Nuclear Theory in the Supercomputing Era – 2018 (NTSE-2018)
IBS, Daejeon, Korea, 29 October – 2 November 2018

Large-scale shell model calculations of heavy nuclei

Chong Qi
KTH Royal institute of Technology, Stockholm

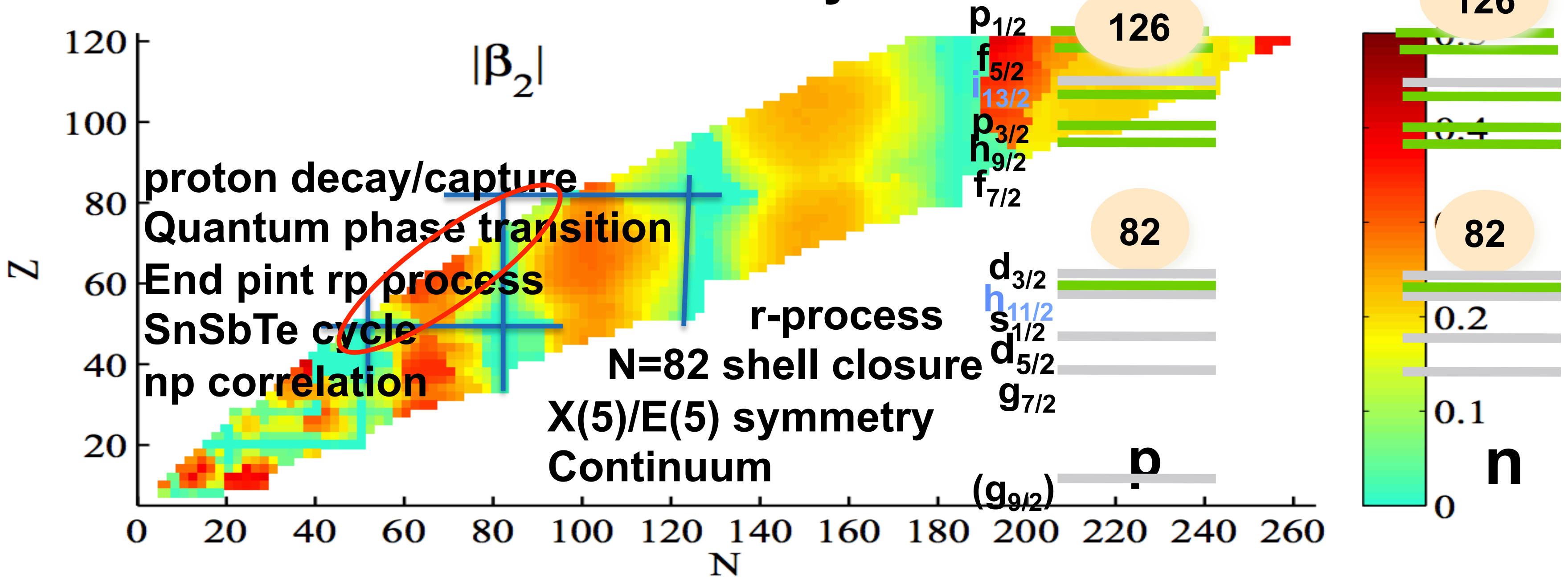
Thanks to
XiaoYu Liu, R. Liotta, R. Wyss, T. Bäck, A. Johnson, B. Cederwall (KTH)
Liyuan Jia, Guanjian Fu (Shanghai)

Outline

- **Brief introduction**
- **Simple truncation/cutoff**
- **Applications**

Motivation

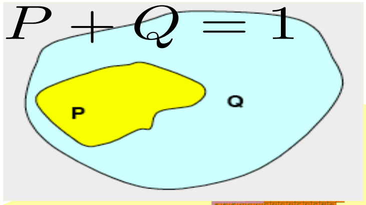
Microscopic large-scale shell-model description of intermediate-mass and heavy nuclei

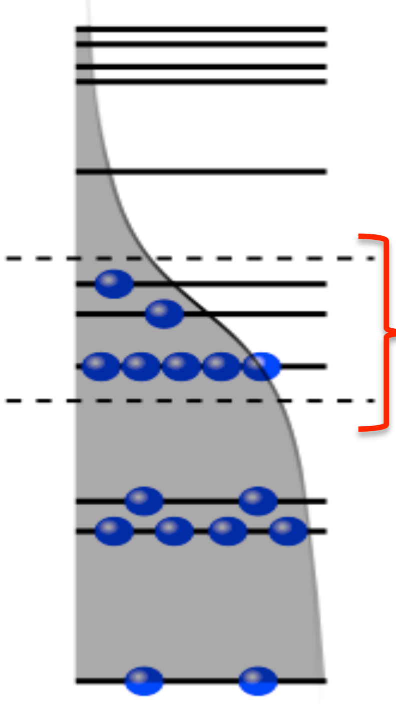


Deformation minima in even-even nuclei by using the *deformed Woods-Saxon potential (not LSSM).*

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

Z. Wu et al., Phys. Rev. C 92, 024306 (2015).





Full configuration interaction shell model

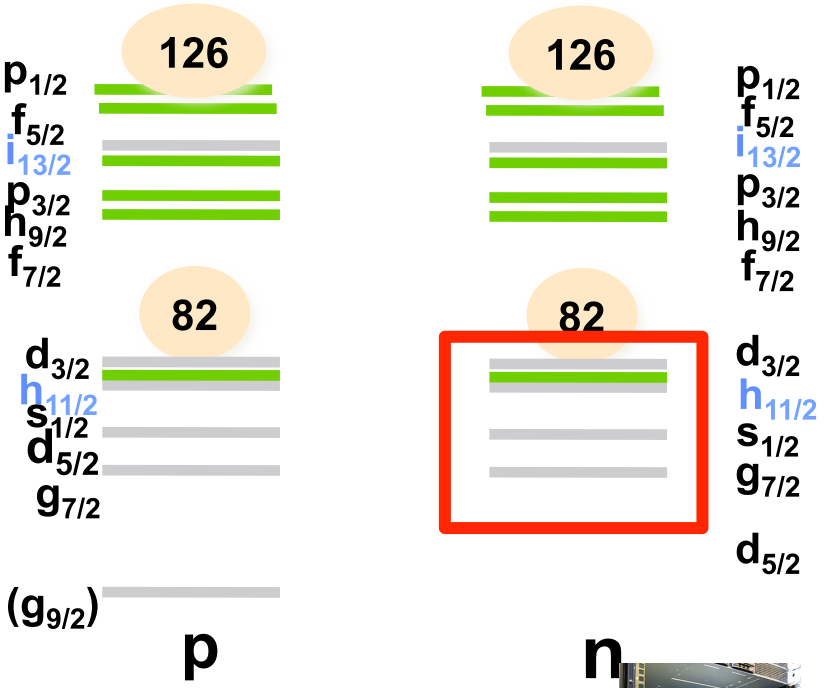
✧Limited number of valence orbitals;

✧No continuum; All quantities are real

✧Sparse Hamiltonian matrix if three-body interaction neglected

- The nuclear shell model it considers the mixing effect of all possible configurations within a given model space.
- The most precise model available on the market

Our ‘ideal’ model space and effective interaction

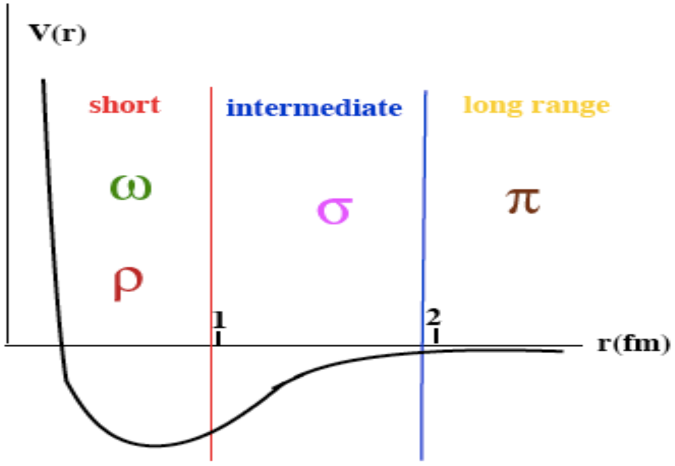


PDC's supercomputer Beskow

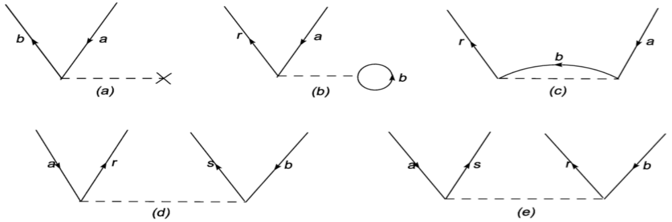
Memory or core, that is a question

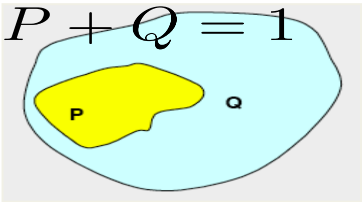
"Bare" Nucleon-Nucleon Potentials:

- Argonne V18: PRC 56, 1720 (1997)
- CD-Bonn 2000: PRC 63, 024001 (2000)
- *N^3LO: PRC 68, 041001 (2003)*
- *N^4LO*
- *N^5LO*



Perturbation treatment

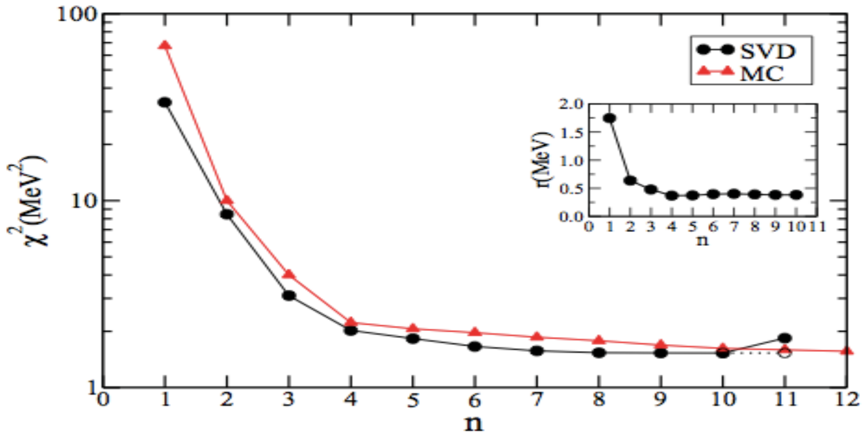




and many other diagrams. Usually we stop at the second or third order;

- No preference for NN potential
- Convergence not guaranteed

Optimization of the monopole interaction



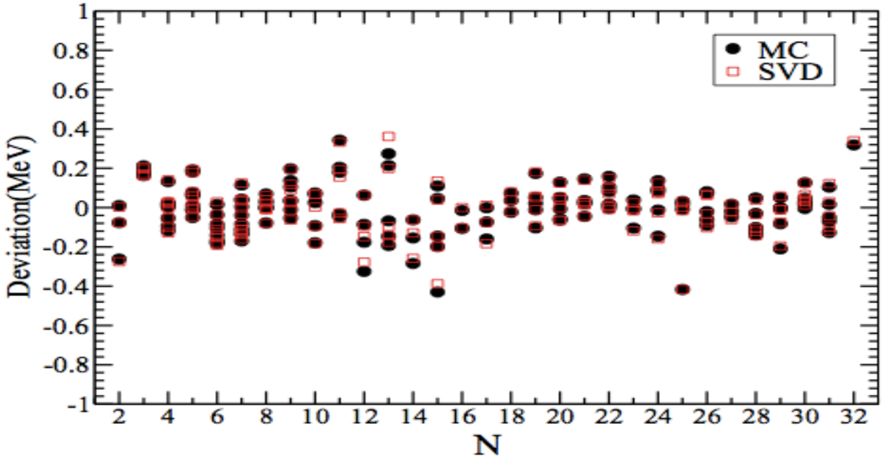


FIG. 4. (Color online) Differences between experimental and calculated binding energies $E_i^{\mathrm{Expt.}} - E_i^{\mathrm{Cal.}}$ as a function of valence neutron number.

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

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

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

Binding energy and odd-even staggering in Pb isotopes after optimzation

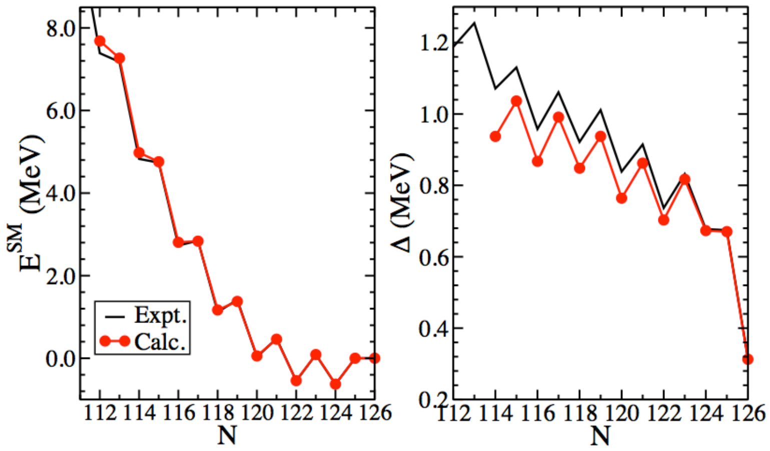


FIG. 9. (color online) Left: Experimental [80] and calculated shell-model correlation energies as a function of neutron number; Right: The empirical pairing gaps as extracted according to Eq. (5).

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

CQ, LY Jia, GJ Fu, Phys. Rev. C 94, 014312 (2016)

Monopole Hamiltonian

Determines average energy of eigenstates in a given configuration

- Angular-momentum averaged effects of two-body interaction

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

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

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

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

- **The monopole interaction itself does not induce any mixture between different configurations.**
- **Important for binding energies, shell gaps**
- **Strong mixture of the wave function is mainly induced by the residual J=0 *pairing* and *QQ* np interaction**

‘EFT-like’ Shell model effective interaction

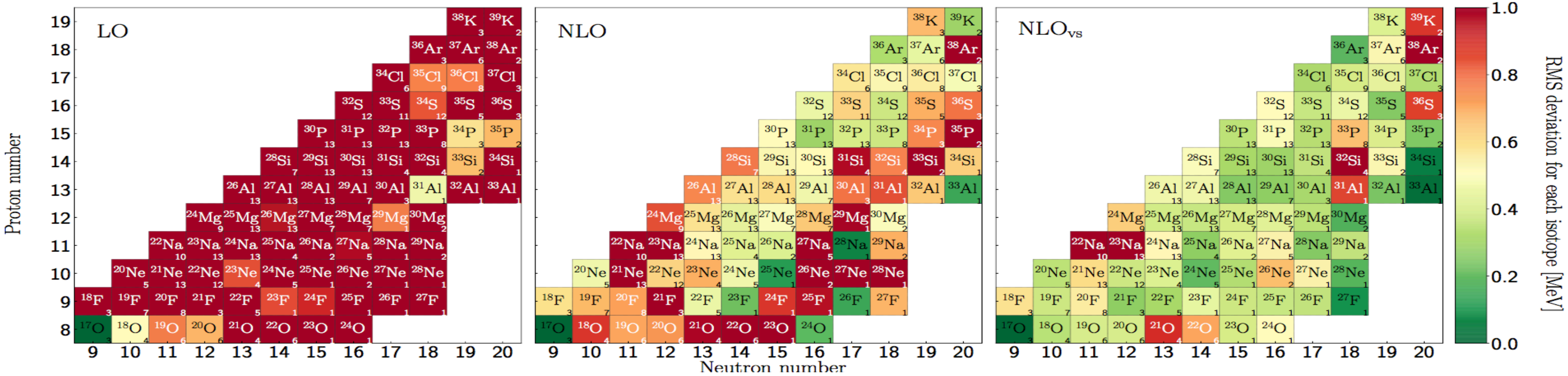


FIG. 3. Graphical representation of the RMS deviation from experiment for each fitted nucleus in the *sd* shell. The figure shows the results for the chiral shell-model interactions

Shell-model interactions from chiral effective field theory

L. Huth, V. Durant, J. Simonis, and A. Schwenk
Phys. Rev. C **98**, 044301 – Published 2 October 2018

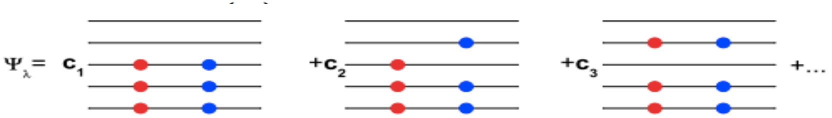
'Monopole' truncation

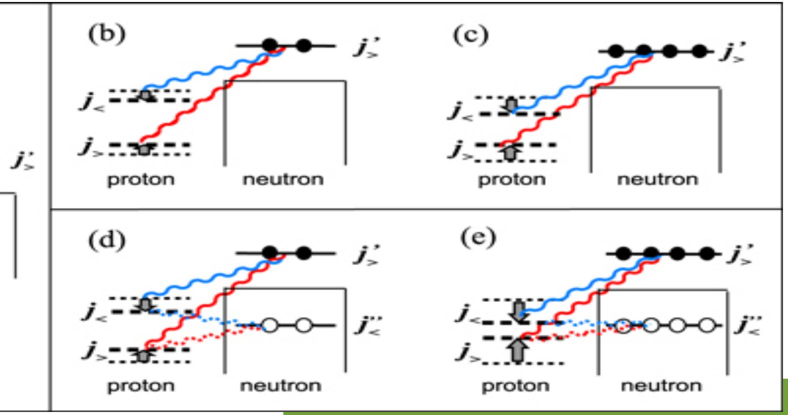
$$H = H_m + H_M$$

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

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

$$+ \langle \Psi_I | H_M | \Psi_I \rangle,$$





Effective single-particle energy evolution due to monopole interaction

We treat the total monopole energy as a whole and define model space accordingly

from T Otsuka and Y Tsunoda, JPG 2016

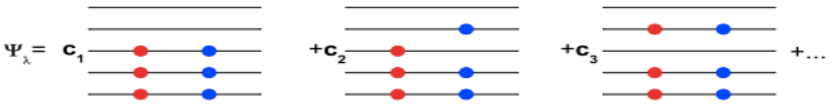
‘Monopole’ truncation

$$H = H_m + H_M$$

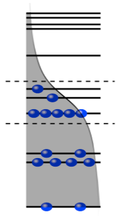
$$E^{\rm SM} = \langle \Psi_I | H | \Psi_I \rangle$$

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

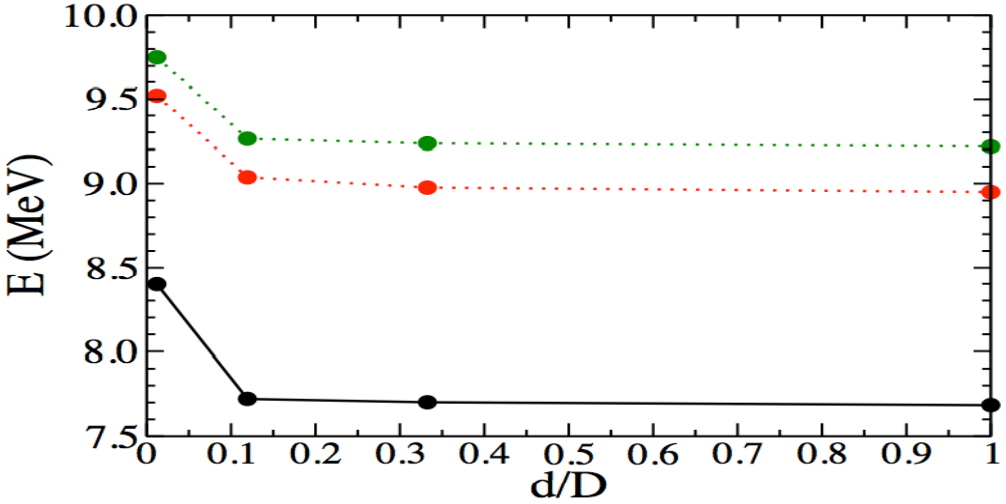
$$+ \langle \Psi_I | H_M | \Psi_I \rangle,$$



- Similar to ‘npnh’ and Nmax if no monopole considered.
- But monopole interaction can change significantly the (effective) mean field and invalidate npnh.
- Easy to implement and keeps the simplicity of the M-schen algorithm
- Possibility to include certain intruder configurations



Convergence for ^{194}Pb



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

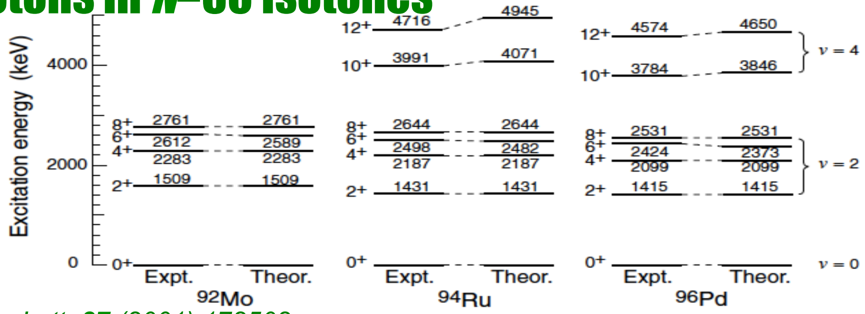
CQ, LY Jia, GJ Fu, PRC 2016

Seniority truncation

$$|\mathrm{g.s.}\rangle = |\nu = 0; J = 0\rangle = (P_j^+)^{n/2}|\Phi_0\rangle$$

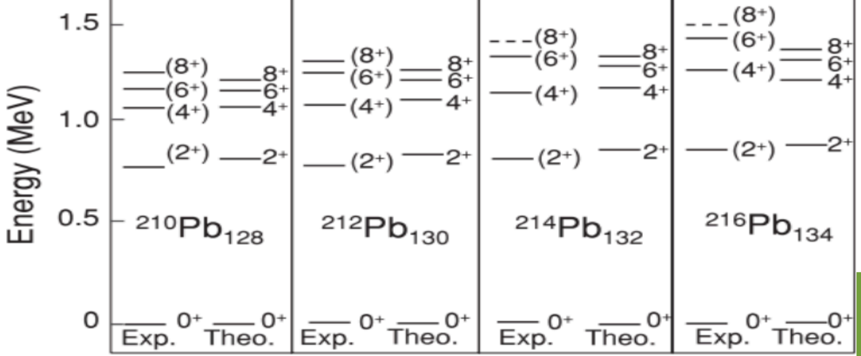
$$|\nu = 2; JM\rangle = (P_j^+)^{(n-2)/2}A^+(j^2JM)|\Phi_0\rangle$$

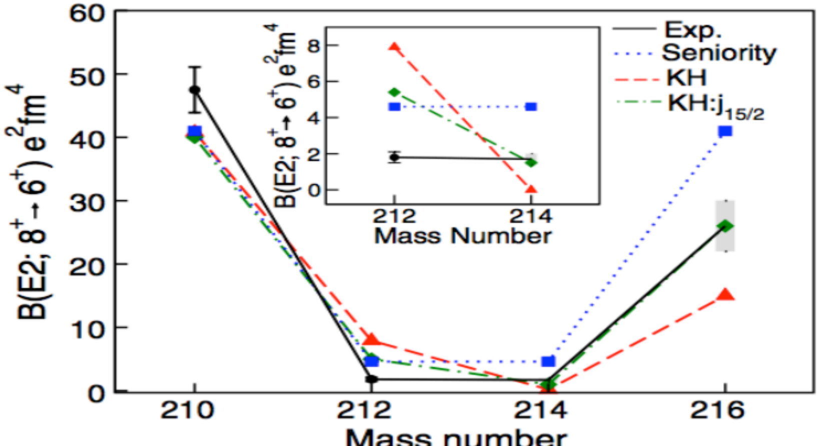
Energy levels of $0g_{9/2}$ protons in N=50 isotones



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)

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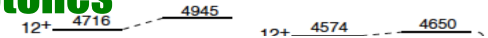
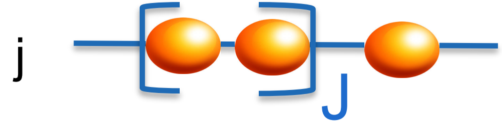
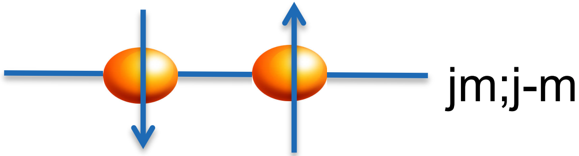
Energy levels of $0g_{9/2}$ protons in *N*=50 isotones



Is 'M=0' pair a relevant degree of freedom





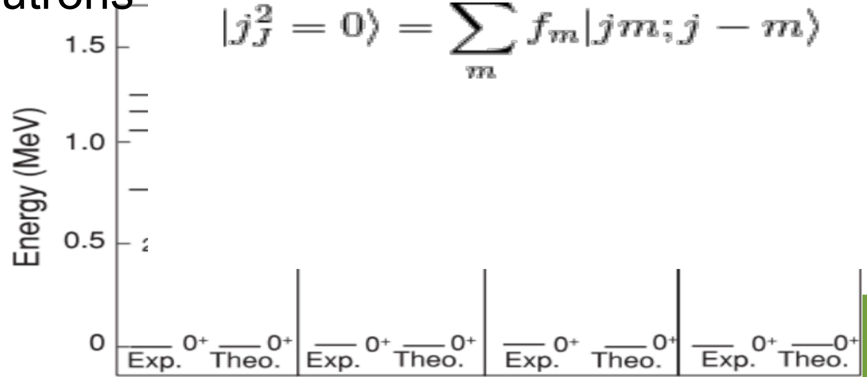
D.J. Rowe and G

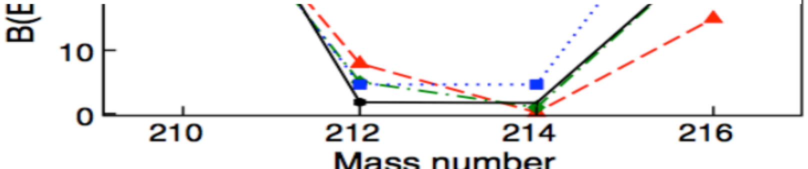
Neutrons

$$|j_J^2 = 0\rangle = \sum_m f_m|jm;j-m\rangle$$

M=0

J=0,2,4…

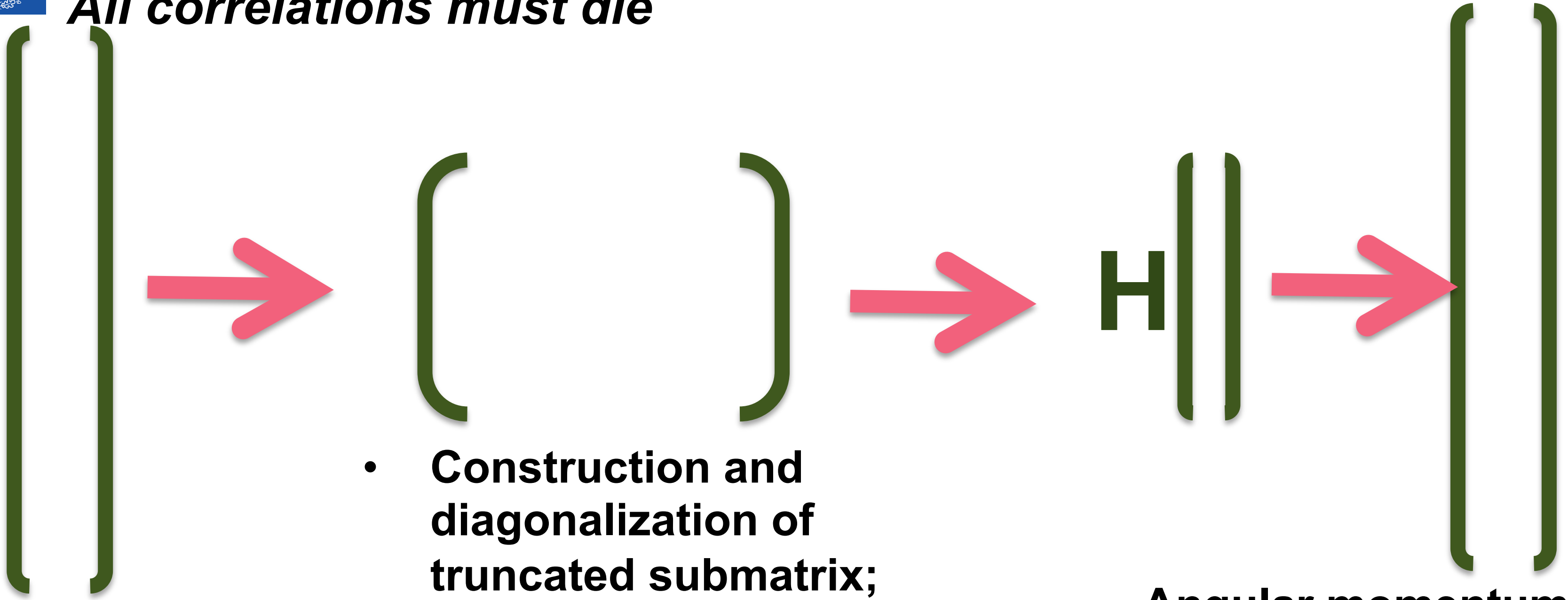




A. Gottardo et al., PRL 109, 162502 (2012)

Construction of ‘ideal’ trial wave function *by hand*

All correlations must die



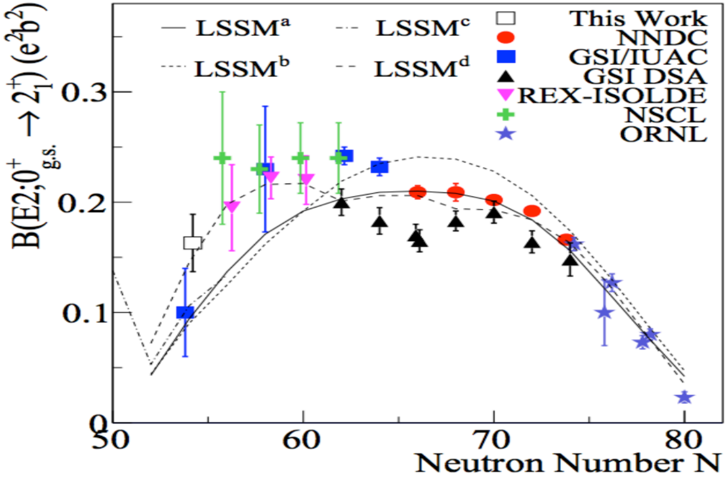
- **Construction and diagonalization of truncated submatrix;**
- **‘Eigen function’ with approximate angular momentum**

Angular momentum restoration

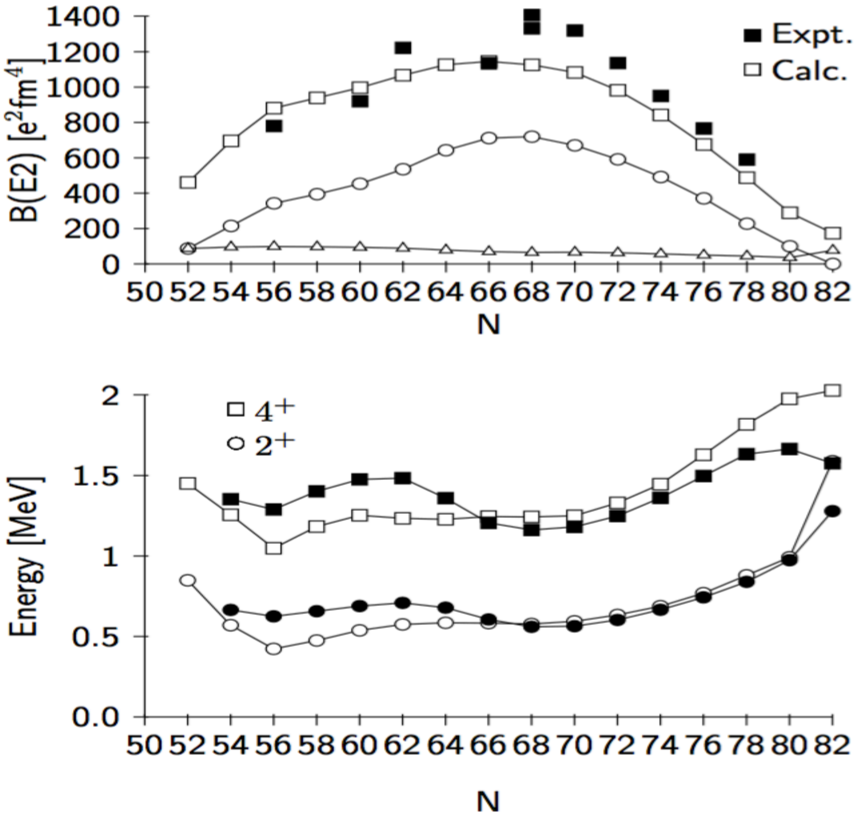
Full uncorrelated M-scheme basis

Together with XiaoYu Liu, N. Shimizu, T. Otsuka

Experimental and calculated B(E2) for Sn and Te isotopes



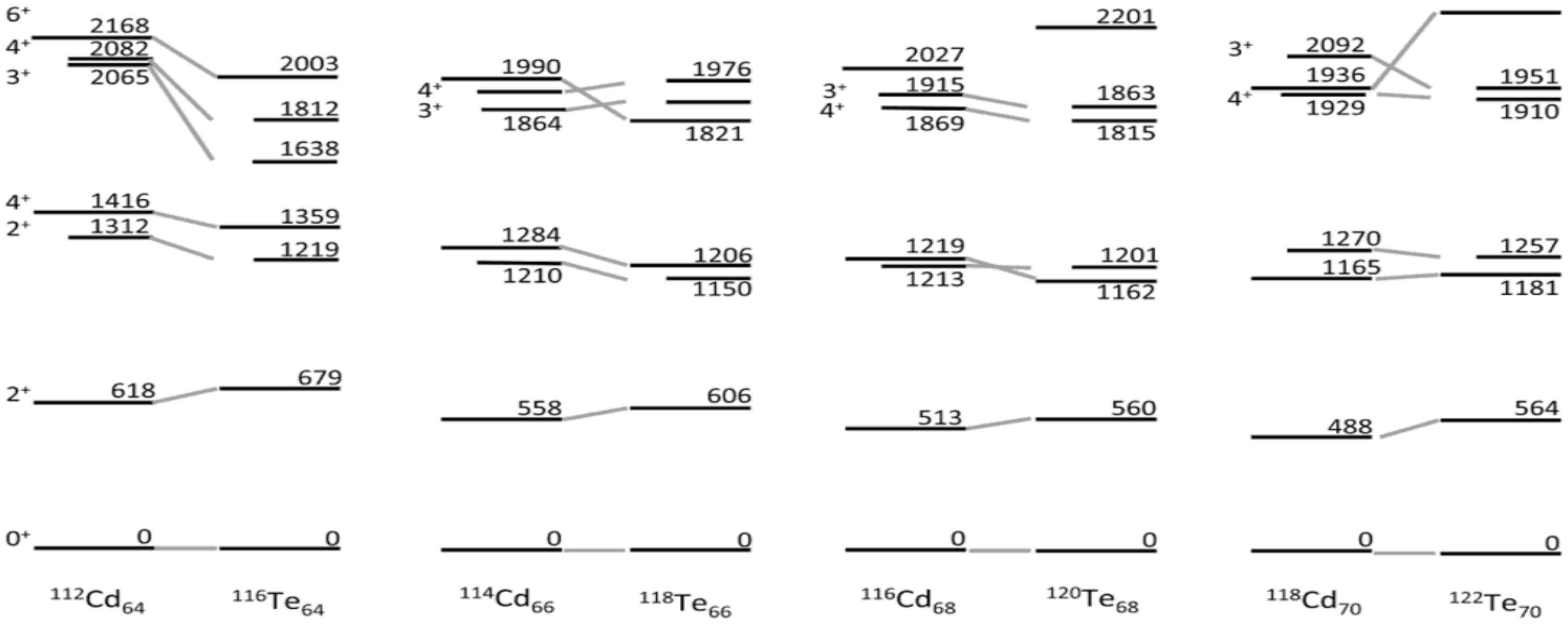
P. Doornenbal et al,arxiv.org/abs/1305.2877



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

CQ, Phys. Rev. C 94, 034310 (2016); data from M. Doncel, CQ et al, PRC 91, 061304(R) (2015) and Nudat2.4

Cd and Te isotopes long considered as best candidates for quadrupole vibration



J.L. Wood, Emergent Phenomena in Atomic Nuclei from Large-Scale Modeling: A Symmet
edited by Kristina D Launey

Cd and Te isotopes long considered as best candidates for quadrupole vibration

6^+ 2168 2201

PHYSICAL REVIEW C **92**, 064309 (2015)

Effective field theory for nuclear vibrations with quantified uncertainties

E. A. Coello Pérez[1] and T. Papenbrock[1,2]
[1]*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*
[2]*Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
(Received 9 October 2015; published 14 December 2015)

We develop an effective field theory (EFT) for nuclear vibrations. The key ingredients—quadrupole degrees of freedom, rotational invariance, and a breakdown scale around the three-phonon level—are taken from data. The EFT is developed for spectra and electromagnetic moments and transitions. We employ tools from Bayesian statistics for the quantification of theoretical uncertainties. The EFT consistently describes spectra and electromagnetic transitions for ^{62}Ni , ^{98,100}Ru , ^{106,108}Pd , ^{110,112,114}Cd, and ^{118,120,122}Te within the theoretical uncertainties. This suggests that these nuclei can be viewed as anharmonic vibrators.

$^{112}Cd_{64}$ $^{116}Te_{64}$ $^{114}Cd_{66}$ $^{118}Te_{66}$ $^{116}Cd_{68}$ $^{120}Te_{68}$ $^{118}Cd_{70}$ $^{122}Te_{70}$

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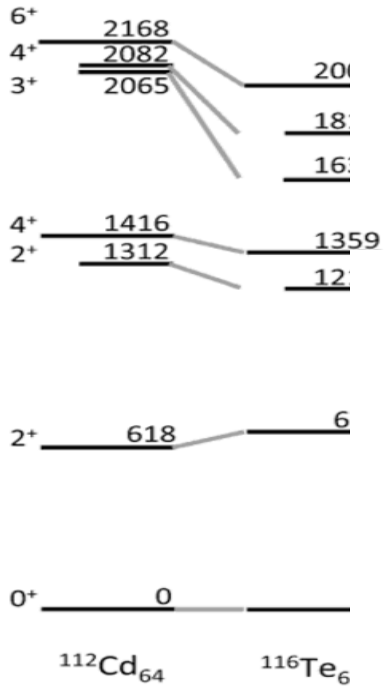

PHYSICAL REVIEW C **71**, 064324 (2005)

$E2$ transition probabilities in ^{114}Te: A conundrum

O. Möller, N. Warr, J. Jolie, A. Dewald, A. Fitzler, A. Linnemann, and K. O. Zell
Institut für Kernphysik, Universtät zu Köln, Zülpicher Straße 77, D-50937 Köln, Germany

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Lawrence Livermore National Laboratory, Livermore, California 94551, USA

S. W. Yates
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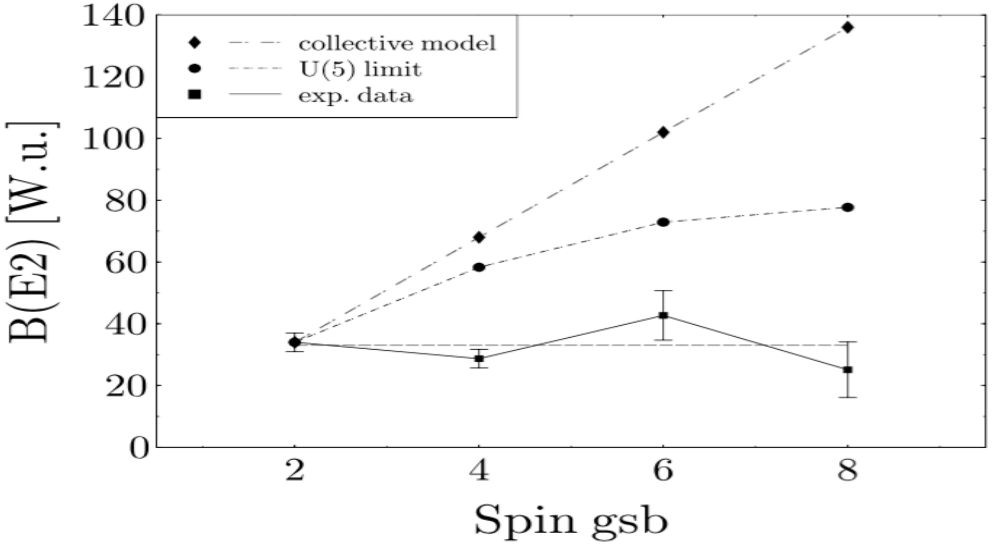
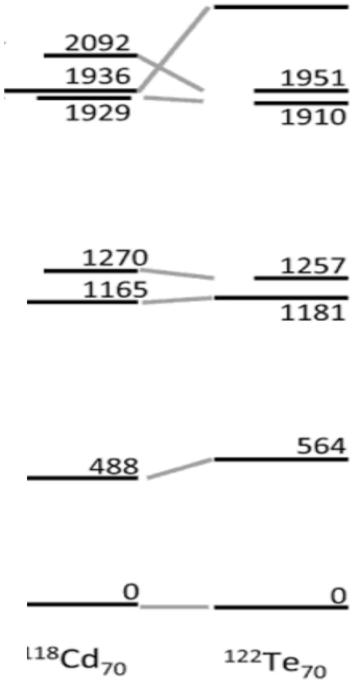
(Received 11 February 2005; published 30 June 2005)





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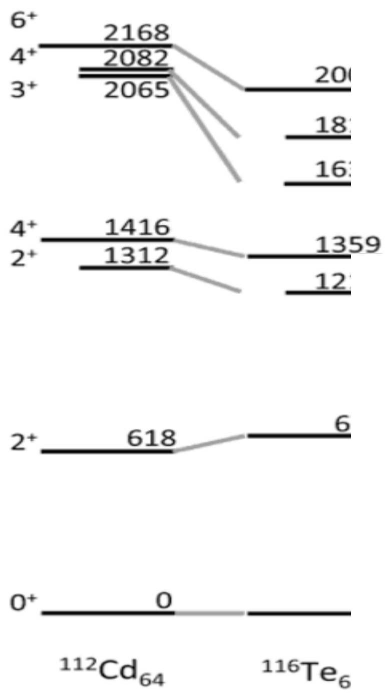

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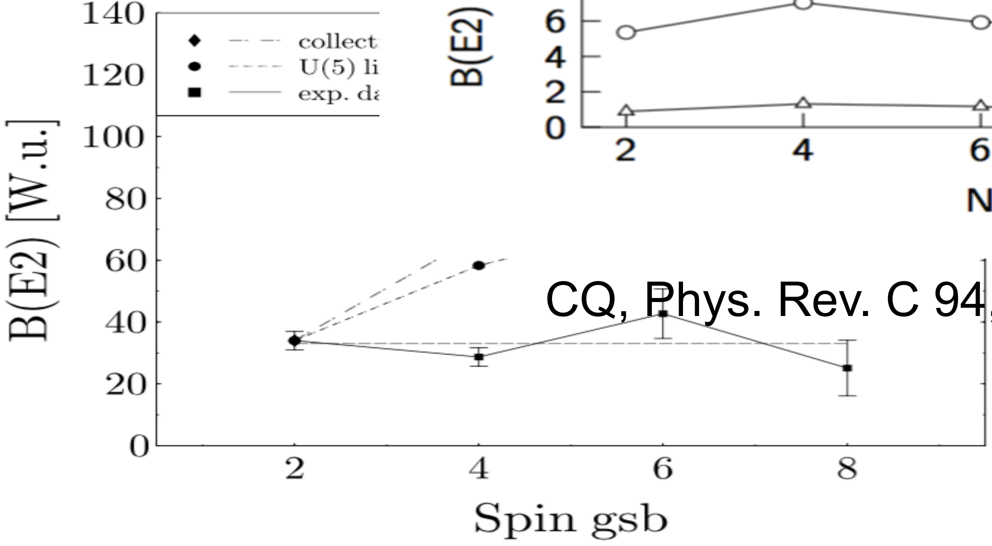

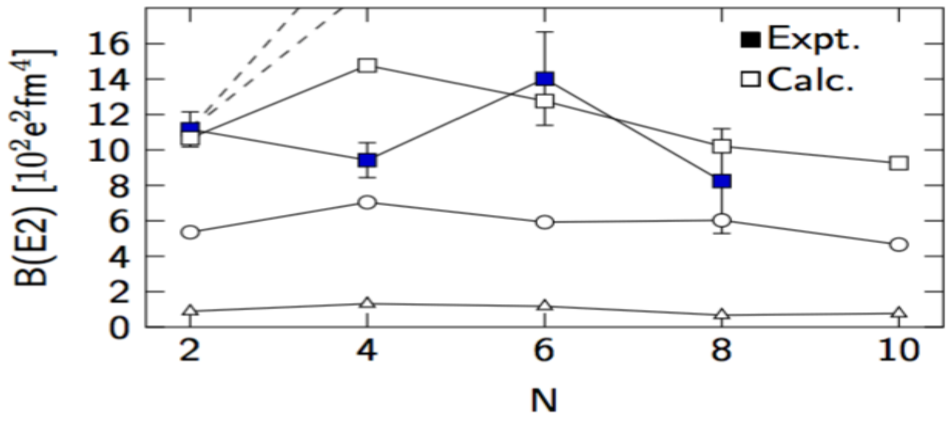

CQ, Phys. Rev. C 94, 034310 (2016)

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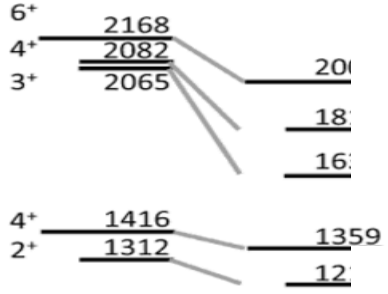
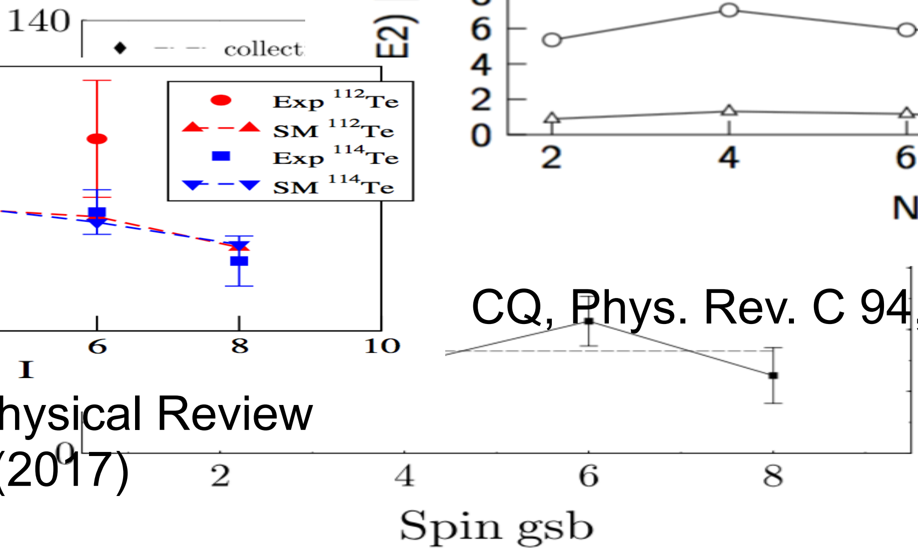
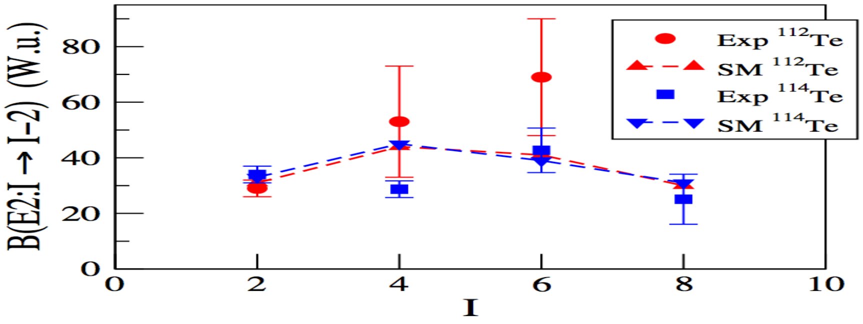
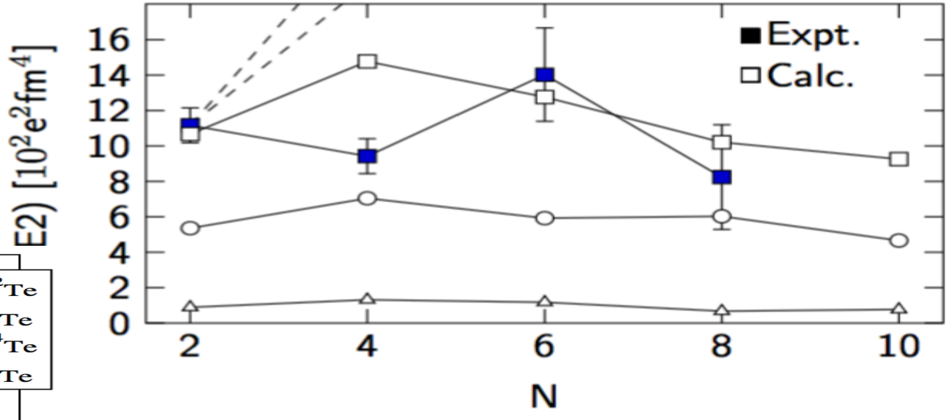
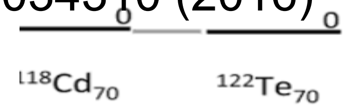






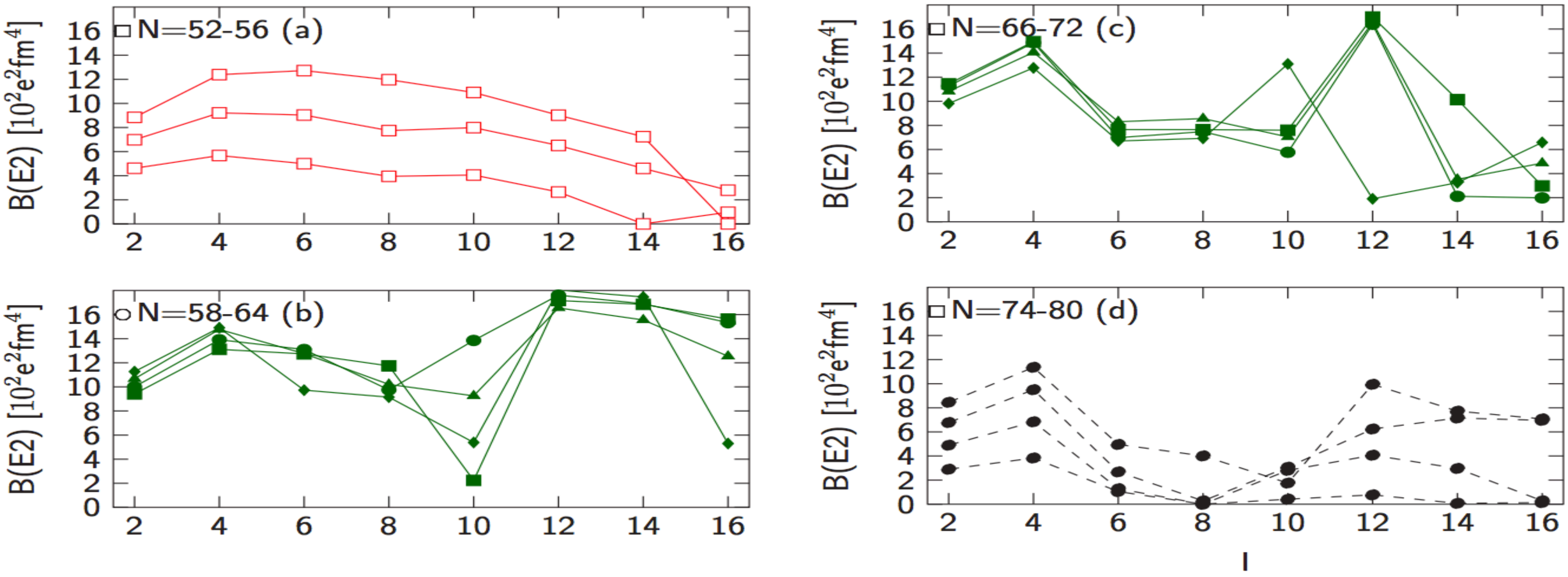




CQ, Phys. Rev. C 94, 034310 (2016)

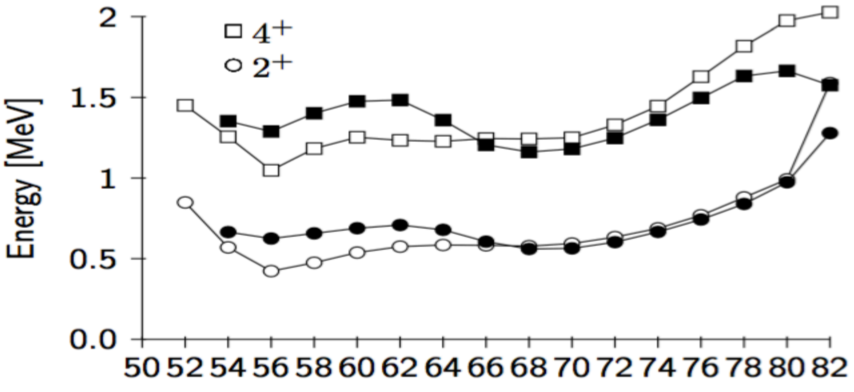
M. Doncel et al, Physical Review C 96 (5), 051304 (2017)

J.L. Wood, Emerge… Modeling: A Symmet
edited by Kristina D Launey



CQ, Phys. Rev. C 94, 034310 (2016)

Enhanced np correlation when N approaches 50?



CQ, Phys. Rev. C 94, 034310 (2016); data from M. Doncel, CQ et al, PRC 91, 061304(R) (2015) and Nudat2.4

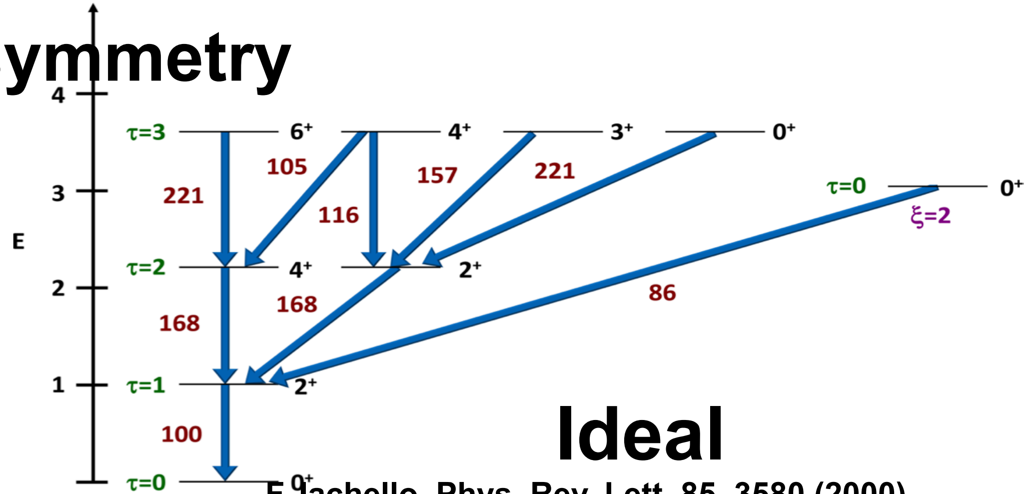
PHYSICAL REVIEW C **82**, 024307 (2010)

Investigations of proton-neutron correlations close to the drip line

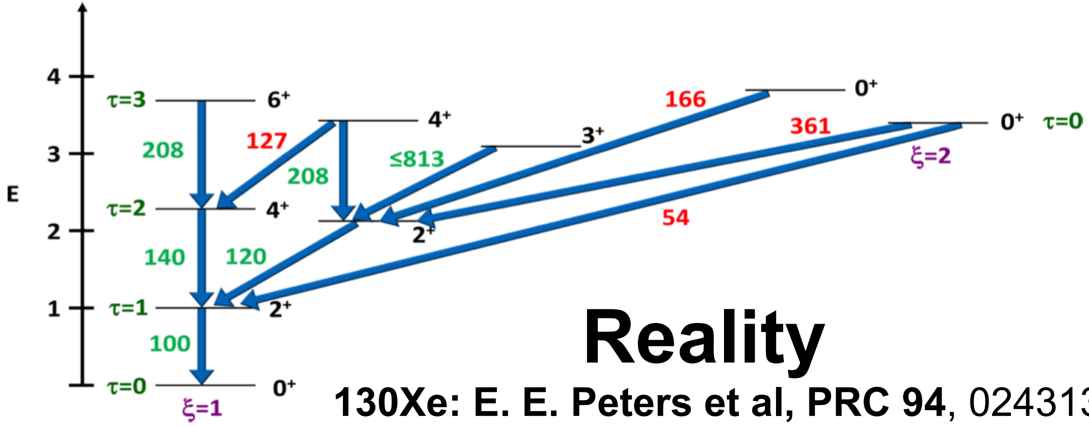
D. S. Delion,[1,2] R. Wyss,[3] R. J. Liotta,[3] Bo Cederwall,[3] A. Johnson,[3] and M. Sandzelius[3]
[1] *"Horia Hulubei" National Institute of Physics and Nuclear Engineering, 407 Atomistilor, RO-077125 Bucharest-Măgurele, Romania*
[2] *Academy of Romanian Scientists, 54 Splaiul Independentei, RO-050085 Bucharest, Romania*
[3] *Royal Institute of Technology, AlbaNova University Center, SE-10691 Stockholm, Sweden*
(Received 22 December 2009; revised manuscript received 28 June 2010; published 9 August 2010)

E(5) critical-point symmetry

- ^{134}Ba may be best candidate for E(5)
- Xe ruled out?
- ^{132,134}Ba 'largest' systems one can treat in shell model calculations
- Shell model gives strong $2^+_3 \rightarrow 0^+_2$ transitions in all $^{128-132}$Xe



F. Iachello, Phys. Rev. Lett. 85, 3580 (2000).
R. F. Casten and N. V. Zamfir, Phys. Rev. Lett. 85, 3584



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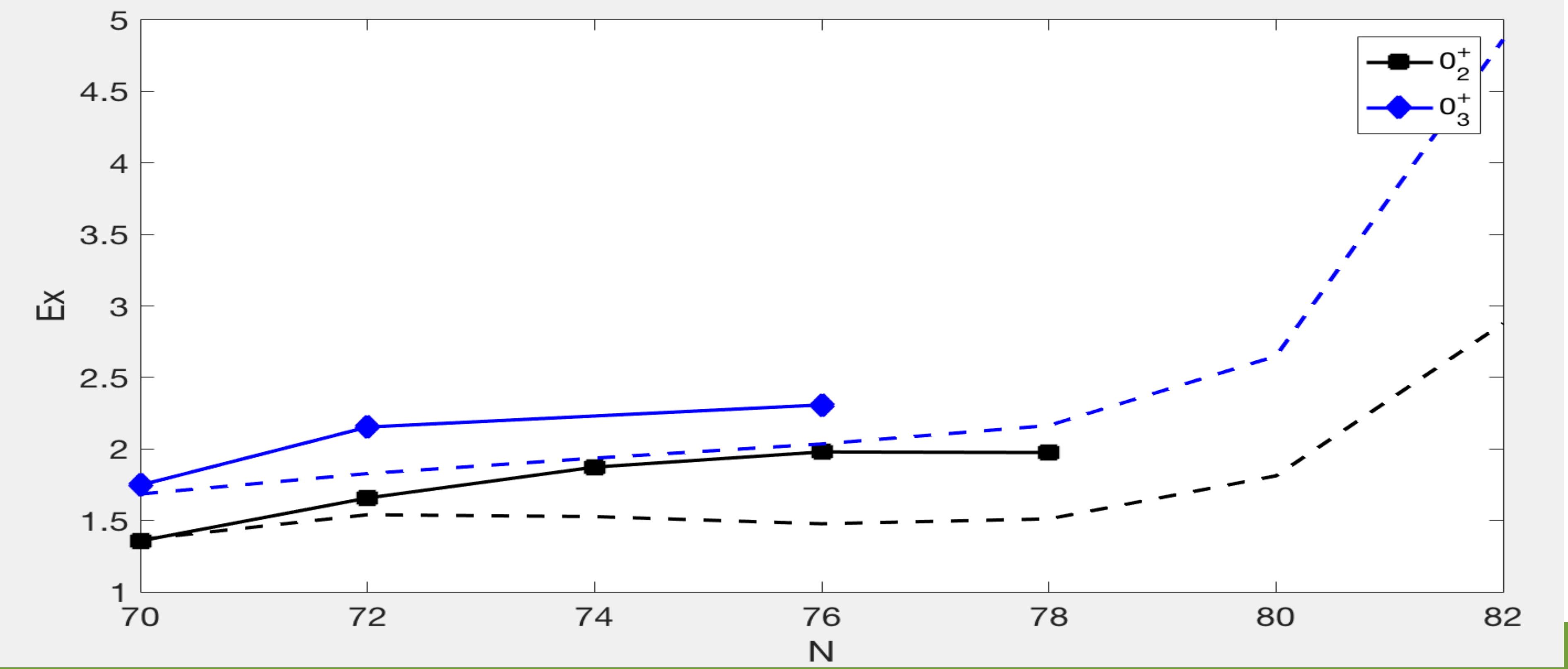
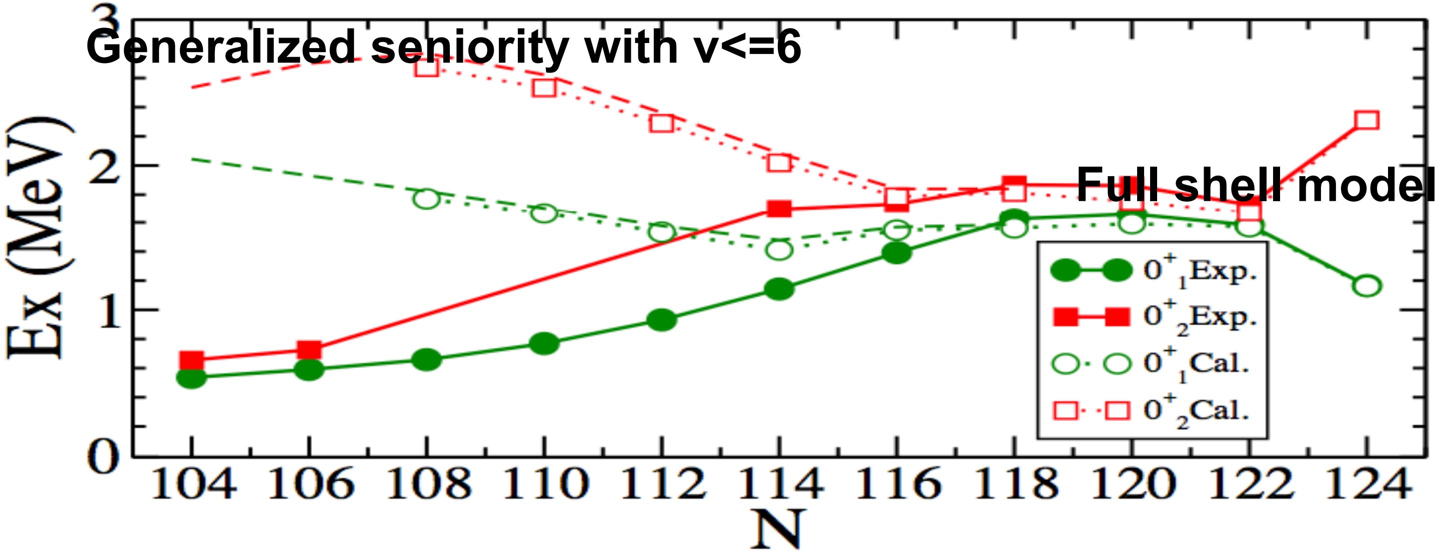
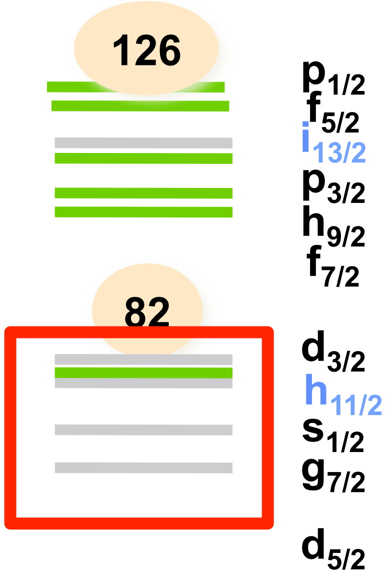
Experimental and calculated 0+ states in Te isotopes



The excited 0+ states in Pb isotopes

Present model space **not sufficient** for those deformed 0+ states





CQ, LY Jia, GJ Fu, Phys. Rev. C 94, 014312 (2016)

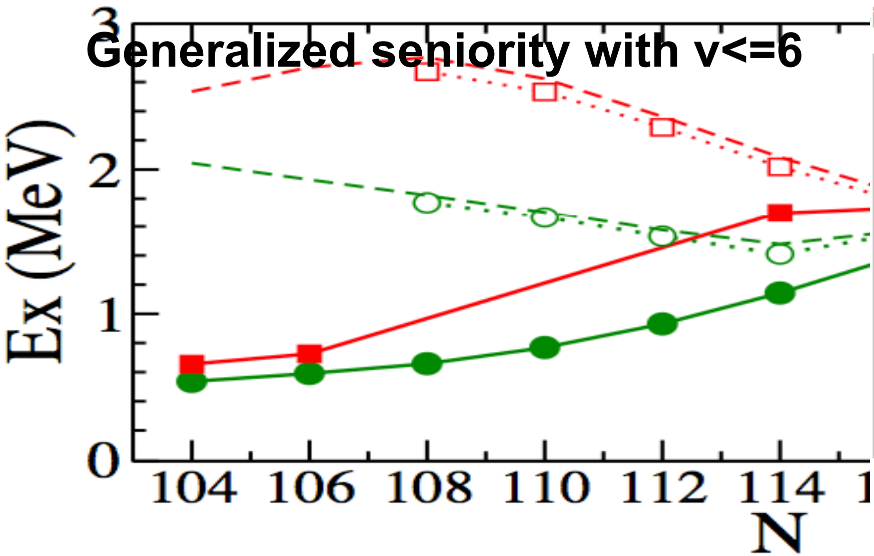
n

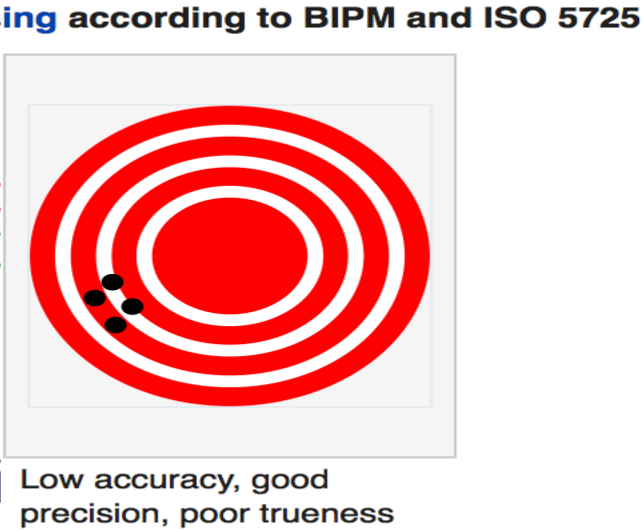
$$0_1^+ = +a|sph\rangle + b|def\rangle$$

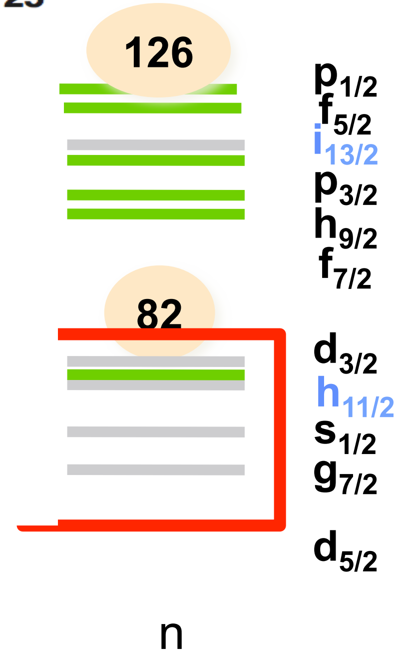
$$0_2^+ = -b|sph\rangle + a|def\rangle$$

The excited 0+ states in Pb isotopes

Present model space **not sufficient** for those deformed 0+ states







CQ, LY Jia, GJ Fu, Phys. Rev. C 94, 014312 (2016)

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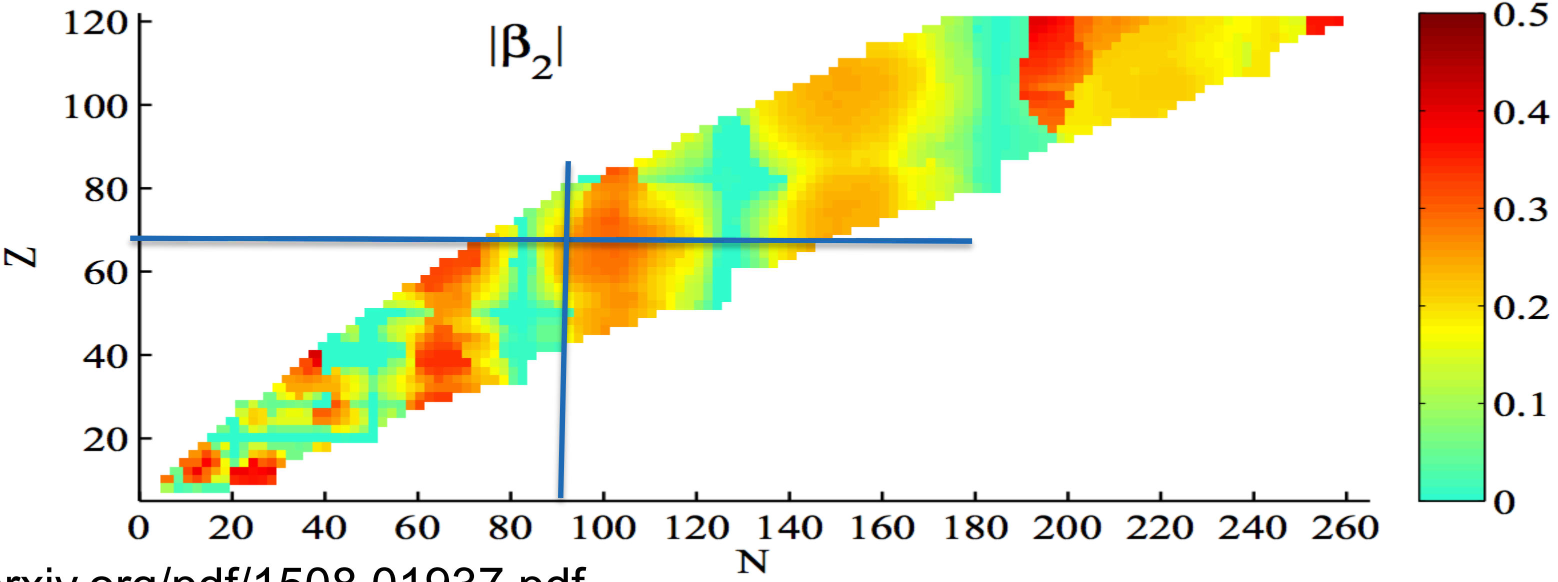
Quantum phase transitions around N=60/90



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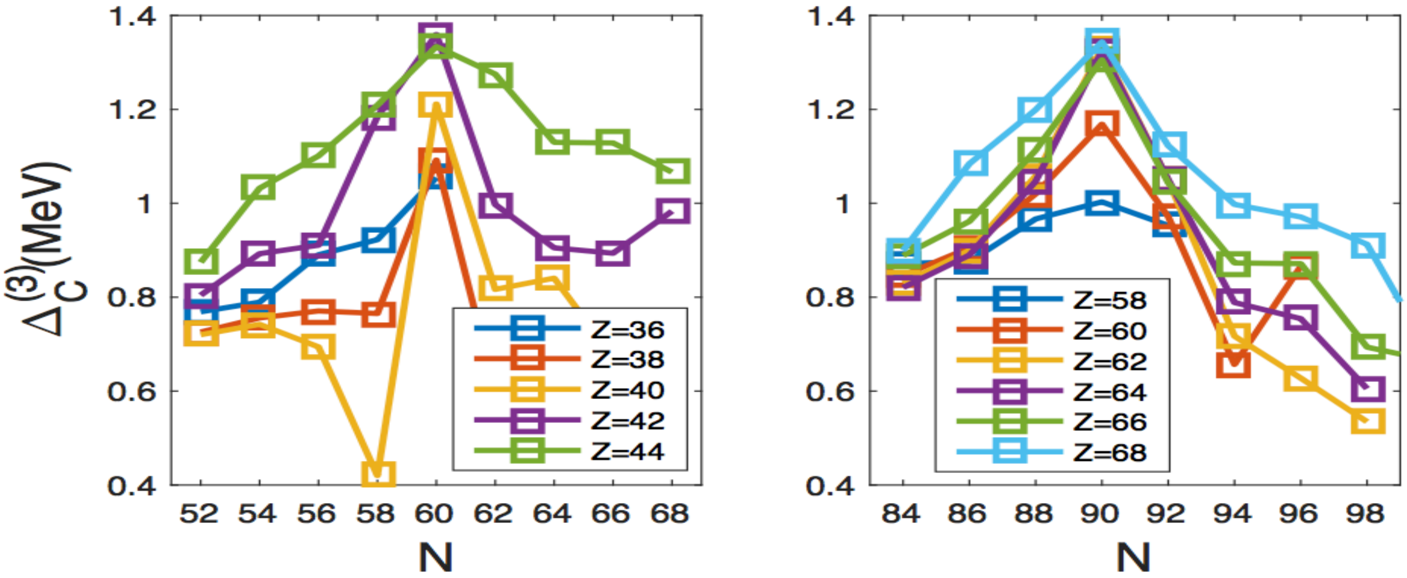
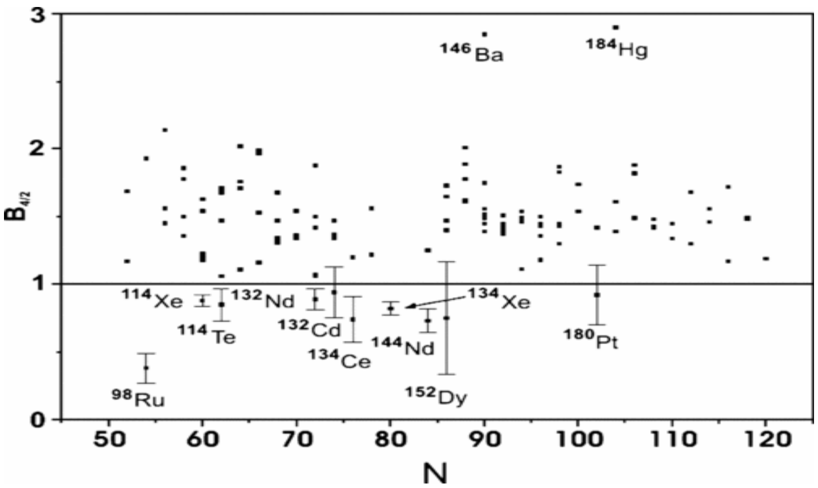
For reviews on the subject, see

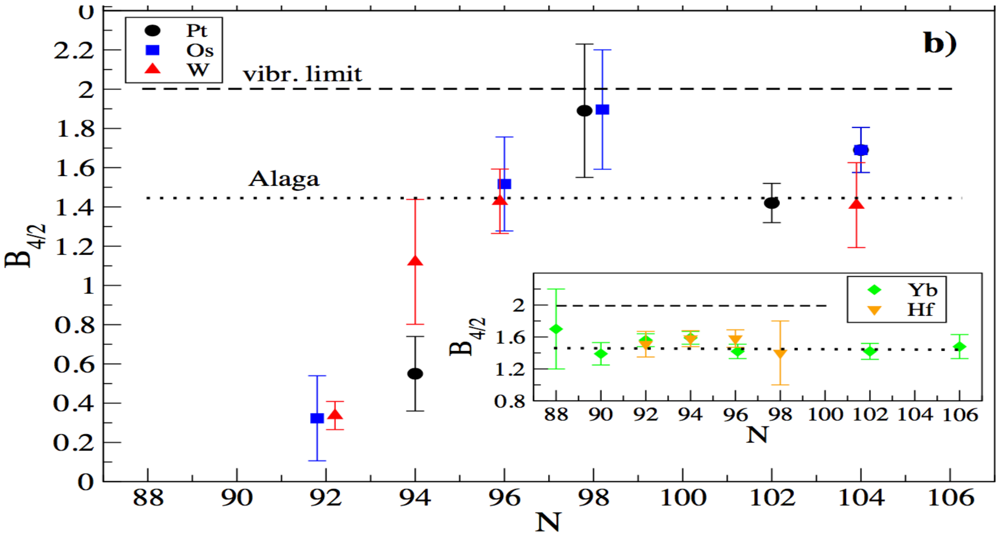
Pavel Cejnar, Jan Jolie, and Richard F. Casten, Rev. Mod. Phys. 82, 2155 , 2010

T. Otsuka, Y. Tsunoda, T. Togashi, N. Shimizu, T. Abe, arXiv:1711.02275

Binding energy odd-even staggering and sudden onset of deformation around N=90

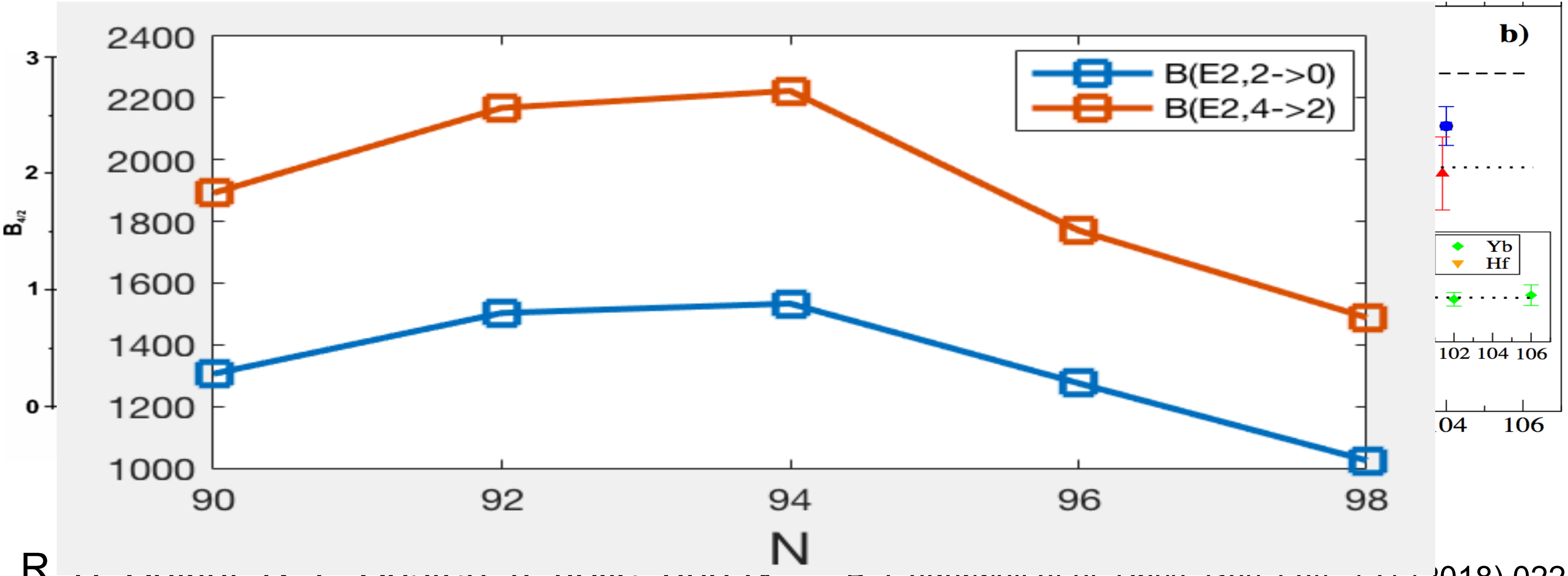






R. B. Cakirli, R. F. Casten, J. Jolie, and N. Warr
Phys. Rev. C 70, 047302 (2004)

B. Cederwall et al, Phys. Rev. Lett. 121 (2018) 022502
CQ etal, to be submitted



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B. Cederwall et al, Phys. Rev. Lett. 121 (2018) 02250
CQ etal, to be submitted

Onset/Breaking of the seniority symmetry

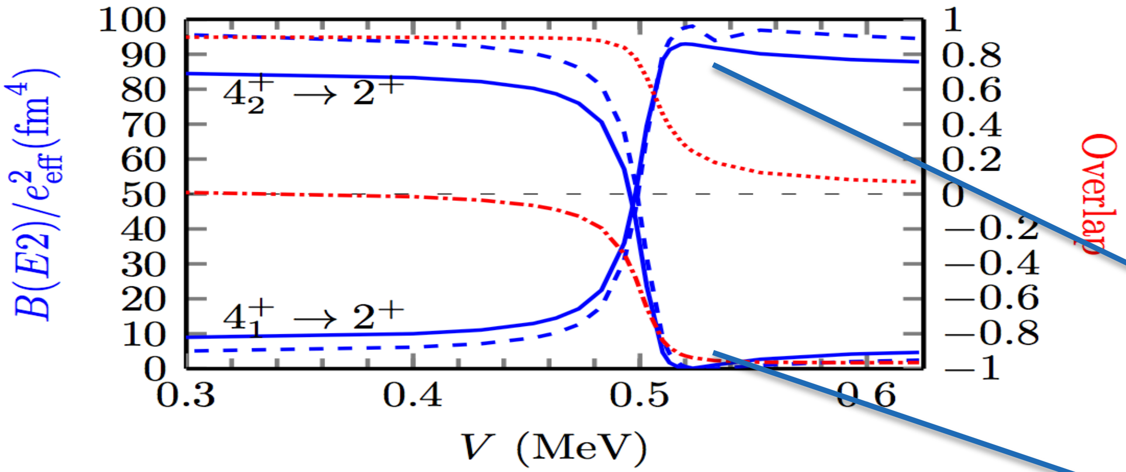


Figure 5. E2 transition strengths (solid lines) for the tran sitions $4^+_{1,2} \rightarrow 2^+_1$ in ^{96}Pd calculated in a minimal mode space $p_{1/2,3/2}g$ calculated by varying the strength of the non-diagonal matrix element $V^{J=2}_{p_{3/2}p_{3/2}g_{9/2}g_{9/2}}$. The dashe lines correspond to the transition from $4^+_{1,2}$ to the stat $|g^{-4}_{9/2}, v = 2, I = 2\rangle$. The dotted and dash-dotted lines (red show the overlaps between 4^+_1 and the seniority $v = 2$ an

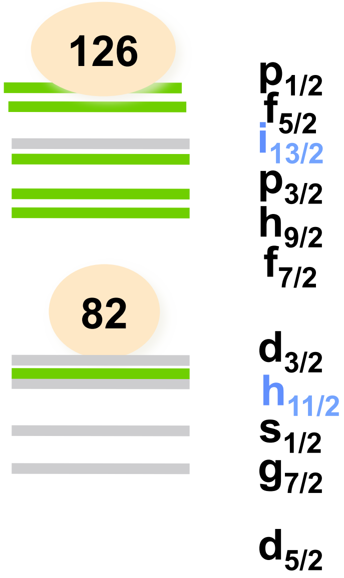
Table 1. Experimental and calcu states in ^{94}Ru, ^{96}Pd and ^{98}Cd. Th results from this work are marke the theoretical calculations marke

$J_i \rightarrow J_f$	Exp	B
^{94}Ru		
$2 \rightarrow 0$	$\geq$9.5 [a]	266
$4 \rightarrow 2$	$\geq$46 [a]	
$6 \rightarrow 4$	2.89(10)	6.6
$8 \rightarrow 6$	0.090(5)	3.1
^{96}Pd		
$2 \rightarrow 0$	$\geq$6 [a]	
$4 \rightarrow 2$	3.8(4) [a]	
$6 \rightarrow 4$	24(2) [a]	
$8 \rightarrow 6$	8.9(13)	
^{98}Cd		
$8 \rightarrow 6$	31(4), $14.5^{+7.5}_{-3.5}$	

C Qi Physics Letters B 773, 616-619 (2017)

Summary

- Monopole optimized interaction
- Truncation methods
- ‘Vibrational’ nuclei around ^{100}Sn
- N=90 transitional nuclei
- Exotic EM transition properties in certain nuclei with ‘regular’ nuclear spectra



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Thank you!