High-Performance Algorithm for Calculating Non-Spurious Spin- and Parity-Dependent Nuclear Level Densities

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◊ **Support from DOE grant DF-FC02-09ER41584 is acknowledged**

Year-5 deliverables

- Develop and test the Moments Method nuclear level density code that removes the center-of-mass spurious states
- Use the new Moments Method code to calculate nuclear level densities and reaction rates in the rp-process path

Nuclear Level Densities

- need to know nuclear level densities (NLD) for nuclear reactions, astrophysics, and applications
- theories and methods:
  - Fermi Gas Model: combinatorics of single-particle excitations near the Fermi surface. H. A. Bethe, 1936

$$\rho(E, J, \pi) = \frac{1}{2} F(U, J) \rho_{FG}(U), \quad \text{where} \quad U = E - \Delta$$

  - Hartree-Fock-Bogolyubov model: also combinatorics

S. Goriely, Nucl. Phys. **A605**, 28 (1996)
Demetriou and Goriely, Nucl. Phys. **A695**, 95 (2001)
S. Goriely, S. Hilaire, and A.J. Koning, Phys. Rev. C **78** 064307 (2008)
Goriely et al., Nucl. Phys. **A773**, 279 (2006); http://www.astro.ulb.ac.be/Html/nld_comb.html

  - Shell Model calculations. Moments Method: describes statistical properties of nuclei

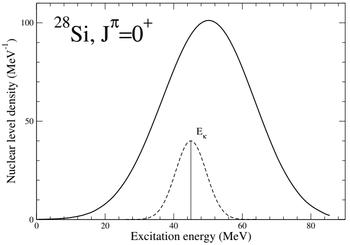
J. B. French and K. F. Ratcliff, Phys. Rev. C**3**, 94 (1971)
S. S. M. Wong, *Nuclear Spectroscopy*, 1986
M. Horoi et al.: PRC **69** 041307(R), (2004); NPA **785**, 142 (2005); PRL **98**, 262503 (2007)

Moments Method. Statistical Spectroscopy

$$\rho(E,\alpha) = \sum_{\kappa} D_{\alpha\kappa} \cdot G(E + E_{gs} - E_{\alpha\kappa}, \sigma_{\alpha\kappa})$$

$\alpha = \{n, J, T_z, \pi\}$ - set of quantum numbers, $G(E,\sigma)$ - Gaussian function

κ - configurations, e.g. 6 particles in *sd* shell:



κ	$d\frac{5}{2}$	$s\frac{1}{2}$	$d\frac{3}{2}$
1	6	0	0
2	5	1	0
3	5	0	1
4	4	2	0
...	...	...	...
15	0	2	4

$D_{\alpha\kappa}$ - number of many-body states with given J that can be built for a given configuration κ

Moments of H for each configuration κ:

$$E_{\alpha\kappa} = \mathrm{Tr}^{(\alpha\kappa)}[H]/D_{\alpha\kappa}$$

$$\sigma^2_{\alpha\kappa} = \mathrm{Tr}^{(\alpha\kappa)}[H^2]/D_{\alpha\kappa} - \left(\mathrm{Tr}^{(\alpha\kappa)}[H]/D_{\alpha\kappa}\right)^2$$

M. Horoi, M. Ghita, and V. Zelevinsky, PRC **69** (2004) 041307(R)

it is important to know the E_{gs} and cut-off parameter η

Moments Method. Statistical Spectroscopy

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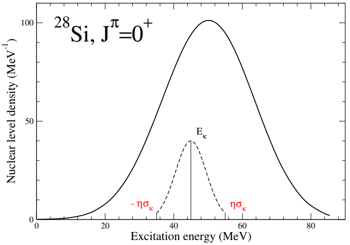

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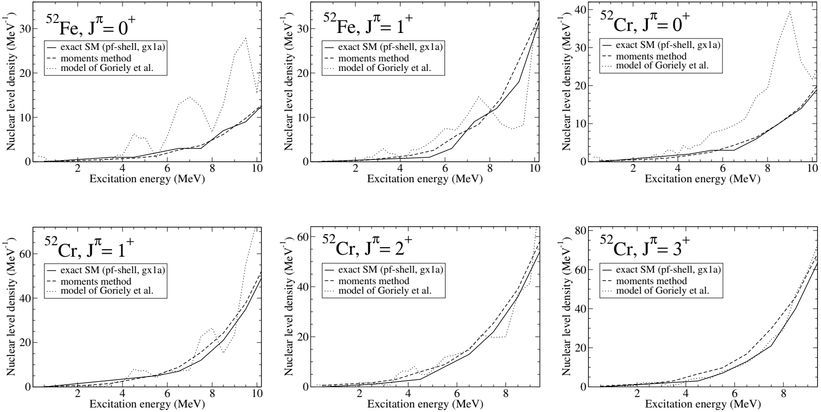
M. Horoi, M. Ghita, and V. Zelevinsky, PRC **69** (2004) 041307(R)

it is important to know the E_{gs} and cut-off parameter η

Results for ^{52}Fe, ^{52}Cr, parity=+1, some *J*. *pf*-shell

Comparison of nuclear level densities between exact Shell Model (solid line), Moments Method (dashed line), and HFB method (dotted line). Cut-off parameter $\eta = 2.6$, interaction GXPF1A.



R. Senkov and M. Horoi, arXiv:1004.5027, Phys. Rev. C **82**, 024304 (2010).

Removal of the center-of-mass spurious states

Lawson method

$$H \rightarrow H' = H + \beta \left[\left(H_{CM} - \frac{3}{2}\hbar\omega \right) \frac{A}{\hbar\omega} \right]$$

D.H. Gloekner and D.R. Lawson, Phys. Lett. B **53**, 313 (1974)

Recursive method

3D-Harmonic oscillator:

$$\mathcal{N}_{pure}(A, K\hbar\omega) = \mathcal{N}_{tot}(A, K\hbar\omega) - \sum_{K'=1}^{K} \mathcal{C}_{K'} \mathcal{N}_{pure}(A, (K - K')\hbar\omega)$$

$$\mathcal{N}_{pure}(A, 0\hbar\omega) = \mathcal{N}_{tot}(A, 0\hbar\omega), \;\; \mathcal{C}_{K'} = (K' + 1)(K' + 2)/2$$

P. Van Isacker, Phys. Rev. Lett. **89**, 262502 (2002)

Nuclear level density:

$$\rho^{(0)}(E, J, K) = \rho(E, J, K) - \sum_{K'=1}^{K} \sum_{J_{K'}=J_{min}}^{K, step\ 2} \sum_{J'=|J-J_{K'}|}^{J+J_{K'}} \rho^{(0)}(E, J', K - K')$$

M. Horoi and V. Zelevinsky, Phys. Rev. Lett. **98**, 262503 (2007)

$N\hbar\omega$ restriction and Width calculation

Before (no restriction):

$$\mathrm{Tr}^{(\alpha\kappa)}[H] = \sum_{\lambda\in\kappa} \langle\lambda|H|\lambda\rangle$$

$$\mathrm{Tr}^{(\alpha\kappa)}[H^2] = \sum_{\lambda\in\kappa}\sum_{\mu} \langle\lambda|H|\mu\rangle\langle\mu|H|\lambda\rangle = \sum_{\lambda\in\kappa} \langle\lambda|H^2|\lambda\rangle$$

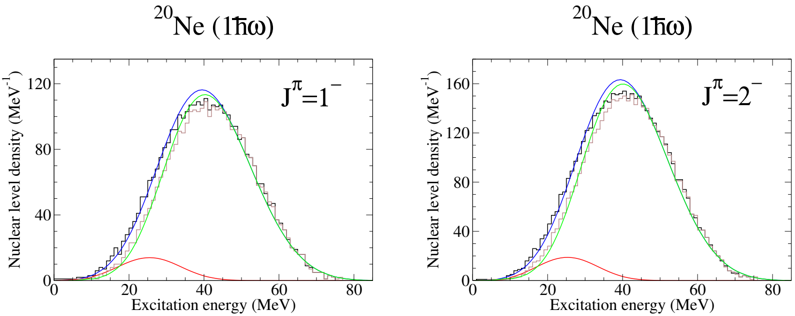
Now (restricted):

$$\mathrm{Tr}^{(\alpha\kappa)}[H] = \sum_{\lambda\in\kappa} \langle\lambda|H|\lambda\rangle$$

$$\mathrm{Tr}^{(\alpha\kappa)}[H^2] \Rightarrow \sum_{\lambda\in\kappa}\sum_{\mu\in R} \langle\lambda|H|\mu\rangle\langle\mu|H|\lambda\rangle \neq \sum_{\lambda\in\kappa} \langle\lambda|H^2|\lambda\rangle$$

R.A. Senkov, M. Horoi, and V.G. Zelevinsky, in press, Phys. Lett. **B**, arXiv:1102.0940

Example: ^{20}Ne, (s-p-sd-pf)-model space, $1\hbar\omega$



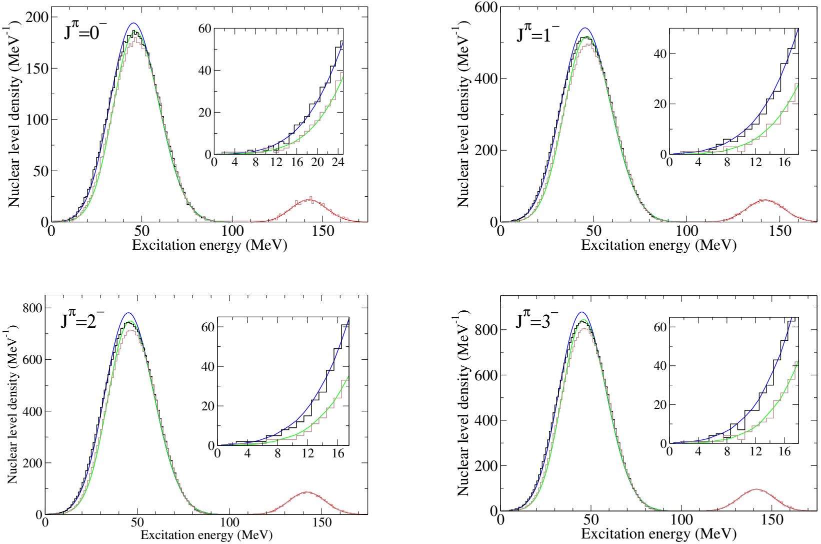
(black), (brown) are shell model calculations with $\beta = 0$ and $\beta = 4$,

(blue), (green), (red) - moments method: ρ, $\rho^{(0)}$, and $\delta\rho = \rho - \rho^{(0)}$

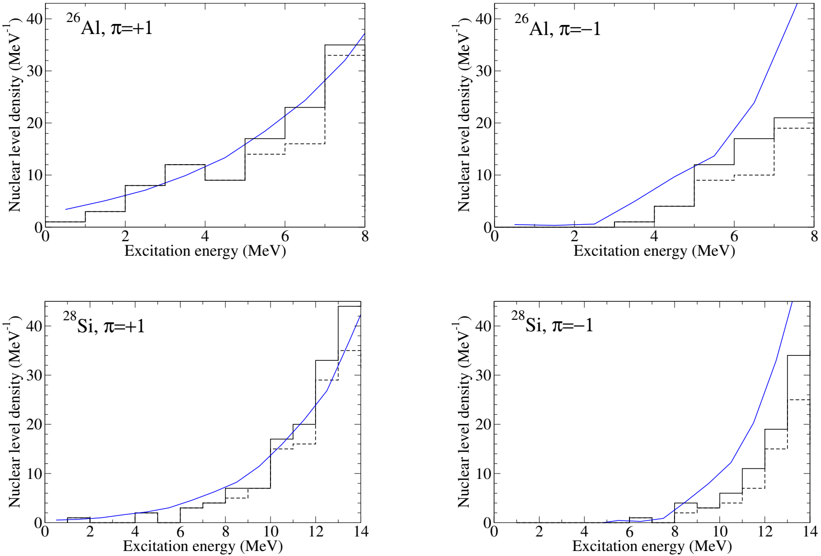
$$J = 1: \quad \rho^{(0)}(E, 1, 1\hbar\omega) = \rho(E, 1, 1\hbar\omega) - \sum_{J'=0}^{2} \rho(E, J', 0\hbar\omega)$$

$$J = 2: \quad \rho^{(0)}(E, 2, 1\hbar\omega) = \rho(E, 2, 1\hbar\omega) - \sum_{J'=1}^{3} \rho(E, J', 0\hbar\omega)$$

^{22}Mg, (s-p-sd-pf)-model space, $1\hbar\omega$, $\beta \cdot A = 110$MeV

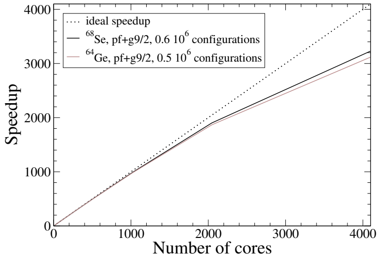


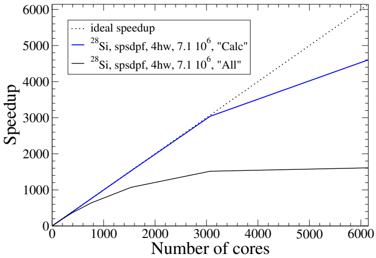
^{26}Al and ^{28}Si, (s-p-sd-pf)-model space, both parities, all J



Code scaling (NERSC/Hopper)

Moments Method Code = “PreCalc” + “Calc”



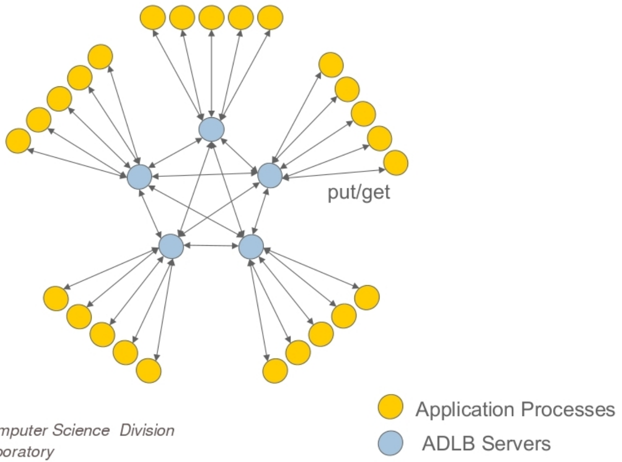


“PreCalc” $\rightarrow N_p + N_n \approx 5.3 \cdot 10^3$ conf. – scales not good
“Calc” $\rightarrow N_p \cdot N_n \approx 7.1 \cdot 10^6$ conf. – scales good

at Number of cores = 1,500: “PreCalc” = 1min, “Calc” = 2.5 min

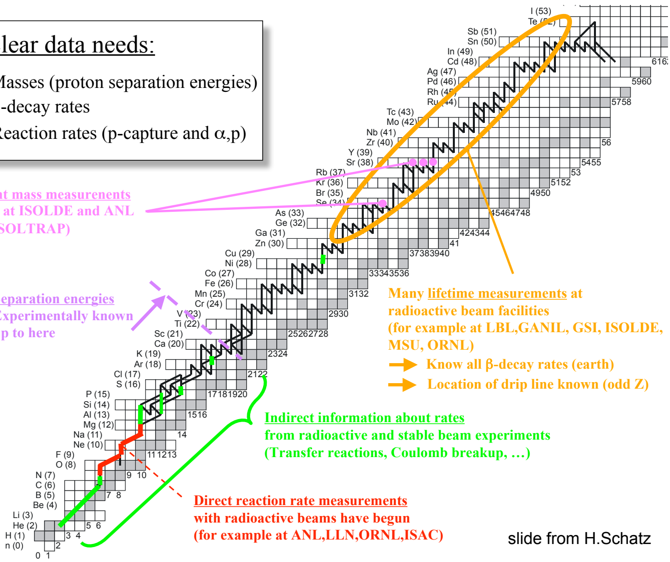
How to improve the “PreCalc” part?

Dynamic load balancing: one Master $\Rightarrow$ several Masters (ADLB)


put/get
Application Processes
ADLB Servers

Nuclear data needs:

- Masses (proton separation energies)
- β-decay rates
- Reaction rates (p-capture and α,p)



Some recent mass measurements
β-endpoint at ISOLDE and ANL
Ion trap (ISOLTRAP)

Separation energies
Experimentally known
up to here

Many lifetime measurements at radioactive beam facilities
(for example at LBL,GANIL, GSI, ISOLDE, MSU, ORNL)

→ **Know all β-decay rates (earth)**

→ **Location of drip line known (odd Z)**

Indirect information about rates
from radioactive and stable beam experiments
(Transfer reactions, Coulomb breakup, …)

Direct reaction rate measurements
with radioactive beams have begun
(for example at ANL,LLN,ORNL,ISAC)

slide from H.Schatz

NLD and Hauser-Feshbach

talys 1.2 : www.talys.eu

NLD-M1

ldmodel 1: Constant temperature + Fermi gas model

ldmodel 2: Back-shifted Fermi gas model

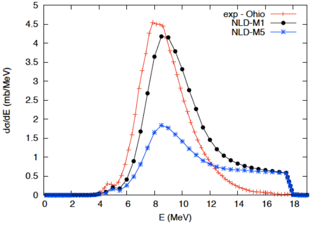
ldmodel 3: Generalised superfluid model

ldmodel 4: Microscopic level densities from Goriely's table

ldmodel 5: Microscopic level densities from Hilaire's table

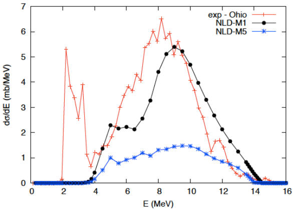
NLD-M5

Exp – Ohio: A. Voinov et al., PRC **76**, 044602 (2007)



$\leftarrow\ ^{58}Fe\left(^{3}He,\alpha\right)$

$\theta = 150^0$



$\leftarrow\ ^{59}Co\left(d,\alpha\right)$

$\theta = 150^0$

Comparison with Moments Densities

talys 1.2 : www.talys.eu

NLD-M1

ldmodel 1: Constant temperature + Fermi gas model

ldmodel 2: Back-shifted Fermi gas model

ldmodel 3: Generalised superfluid model

ldmodel 4: Microscopic level densities from Goriely's table

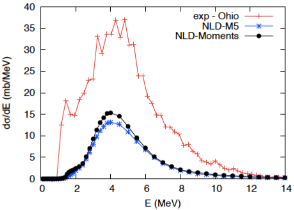
ldmodel 5: Microscopic level densities from Hilaire's table

NLD-M5

Interface:

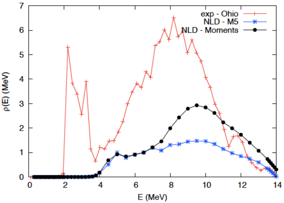
Moments table -> Hilaire's table

Exp – Ohio: A. Voinov et al., PRC **76**, 044602 (2007)



← $^{58}Fe(^{3}He, p)$

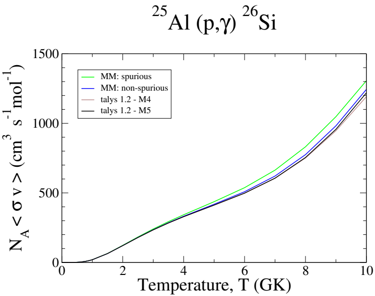
$\theta = 150^0$

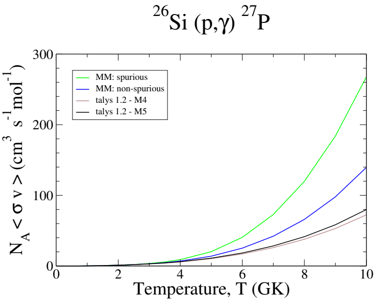


← $^{59}Co(d, \alpha)$

$\theta = 150^0$

Example: reaction rates in rp-process path





TALYS 1.2: http://www.talys.eu/

M4: S. Goriely, F. Tondeur, J.M. Pearson, Atom. Data Nucl. Data Tables 77, 311 (2001).

M5: S. Goriely, S. Hilaire and A.J. Koning, “Improved microscopic nuclear level densities within the HFB plus combinatorial method”, Phys. Rev. C 78, 064307 (2008).

Deliverables for year 5

- new algorithm of removal of the contribution of center-of-mass spurious states was successfully developed and tested
- the code is parallelized and was tested using up to 6,000 processors
- calculations of NLD in large model spaces were performed
- calculations of reaction rates in the rp-process path were made

What's next?

- improve the scaling
- develop interface, scripts
- write documentation, examples. publish the code
- more applications: NLD, reaction rates, schematic interactions

CMU Personnel:

Mihai Horoi, PI
Roman Senkov, postdoc
Jagjit Kaur, student

Publications:

1. “A High-Performance Algorithm to Calculate Spin- and Parity-Dependent Nuclear Level Densities”, R. Senkov and M. Horoi, arXiv:1004.5027, Phys. Rev. C 82, 024304 (2010).

2. “Improved Accuracy Moments Method for Spin-Dependent Shell Model Nuclear Level Densities”, M. Scott and M. Horoi, EPL 91, 52001 (2010).

3. “Can one identify the intrinsic structure of the yrast states in ^{48}Cr after the backhanding?”, Z-C. Gao, M. Horoi, Y. S. Chen, Y. J. Chen, and Tuya, Phys. Rev. C 83, 057303 (2011).

4. “An Update of B(E2) Evaluation for $0_1^+ \to 2_1^+$ Transitions in Even-Even Nuclei near N$\sim$Z$\sim$28”, B. Pritychenko, J. Choquette, M. Horoi, B. Karamy, B. Singh, accepted for publication in At. Data. Nucl. Data. Tabels, arXiv:1102.3365 (BNL-94720-2011-JA).

5. “The Role of Shell Model Nuclear Level Densities for Nuclear Astrophysics”, Proceedings of the International Symposium on Nuclear Astrophysics “Nuclei in Cosmos - XI”, Heidelberg, Germany, July 19-23, 2010, PoS(NIC-X)222, (2010), http://pos.sissa.it/, Horoi, M. and Senkov, R.

6. “Nuclear Shell Model Analyses and Predictions of Double-Beta Decay Observables”, Proceedings of the Carpathian Summer School of Physics “Exotic Nuclei & Nuclear/Particle Astrophysics II. From Nuclei to Stars’, Sinaia, Romania, June 20 - July 3, 2010, AIP Proceedings 1304, 106 (2010), Horoi, M.

7. “High-Performance Algorithm for Calculating Non-Spurious Spin- and Parity-Dependent Nuclear Level Densities” , R. Senkov, M. Horoi, and V. Zelevinsky, accepted by Phys. Lett. B, arXiv:1102.0940

Invited talks:

1. M. Horoi, “Challenges for a reliable shell-model description of the neutrinoless double beta decay matrix elements”, MEDEX’11 Workshop, Prague, June 13-16, 2011.

2. M. Horoi, “Updates on Nushellx”, LCCI collaboration meeting, BLNL, March 17-19, 2011.

3. M. Horoi, “Effective Forces Responsible for Enhanced Proton-Neutron Correlations in N $\approx$ Z Nuclei”, ECT* workshop “Effective Theories and the Nuclear Many-Body Problem”, Trento, Italy, March 7-11, 2011.

4. M. Horoi, “Nuclear Structure Theory Relevant to the Facility for Rare Isotope Beams”, colloquium at Western Michigan University, Kalamazoo, MI, January 24, 2011.

5. M. Horoi, “Proton-neutron pairing correlations in nuclei: a shell model perspective”, invited talk at the International Workshop Probing Proton-Neutron Pair Correlations held at Nishina Center, RIKEN Wako-shi campus, Japan, November 19-20, 2010.

6. M. Horoi, “Structure Theory for the Facility of Rare Isotope Beams”, invited talk at the Annual Meeting of Division of Nuclear Physics of the American Physical Society, Santa Fe, New Mexico, November 4, 2010.

7. M. Horoi, “Nuclear Shell Model Analyses and Predictions of Double-Beta Decay Observables”, invited talk at the Carpathian Summer School of Physics ’Exotic Nuclei & Nuclear/Particle Astrophysics II. From Nuclei to Stars’, Cyclotron Institute at Texas A&M, International Center for Theoretical Physics Trieste, Horia Hulubei National Institute of Physics and Nuclear Engineering, Romania, Sinaia, Romania (June 30, 2010).

Accepted talks:

1. R. Senkov and M. Horoi, “High Performance Algorithm for Non-Spurious Spin- and Parity-Dependent Nuclear Level Density”, Annual Meeting of Division of Nuclear Physics of the American Physical Society, Santa Fe, New Mexico, November 4, 2010.

2. S. Stoica, A. Neacsu, and M. Horoi, “Shell model calculations of double-beta decay lifetimes of ^{76}Ge and ^{82}Se”, Annual Meeting of Division of Nuclear Physics of the American Physical Society, Santa Fe, New Mexico, November 4, 2010.