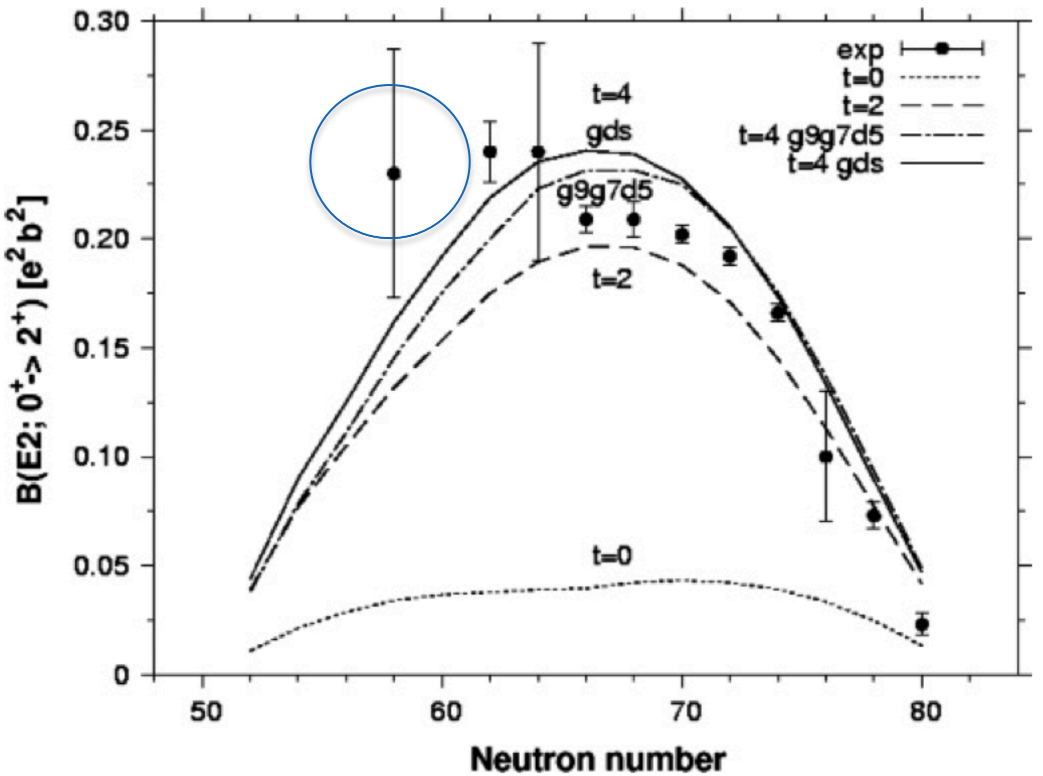
FIG. 8. (Color Online) Experimental [79, 80] and calculated $B(E2)$ values on the transitions of the 10_1^+ states in even Sn isotopes. The lower panel gives the calculated occpancies of the $0h_{11/2}$ orbital in the 10^+ and 8^+ states.

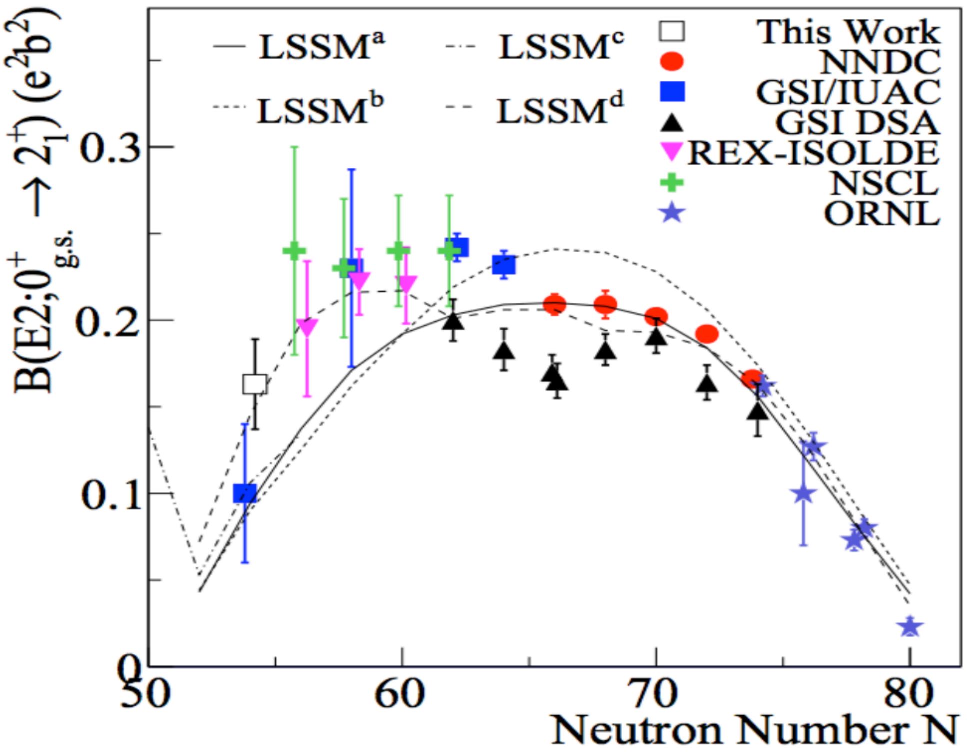
The robustness of the N=Z=50 shell closures

PHYSICAL REVIEW C **72**, 061305(R) (2005)

^{108}Sn studied with intermediate-energy Coulomb excitation

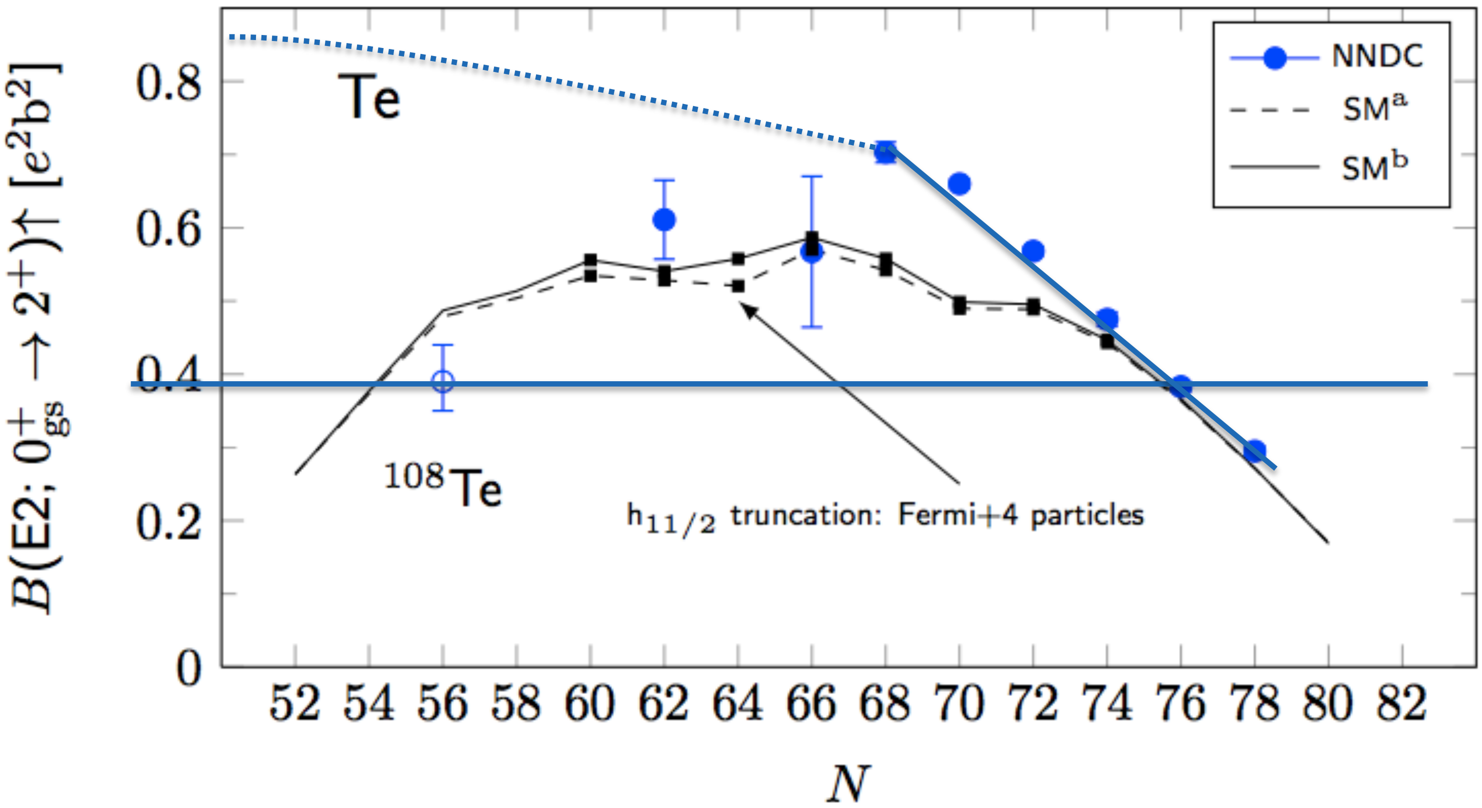
A. Banu,[1,2,*] J. Gerl,[1] C. Fahlander,[3] M. Górska,[1] H. Grawe,[1] T. R. Saito,[1] H.-J. Wollersheim,[1] E. Caurier,[4] T. Engeland,[5]
A. Gniady,[4] M. Hjorth-Jensen,[5] F. Nowacki,[4] T. Beck,[1] F. Becker,[1] P. Bednarczyk,[1,6] M. A. Bentley,[7] A. Bürger,[8]
F. Cristancho,[3,†] G. de Angelis,[9] Zs. Dombrádi,[10] P. Doornenbal,[1,11] H. Geissel,[1] J. Grębosz,[1,6] G. Hammond,[12,‡]
M. Hellström,[1,§] J. Jolie,[11] I. Kojouharov,[1] N. Kurz,[1] R. Lozeva,[1,||] S. Mandal,[1,¶] N. Mărginean,[9] S. Muralithar,[1,**] J. Nyberg,[13]
J. Pochodzalla,[2] W. Prokopowicz,[1,6] P. Reiter,[11] D. Rudolph,[3] C. Rusu,[9] N. Saito,[1] H. Schaffner,[1] D. Sohler,[10] H. Weick,[1]
C. Wheldon,[1,††] and M. Winkler[1]





P. Doornenbal et al,arxiv.org/abs/1305.2877

T. Bäck, CQ et al, PRC **87**, 031306(R) (2013)



T. Bäck, CQ et al, PRC (R), 84 (4), 041306 (2011)

Te isotopes
2015 update

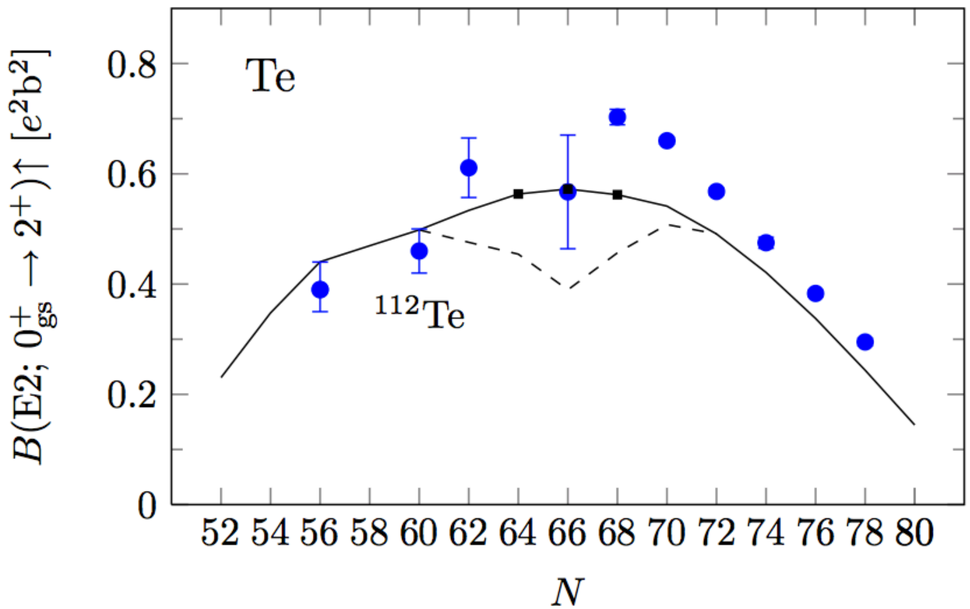
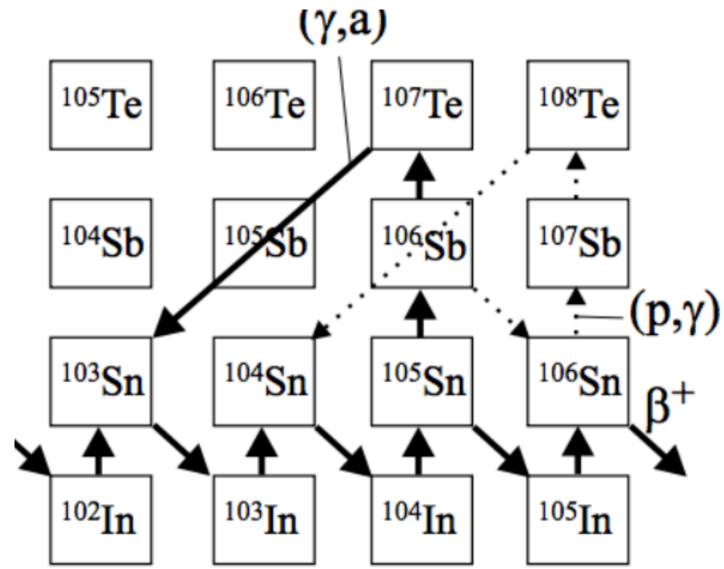


FIG. 3. (Color online) Comparison of the theoretical and experimental $B(E2;0^+_{\mathrm{g.s.}} \to 2^+)$ values for the Te isotopic chain. The solid line corresponds to the calculation in which the full model space ($g_{7/2}$, $d_{5/2}$, $d_{3/2}$, $s_{1/2}$, and $h_{11/2}$) has been considered for all nuclei except $^{116-120}$Te (marked by small solid squares) while the dashed line represents the calculation in the smaller space, see the main text for more details.

endpoint of rp process?



H. Schatz et al, PRL86, 3471 (2001)

M. Doncel, CQ et al, PRC 91, 061304(R) (2015)

CQ, to be published

The unbound nucleus ^{109}I

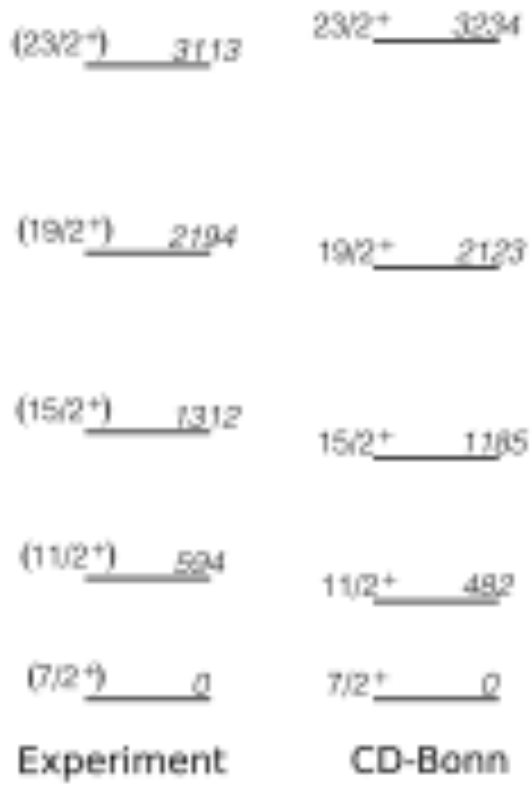
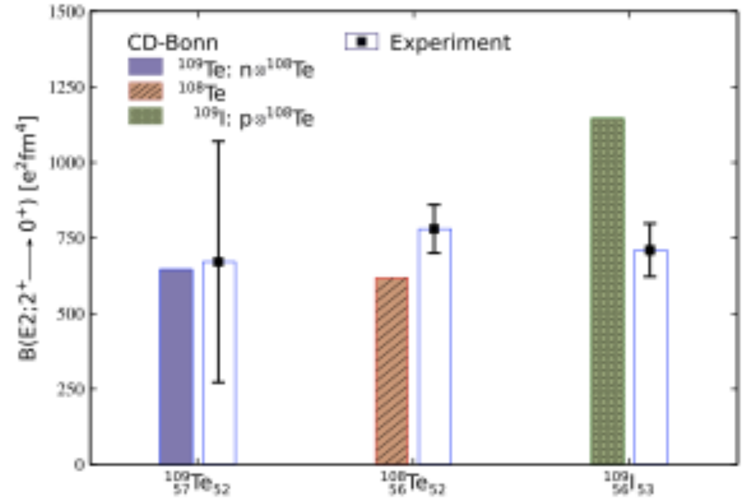
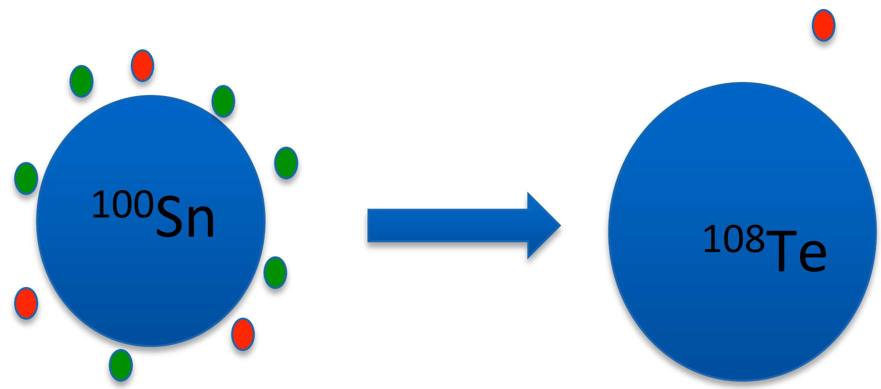


Fig. 3. Experimental excitation energies of ^{109}I (left). All excitation energies are quoted relative to the $(7/2^+)$ state. Theoretical CD-Bonn calculated excitation energies (right) are shown for comparison. The excitation energies of the ground-state band levels are shown to the right of each state.





M.G. Procter et al, Physics Letters B 704 (2011) 118–122

Nucleon-pair approximation:
H Jiang, C Qi, Y Lei, R Liotta, R Wyss, YM Zhao, Physical Review C 88 (4), 044332 (2013).

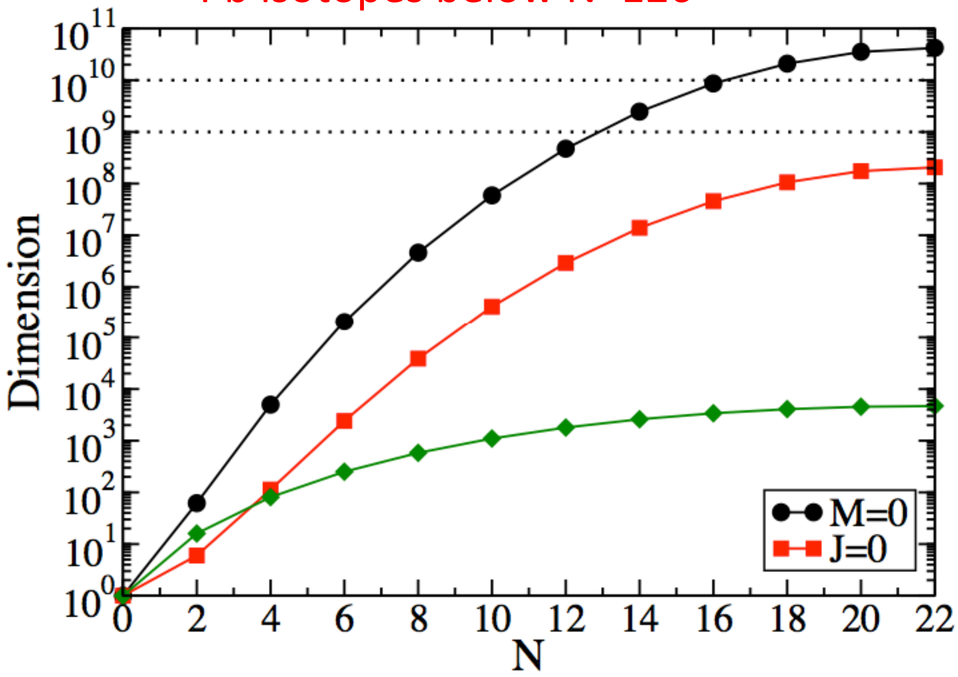
Summary

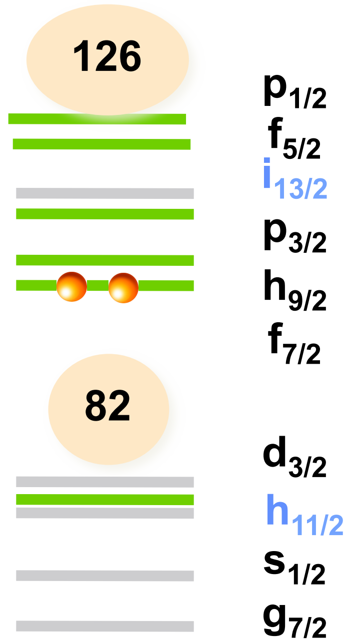
- **Introduction to the nuclear shell model/full configuration interaction approach**
  - ❖Properties of the effective interaction
  - ❖Truncation methods
  - ❖Truncation based an a correlated basis
- **Applications in Sn, Pb and neighboring isotopes**
  - ❖(Empirical) shell model can be a reliable tool for simulating the spectroscopy of intermediate mass and heavy nuclei
  - ❖Future looks prosperous

Thank you

Computational challenge

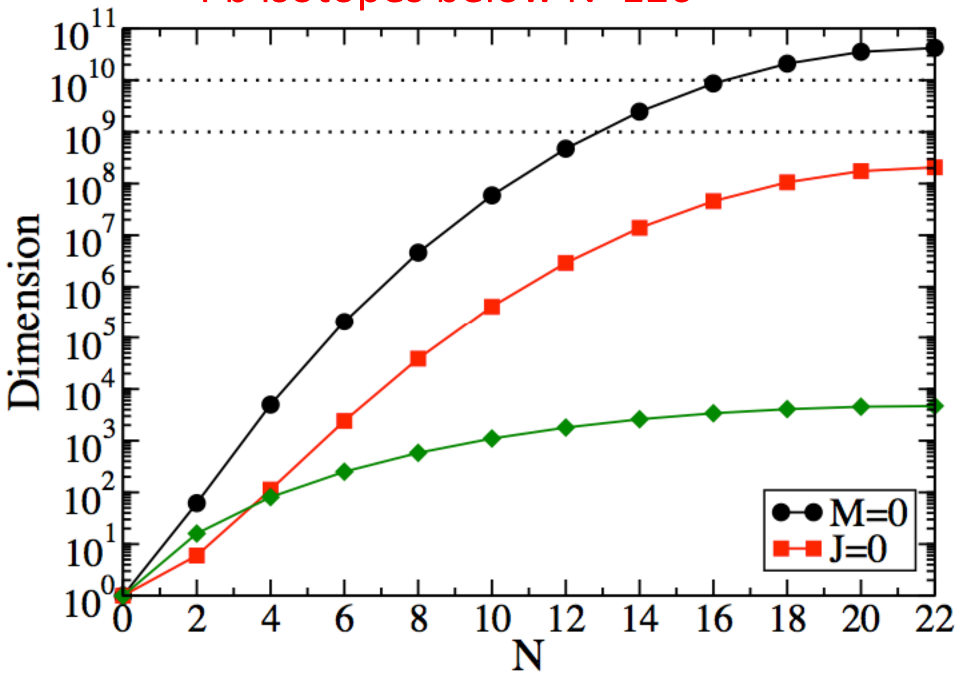
Pb isotopes below N=126

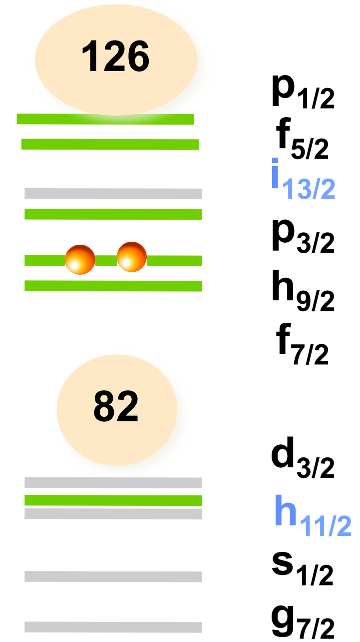




Computational challenge

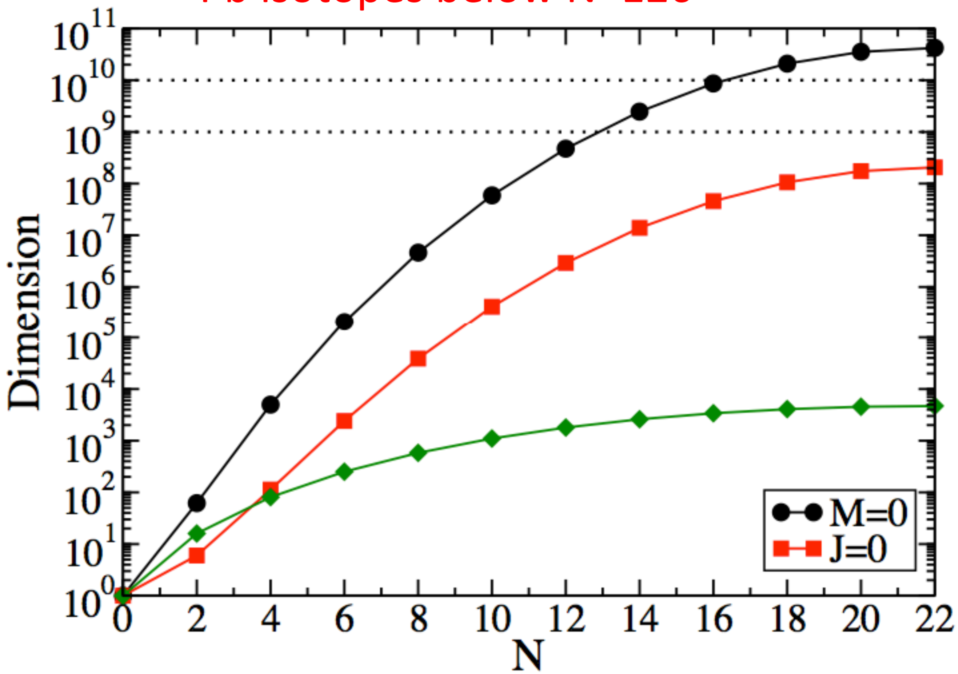
Pb isotopes below N=126

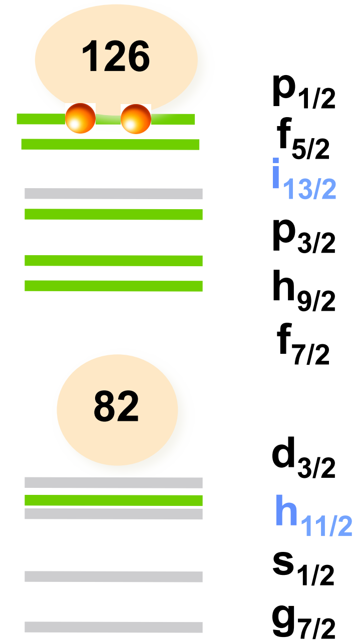




Computational challenge

Pb isotopes below N=126





- Most shell-model codes are in M-scheme: Simple algorithm; avoid the complicated angular momentum coupling
- N~Z Systems are relatively easier to solve by applying the so-called factorization technique (as in ANTOINE)
- System with identical particles can be more difficult to treat. Possible factorization under development.

Two new computers became available this year

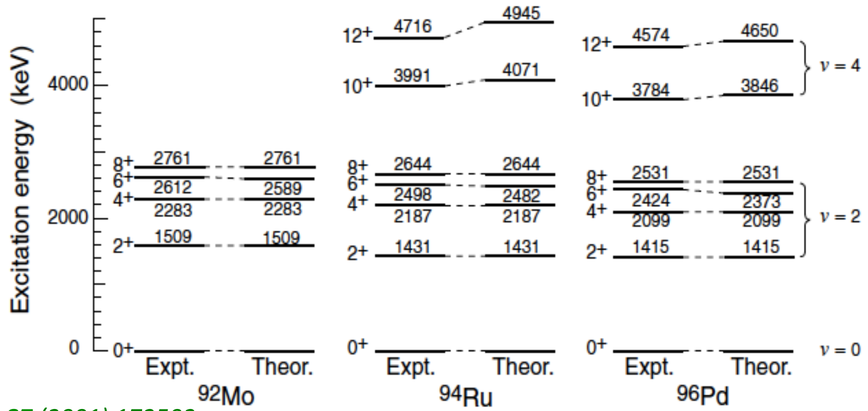
PDC's supercomputer Beskow

Alice Tegnér

Seniority coupling scheme

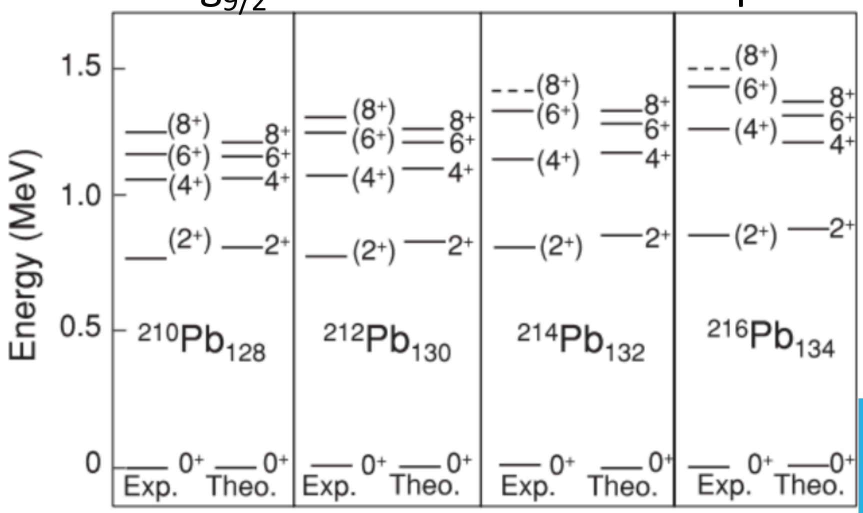
$$|\text{g.s.}\rangle = |\nu = 0; J = 0\rangle = (P_j^+)^{n/2}|\Phi_0\rangle$$
$$|\nu = 2; JM\rangle = (P_j^+)^{(n-2)/2} A^+(j^2 JM)|\Phi_0\rangle$$

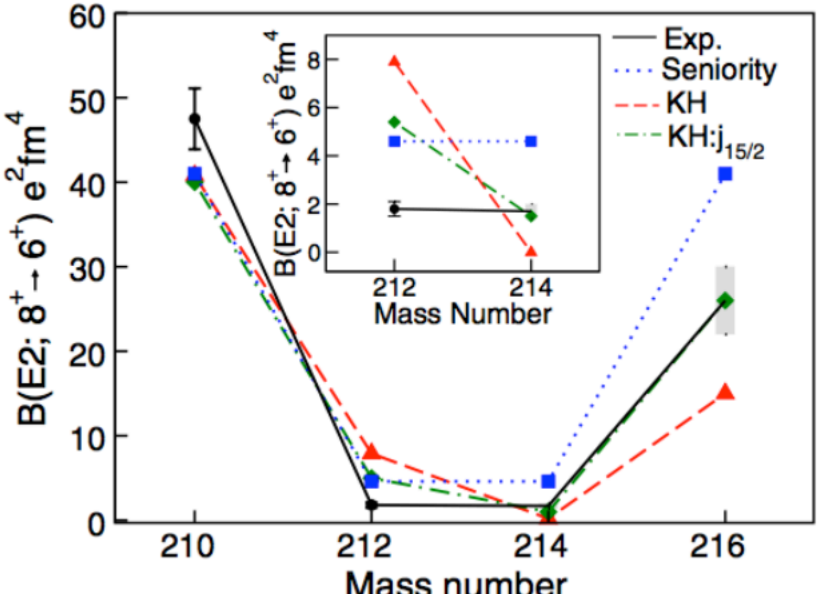
Energy levels of $0g_{9/2}$ protons in *N*=50 isotones



D.J. Rowe and G. Rosensteel, Phys. Rev. Lett. ***87*** *(2001) 172502*

Neutrons in $1g_{9/2}$ in neutron-rich Pb isotopes





A. Gottardo et al., PRL 109, 162502 (2012)

jj coupling instead of LS coupling

General properties of the effective interaction

The two-body interaction matrix elements in a single j shell $\langle j^2;JT|V|j^2;JT\rangle$

- Isovector (T=1): J=0,2,..,2J-1, J=0 term attractive *(pairing),* others close to zero
- Isoscalar (T=0): J=1,3,..,2j
  - ✧**strongly attractive monopole interaction (mean field)**
  - ✧ ***Strong Quadrupole-Quadrupole correlation (which induces 'deformation')***
  - ✧***The np interaction breaks the seniority coupling***

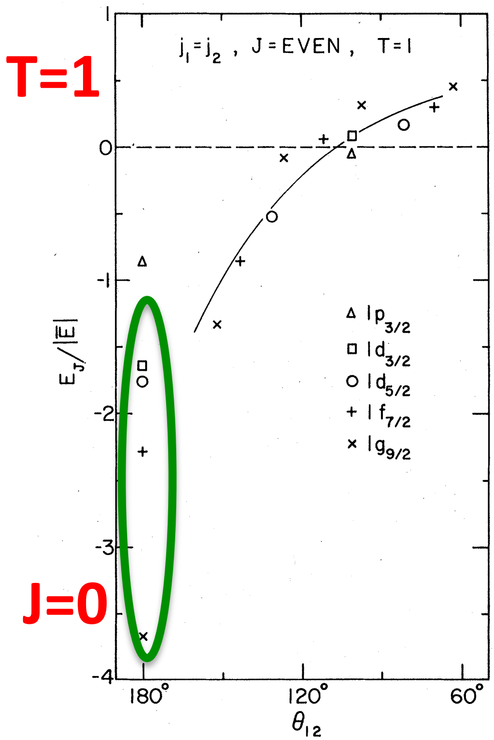


FIG. 3. Comparison of data from various multiplets with $j_1 = j_2$ and $T=1$. The values of the matrix elements are divided by $\bar{E} \equiv \sum_J [J] E_J / \sum_J [J]$ to display the similarities in the J dependence (or θ dependence) of the various multiplets.

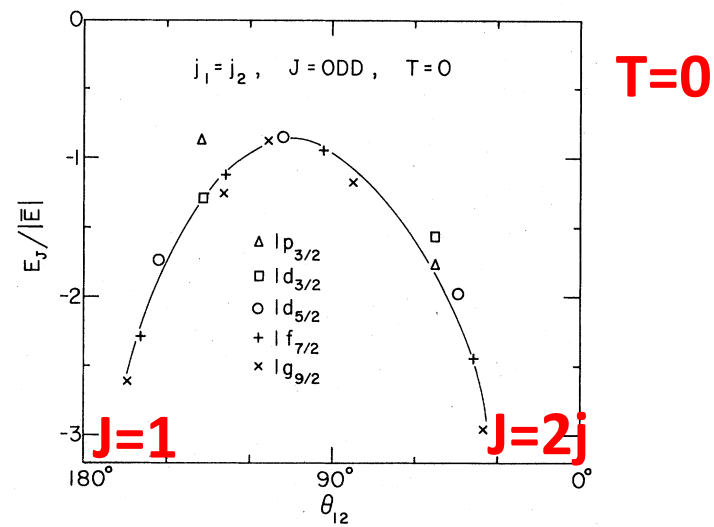


FIG. 2. Comparison of data from various multiplets with $j_1 = j_2$ and $T=0$. The values of the matrix elements are divided by $\bar{E} \equiv \sum_J [J] E_J / \sum_J [J]$ to display the similarities in the J dependence (or θ dependence) of the various multiplets.

$$\cos\theta_{12} = \frac{J(J+1)}{2j(j+1)} - 1$$

J.P. Schiffer and W.W. True, Rev.Mod.Phys. 48,191 (1976)