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Novel High Performance Computational Aspects of the Shell Model Approach for Medium Nuclei

Mihai Horoi

Department of Physics, Central Michigan University,

Mount Pleasant, Michigan 48859, USA

Collaborators: R. Senkov, M. Scott, V. Zelevinsky, B.A. Brown

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Overview

- New shell model ideas for the low-lying states
- Novel developments with shell model nuclear level densities
- Potential impact of the shell model nuclear level densities for nuclear astrophysics predictions

Nuclear Configuration Interaction

Center-of-mass spurious states

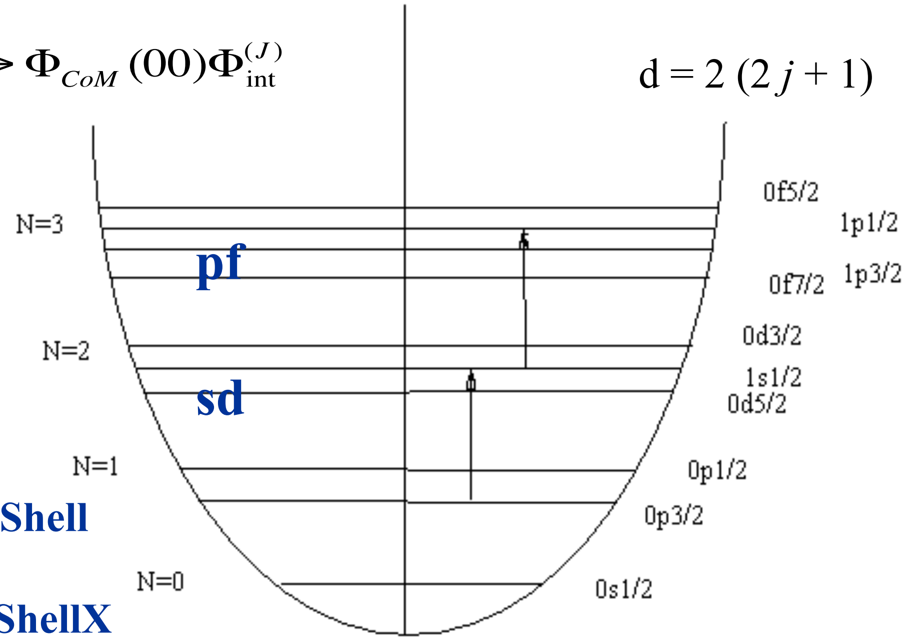
$0\hbar\omega$ $\quad H' = H + \beta(H_{CoM} - 3/2\hbar\omega)$

$1\hbar\omega$ $\quad \Psi^{(J)} = [\Phi_{CoM}(NL)\Phi_{\text{int}}^{(J')}]^{(J)} \rightarrow \Phi_{CoM}(00)\Phi_{\text{int}}^{(J)}$

$(0+2)\hbar\omega$

$(1+3)\hbar\omega$ $\quad$ **N_{max}**

d = 2 (2 j + 1)



$$H = \sum_k \varepsilon_K a_k^+ a_k + \frac{1}{2}\sum_{k\,l\,m\,n} V_{kl;mn} a_k^+ a_l^+ a_n a_m + \cdots$$

$$|\alpha> = \sum_i C_i^\alpha \,|i(JT)>$$ **JT-scheme: OXBASH, NuShell**

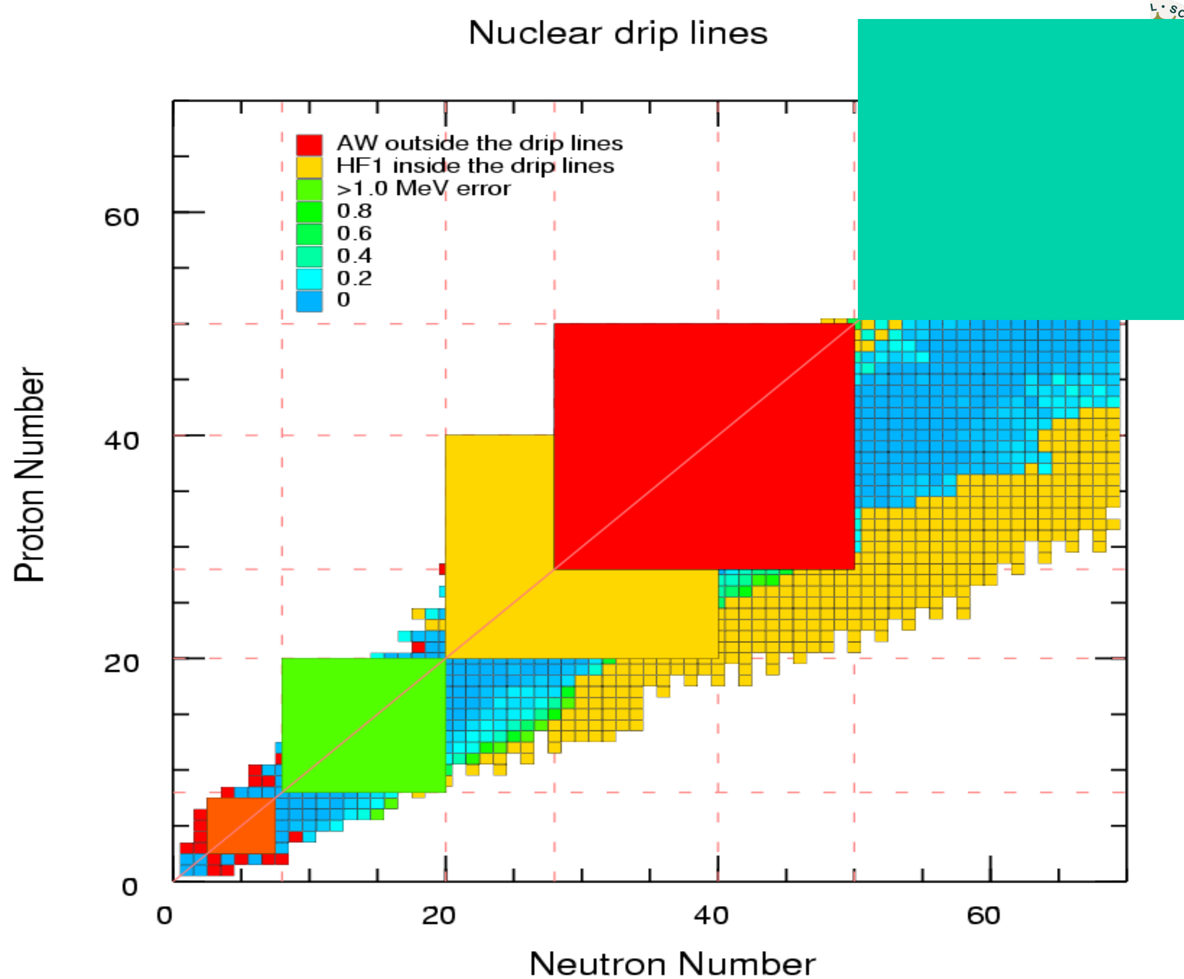
$$|\alpha> = \sum_i C_i^\alpha \,|i(JT_z)>$$ **J-scheme: NATHAN, NuShellX**

$$|\alpha> = \sum_i C_i^\alpha \,|i(MT_z)>$$ **M-scheme: Oslo-code, Antoine, MFDN, MSHELL, CMichSM, …**

$$\sum_j <i|H|j> C_j^\alpha = E_\alpha C_i^\alpha$$

Lanczos algorithm: provides few lower energies, especially the M-scheme codes.

p - 10^2 -1960's
sd - 10^5 - 1980's
pf - 10^9 - 1990's
$pf_{5/2}g_{9/2}$ - 10^{10} - 2006
$g_{7/2}sdh_{11/2}$ - $5x10^{10}$ - '08



Example: ^{76}Sr

$pf_{5/2}g_{9/2}$ dimension

11 090 052 440

Current limit: 10^{10} - 10^{11} –> 46-48 np valence s.p. states

Extensions: Truncations, Exponential Convergence Method,

Coupled Clusters, Projected CI, …

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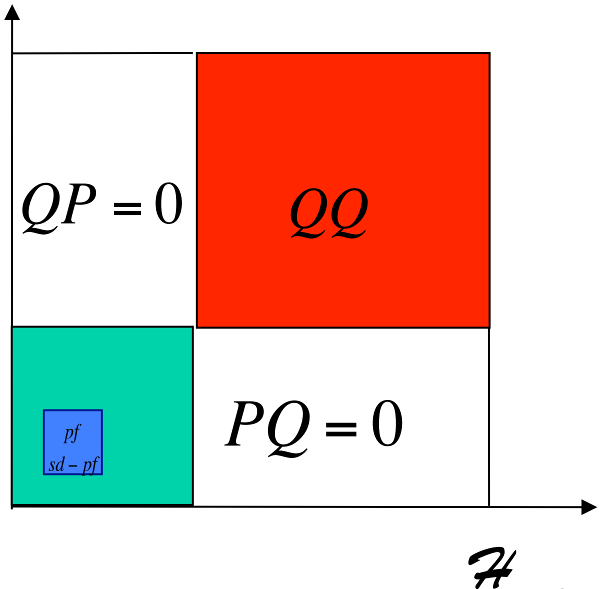
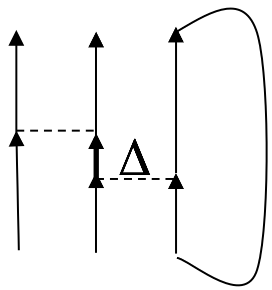
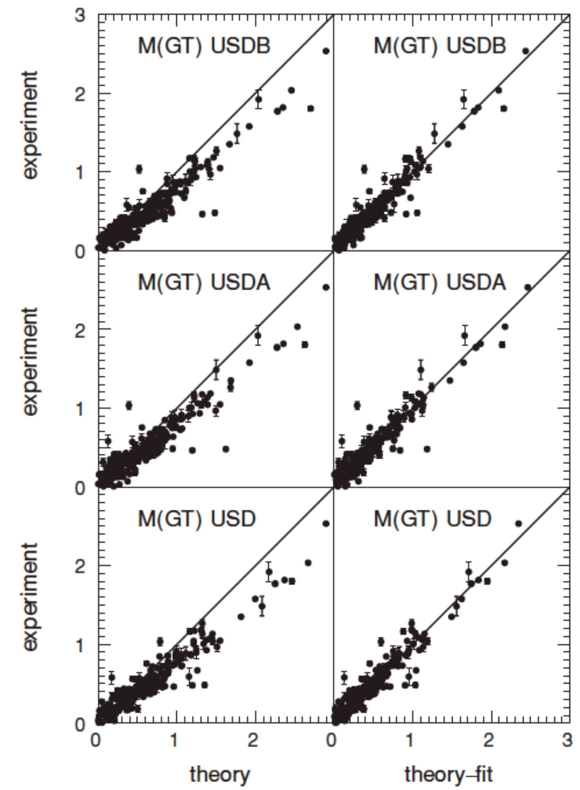
Effective Hamiltonians



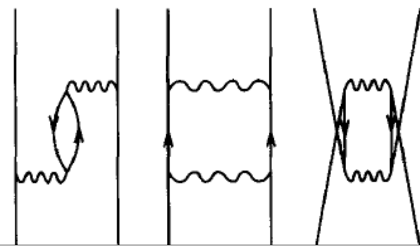


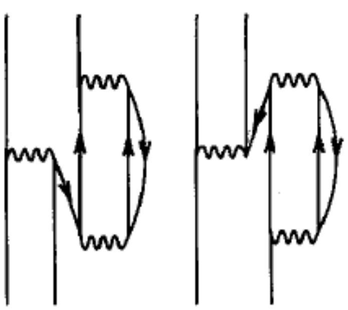
3-body –> two-body

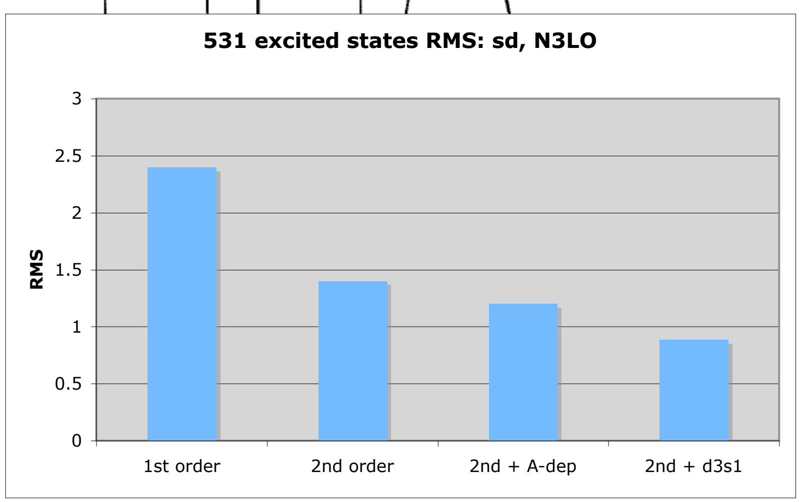


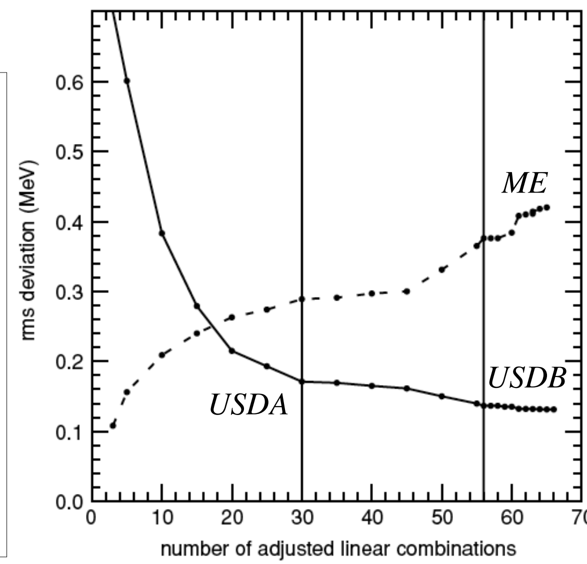
PRC 74, 34315 (2006), 78, 064302 (2008)

core polarization:
Phys.Rep. **261**, 125 (1995)









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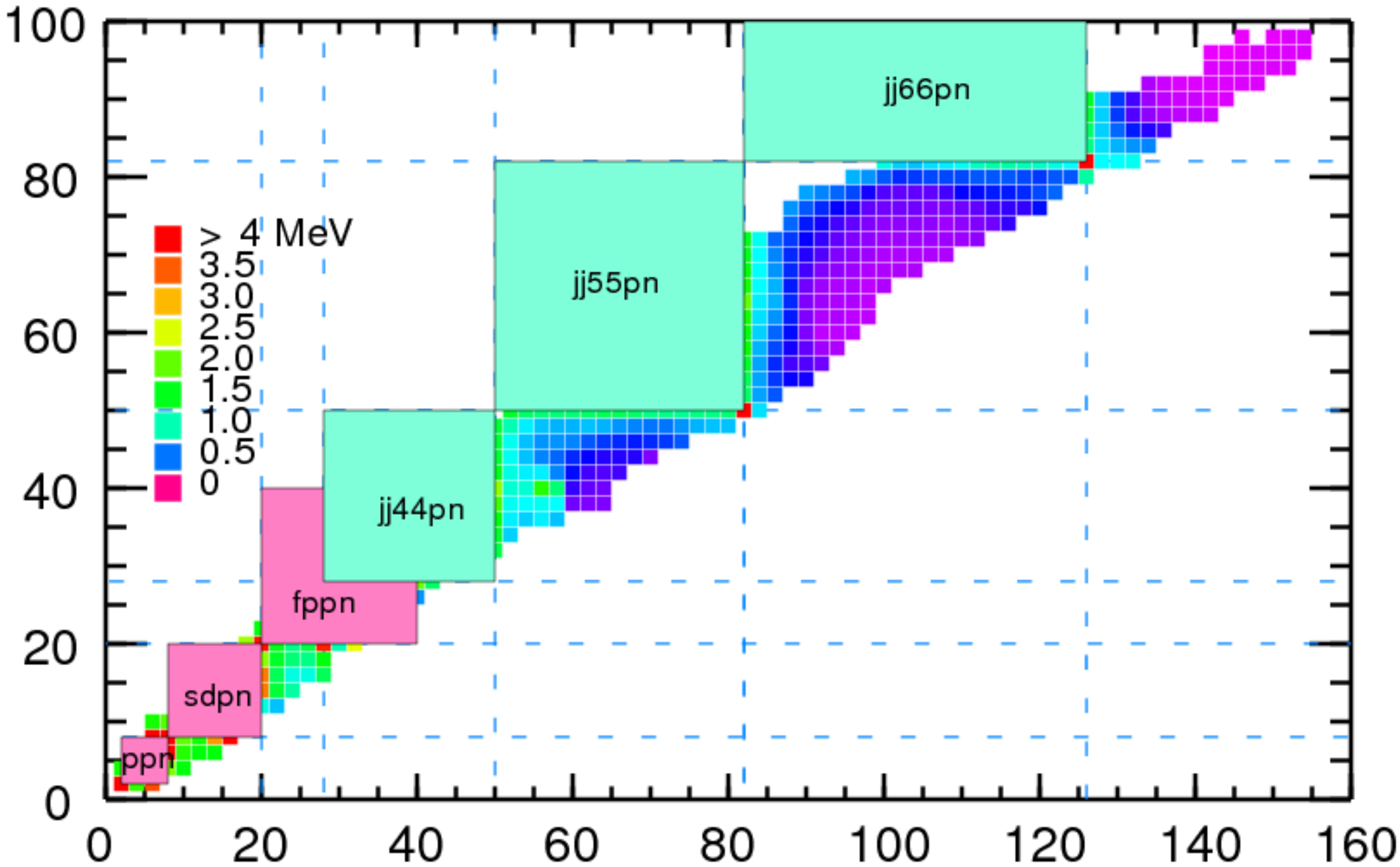
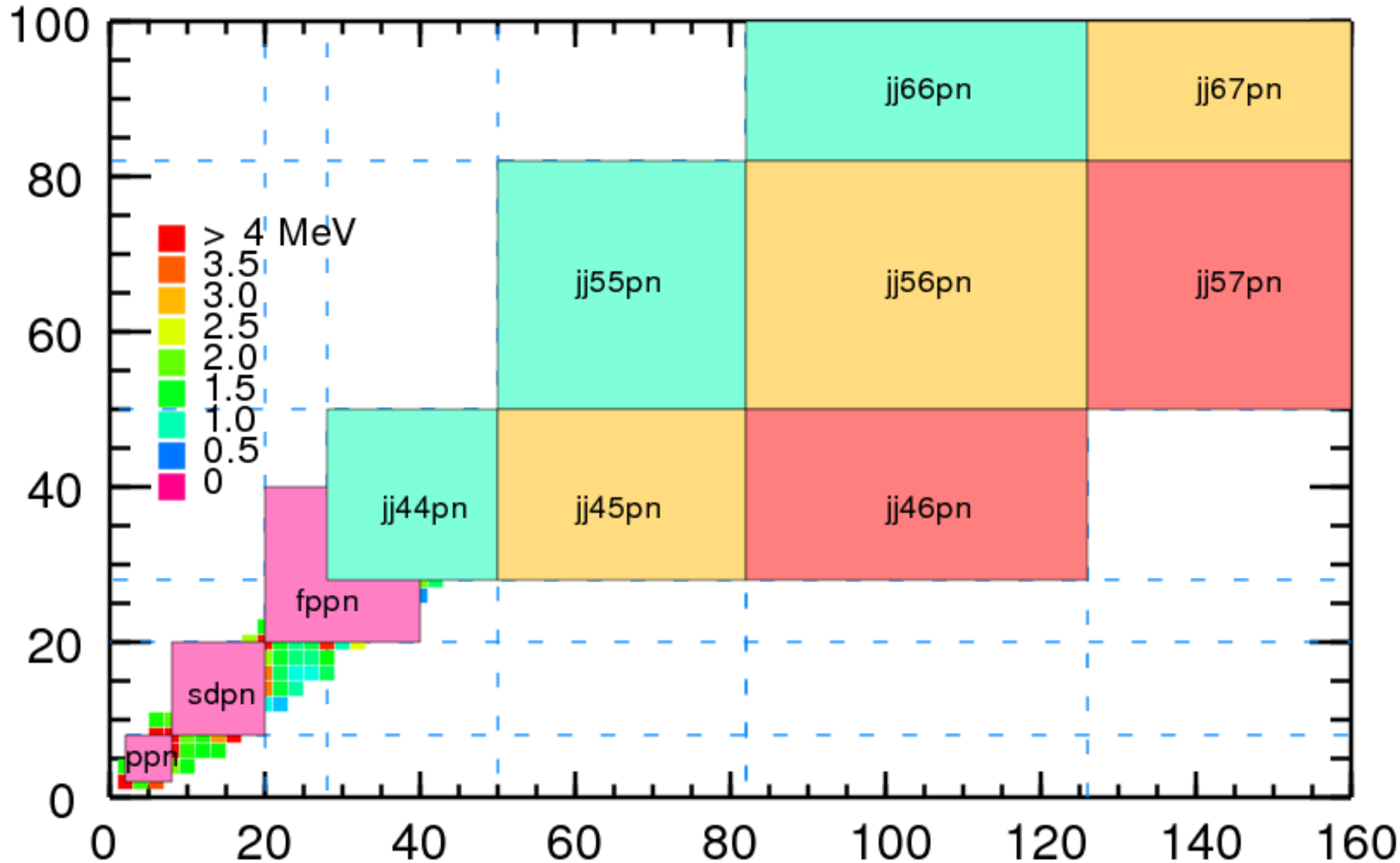


> 4 MeV
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
ppn
sdpn
fppn
jj44pn
jj55pn
jj66pn
0
20
40
60
80
100
0
20
40
60
80
100
120
140
160

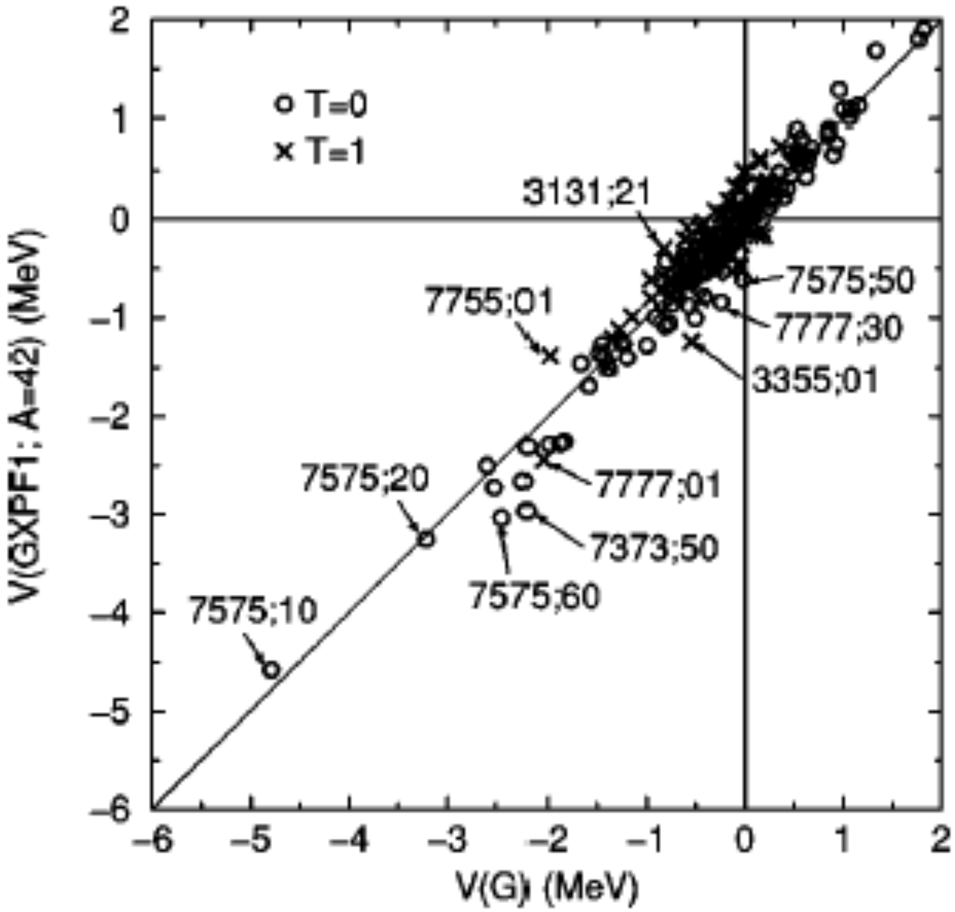

jj66pn
jj67pn
jj55pn
jj56pn
jj57pn
> 4 MeV
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
jj44pn
jj45pn
jj46pn
fppn
sdpn
ppn
100
80
60
40
20
0
0
20
40
60
80
100
120
140
160

GXPF1A Effective Interaction: $f_{7/2}p_{3/2}p_{1/2}f_{5/2}$

Renormalized G-matrix ➔ GXPF1

Phys.Rev. C **69**, 34355 (2004)

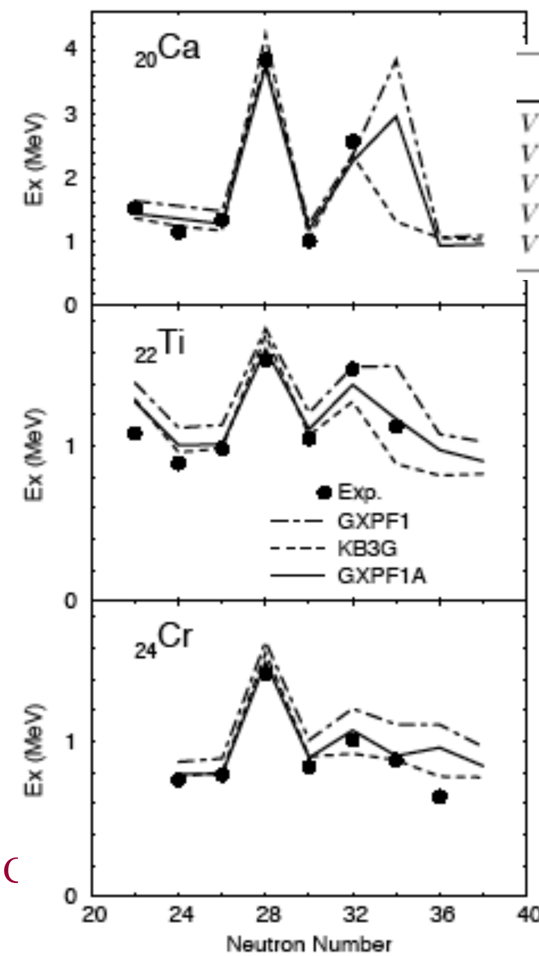
699 energies, 87 nuclei, **rms**=168 keV



GXPF1 ➔ GXPF1A

M. Honma et al, ENAM04

5 matrix elements adjusted for N=34



V	GXPF1	GXPF1A
$V(7777;01)$	−2.439	−2.239
$V(5511;01)$	−0.809	−0.309
$V(1111;01)$	−0.447	+0.053
$V(5151;21)$	−0.152	−0.502
$V(5151;31)$	+0.238	+0.488

^{56}Ni states

J	#
0	1
2	1
4	1
0	2
0	3
6	1
2	2
4	2
4	3
8	1
10	1

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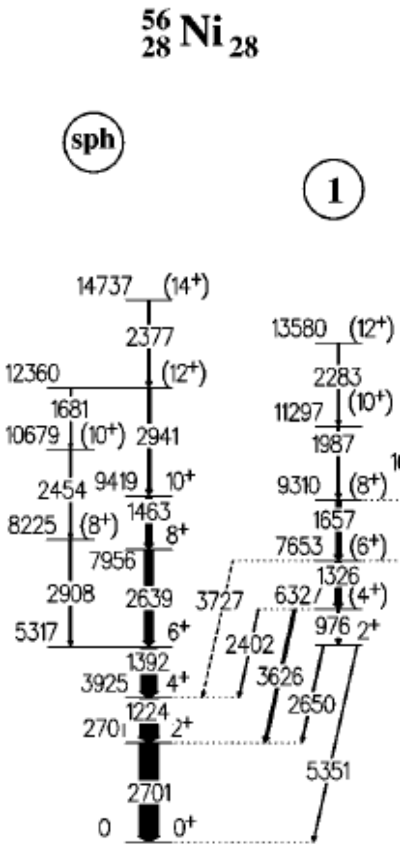
Koeln Low Spin States in ^{56}Ni: complete spectroscopy

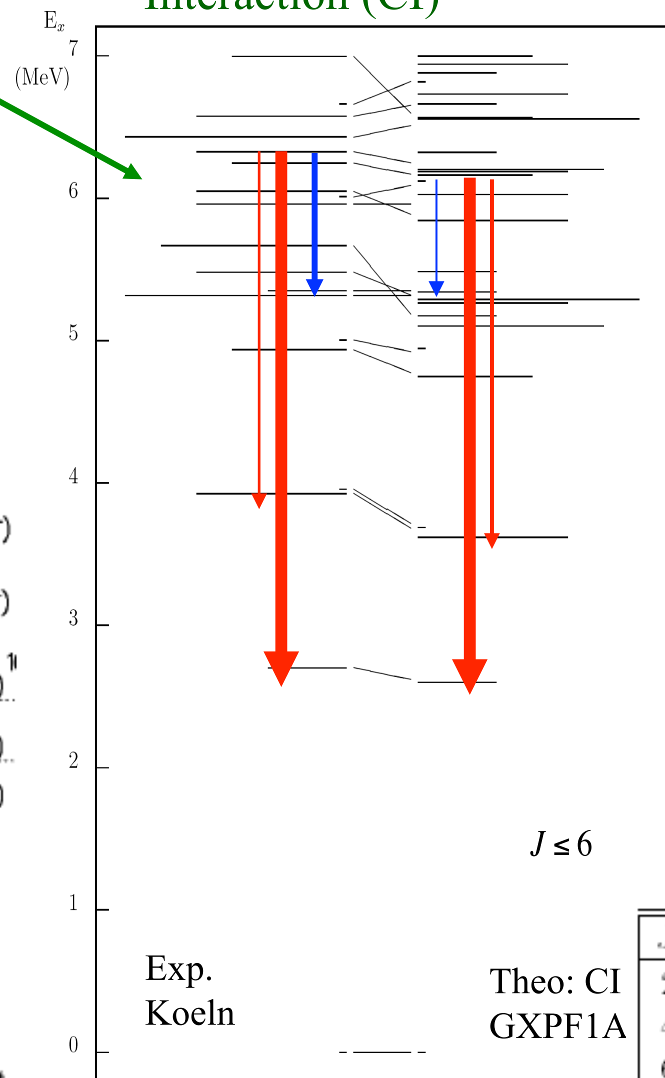
Configuration Interaction (CI)

M. Horoi et al., Phys.Rev. C 73, 061305(R) (2006)

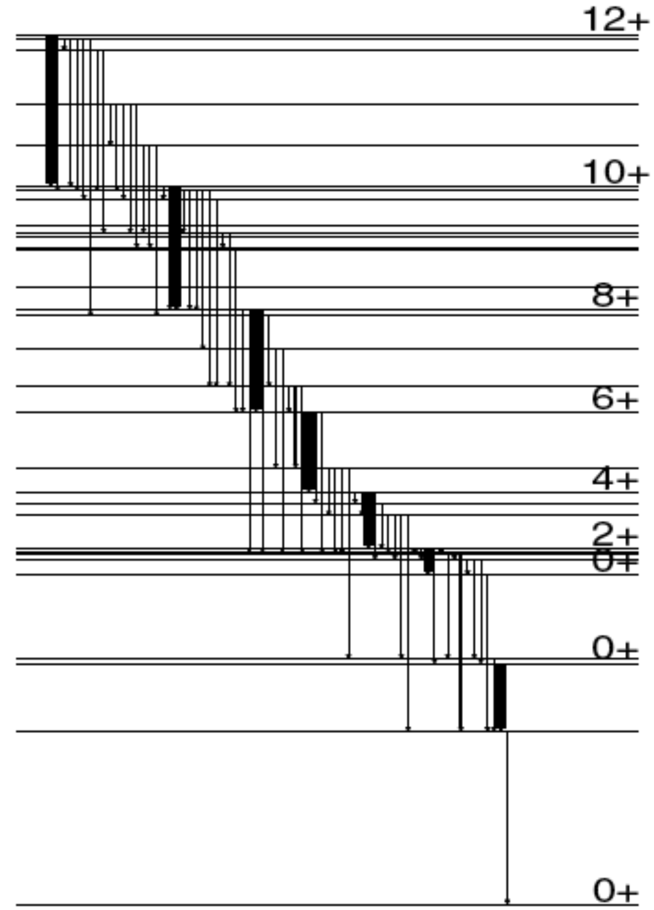


LBNL high spin **experiment**

D.Rudolf et al.,PRL **88**,1999



M. Horoi et al., in preparation



J_n	E_x (MeV)	$< Q >_{J0}$	$(Q_0)_{sp}$	B(E2; $J \rightarrow J-2$)	$\mid Q_0 \mid_{tr}$
2_3	5.342	-41.6	+145.3	413.2	144.1
4_5	6.027	-55.2	+151.9	598.0	143.8
6_3	7.556	-56.2	+140.6	609.3	139.5
8_4	9.300	-47.2	+112.2	558.4	130.5
10_6	10.782	-63.9	+147.0	591.1	132.5
12_5	13.071	-62.7	+141.1	612.3	133.7

$e^p_{eff} = 1.5 \quad e^n_{eff} = 0.5$

Angular Momentum Projected CI (PCI)

Deformed Slater Determinant

Deformed Nilsson Single Particle operator

Spherical H.O.

$$|\Phi_\kappa\rangle = b^\dagger_{i1} b^\dagger_{i2} \ldots b^\dagger_{in} |(\epsilon_2, \epsilon_4)\rangle \qquad b_k = \sum_i W_{ki} c_i$$

Nuclear State Wave-function: $|\Psi^\sigma_{IM}\rangle = \sum_{K\kappa} f^\sigma_{IK\kappa} P^I_{MK} |\Phi_\kappa\rangle$

Angular Momentum Projection

$$\sum_{K'\kappa'} (H^I_{K\kappa,K'\kappa'} - E^\sigma_I N^I_{K\kappa,K'\kappa'}) f^\sigma_{IK\kappa'} = 0$$

Shell Model Hamiltonian

$$H^I_{K\kappa,K'\kappa'} = \langle \Phi_\kappa | H P^I_{KK'} | \Phi_{\kappa'} \rangle \qquad N^I_{K\kappa,K'\kappa'} = \langle \Phi_\kappa | P^I_{KK'} | \Phi_{\kappa'} \rangle$$

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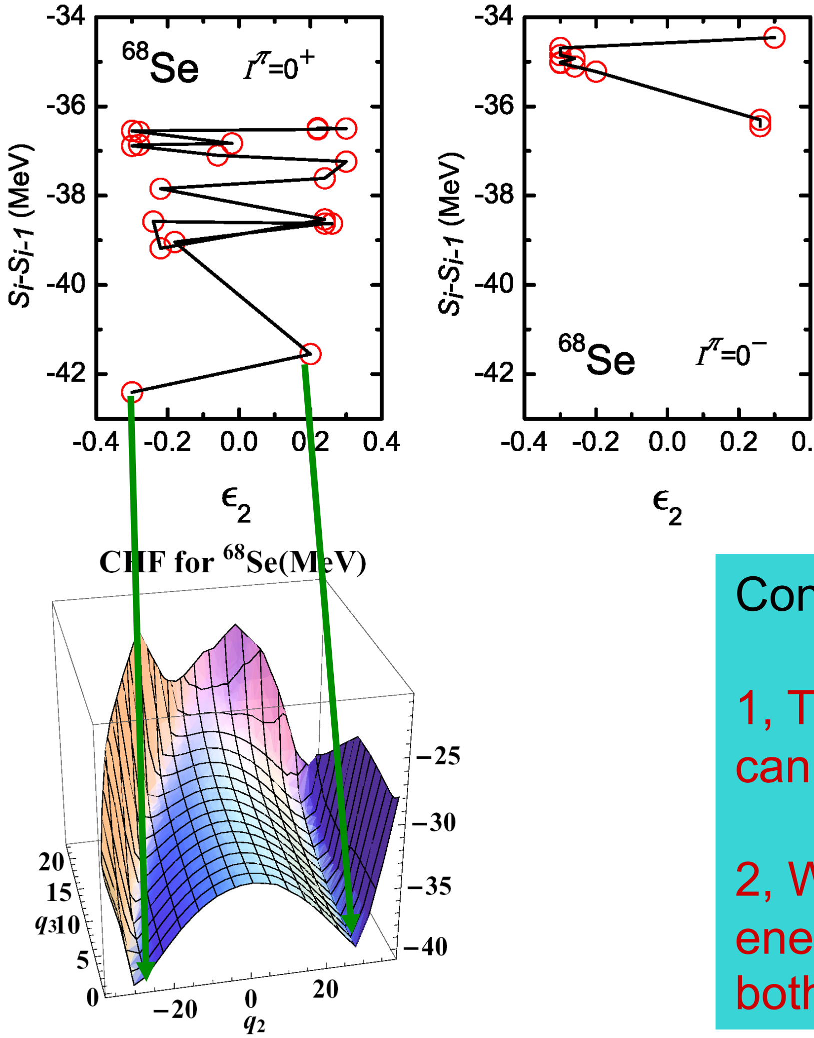
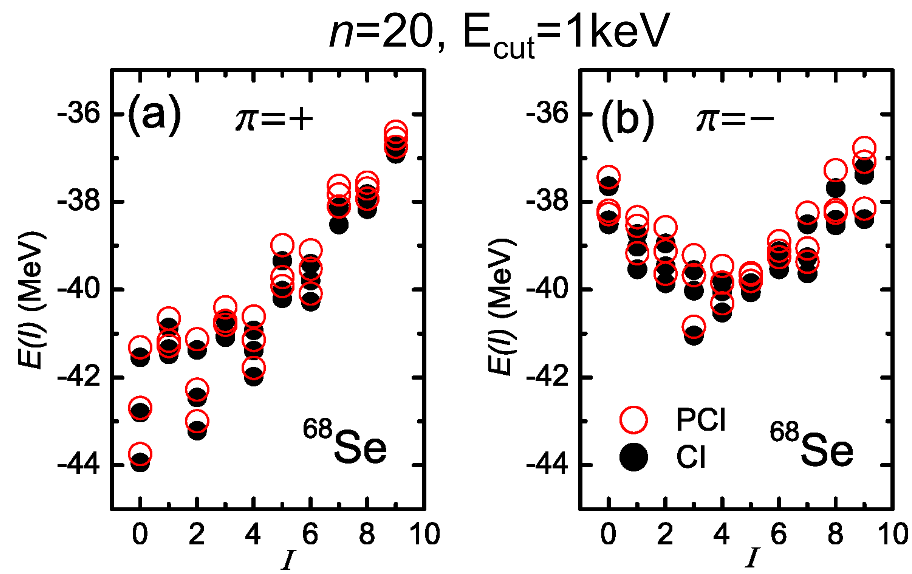
Extension of PCI: Gao, Horoi
PRC **79**, 014311 (2009); PRC **80**, 034325 (2009).

Interaction taken from:
K. Kaneko, M. Hasegawa, and T. Mizusaki, Phys. Rev. C 70, 051301(R) (2004).





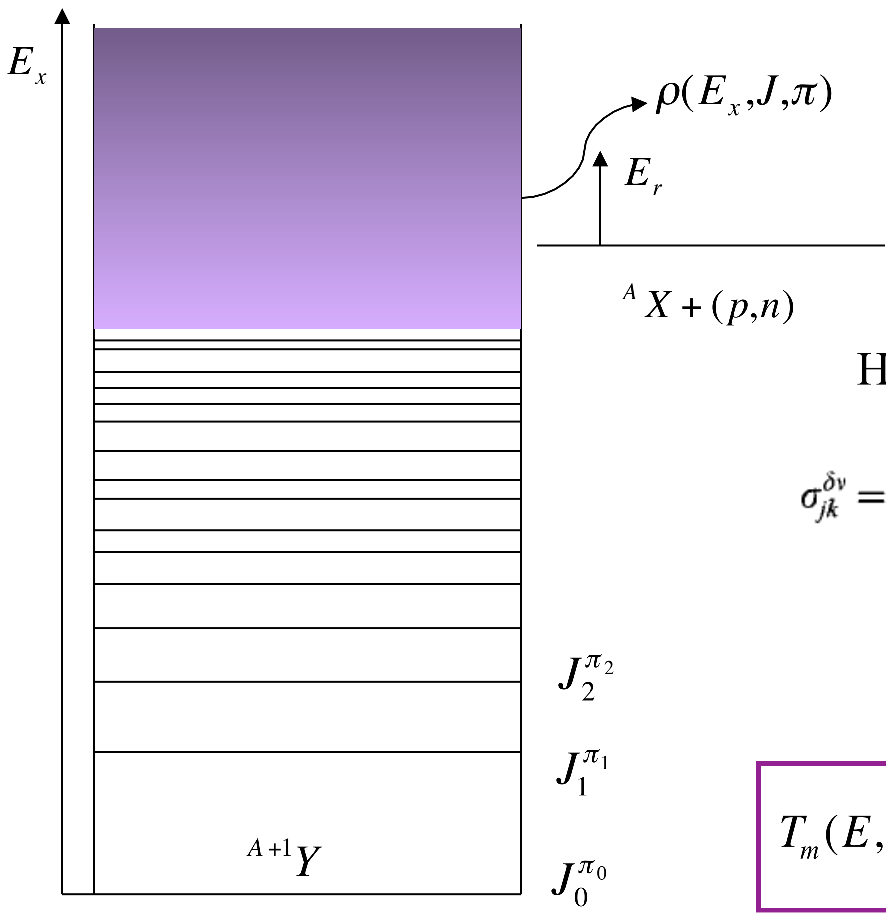
Conclusions:

1, The physics of shape coexistence in ^{68}Se can be clearly seen from the PCI basis.

2, With new method of basis selection the PCI energies are very close to those of full CI for both positive parity and negative parity states.

SciDAC

Nuclear Level Densities (NLD)



$(n,\gamma),\ (n,xn),\ (n,n'),\ (n,p),\ (n,f),\ldots$

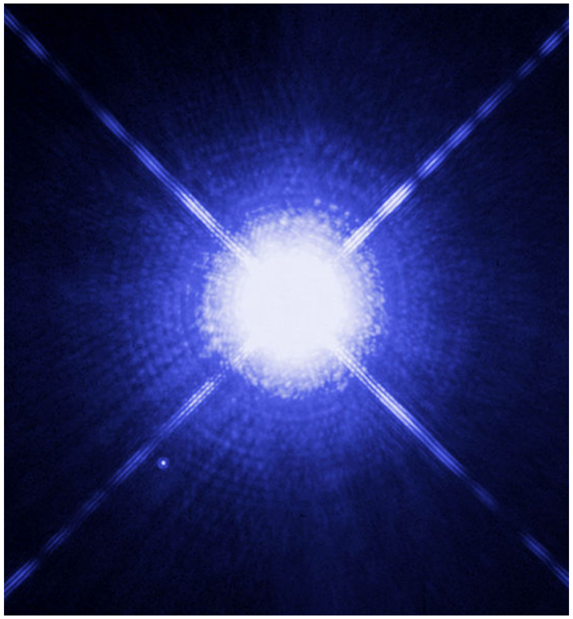
Hauser and Feshbach, Phys. Rev **87**, 366 (1952)

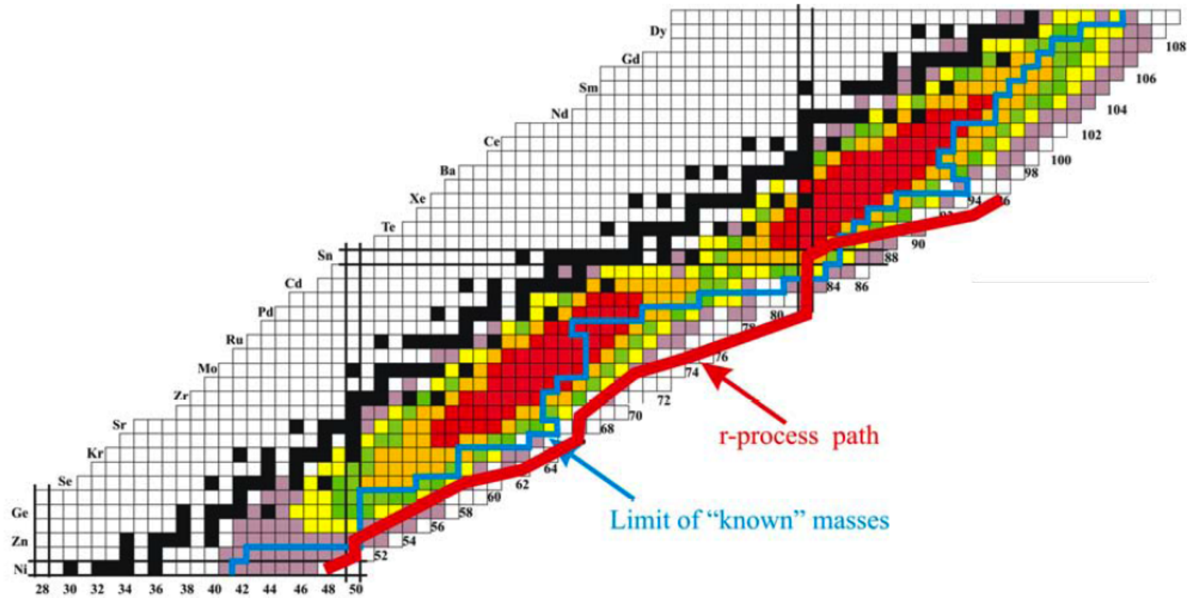
$$\sigma_{jk}^{\delta\nu} = \frac{\pi\hbar^2}{2\mu_{ij}E_{ij}} \frac{1}{(2J_i^{\delta}+1)(2J_j+1)} \times \sum_{J,\pi}(2J+1)\frac{T_j^{\delta}(E,J,\pi,E_j^{\delta},J_j^{\delta},\pi_j^{\delta})\,T_k^{\nu}(E,J,\pi,E_k^{\nu},J_k^{\nu},\pi_k^{\nu})}{\sum_m T_m(E,J,\pi)}$$

$$T_m(E,J,\pi) = \int_{E_{\min}}^{E_{\max}} T(E,J,\pi;E_x,J_x,\pi_x)\,\rho(E_x,J_x,\pi_x)\,dE_x$$

Where are NLD Needed: Nuclear Astrophysics

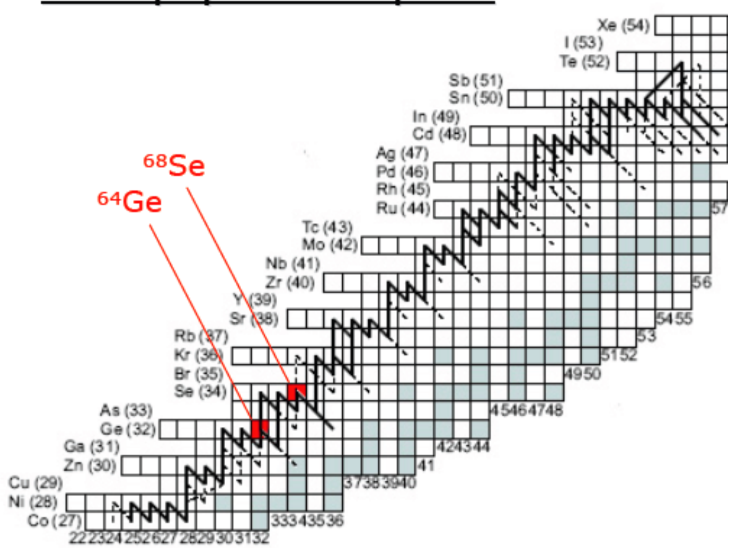
Binary stars XRB: Sirius





SN 1987 A

the rp-process path



Schatz et al. Phys. Rep 294 (1998) 167-298

M. Horoi CMU

The Back-Shifted Fermi Gas Model for Nuclear Level Density

Rauscher at al, Phys. Rev. C 56, 1613 (1997)

Y. Alhassid, G. F. Bertsch, S. Liu, and H. Nakada, Phys. Rev. Lett. **84**, 4313 (2000).

D. Mocelj, T. Rauscher, G. Martinez-Pinedo, and Y. Alhassid, Nucl. Phys. **A718**, 750c (2003).

$$\rho(U,J,\pi)=\frac{1}{2}\mathcal{F}(U,J)\rho(U), \qquad (8)$$

with

$$\rho(U)=\frac{1}{\sqrt{2\pi}\sigma}\frac{\sqrt{\pi}}{12a^{1/4}}\frac{\exp(2\sqrt{aU})}{U^{5/4}},$$

$$\mathcal{F}(U,J)=\frac{2J+1}{2\sigma^2}\exp\left(\frac{-J(J+1)}{2\sigma^2}\right), \qquad (9)$$

$$\sigma^2=\frac{\Theta_{\mathrm{rigid}}}{\hbar^2}\sqrt{\frac{U}{a}}, \quad \Theta_{\mathrm{rigid}}=\frac{2}{5}m_u A R^2, \quad U=E-\delta.$$

$$\frac{a}{A}=c_0+c_1 S(N,Z), \qquad (10)$$

$$\delta = \Delta(Z,N)$$

$$\Delta_{\text{even-even}}=\frac{12}{\sqrt{A}},$$

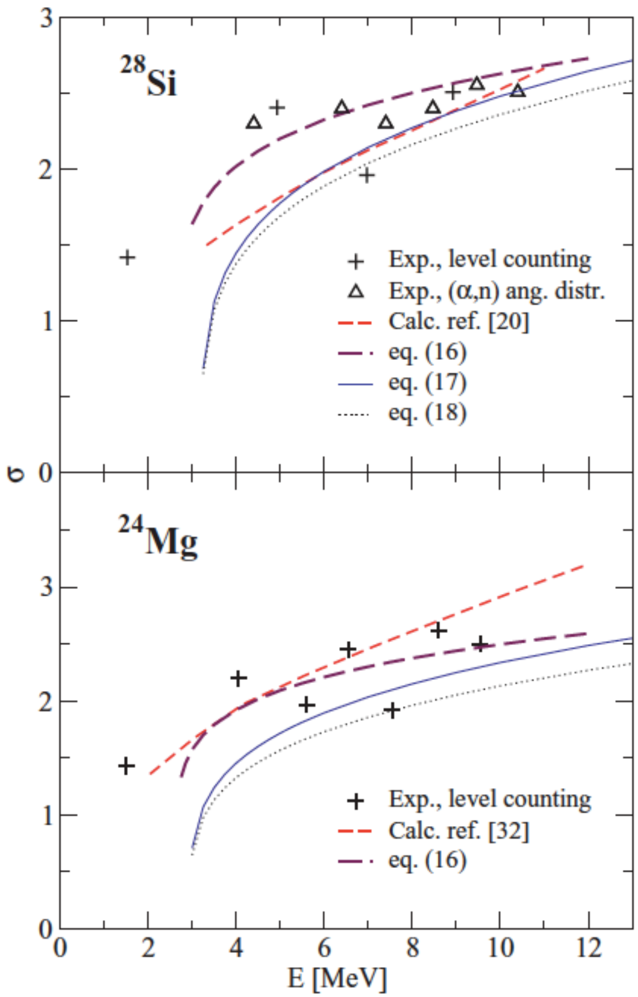
$$\Delta_{\text{odd}}=0, \qquad (12)$$

$$\Delta_{\text{odd-odd}}=-\frac{12}{\sqrt{A}}.$$

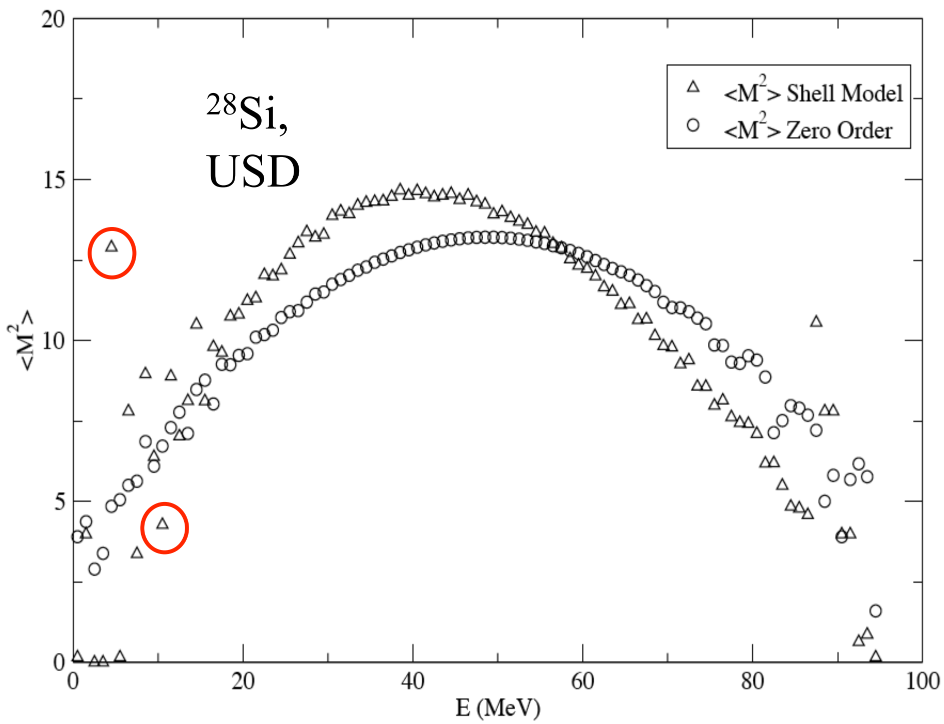
The Spin Cutoff Parameter

$$\left\langle M^2 \right\rangle (E) = \frac{1}{\rho(E)} \sum_{\vec{m}} d_{\vec{m}} (FRG)_{\vec{m}}(E) \left\langle M^2 \right\rangle_{\vec{m}}$$

$$\sigma^2(E) = \left\langle M^2 \right\rangle (E)$$



T. von Egidy & D. Bucurescu, Phys.Rev. C 80, 054310 (2009)



Horoi, Ghita, Zelevinsky, Nucl. Phys. A 758, 142 (2005)

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Other Models of Nuclear Level Densities

$$\rho(E_x, J, \pi) = (1/2)\, \mathcal{F}(U, J)\, \rho_{FG}(U)$$

$$U = E_x - \Delta$$

	Z=10	Z=20	Z=30	Z=40	Z=50	Z=60	Z=70	Z=80	Z=90	Z=100
	Z=11	Z=21	Z=31	Z=41	Z=51	Z=61	Z=71	Z=81	Z=91	Z=101
	Z=12	Z=22	Z=32	Z=42	Z=52	Z=62	Z=72	Z=82	Z=92	Z=102
	Z=13	Z=23	Z=33	Z=43	Z=53	Z=63	Z=73	Z=83	Z=93	Z=103
	Z=14	Z=24	Z=34	Z=44	Z=54	Z=64	Z=74	Z=84	Z=94	Z=104
	Z=15	Z=25	Z=35	Z=45	Z=55	Z=65	Z=75	Z=85	Z=95	Z=105
	Z=16	Z=26	Z=36	Z=46	Z=56	Z=66	Z=76	Z=86	Z=96	Z=106
	Z=17	Z=27	Z=37	Z=47	Z=57	Z=67	Z=77	Z=87	Z=97	Z=107
Z=8	Z=18	Z=28	Z=38	Z=48	Z=58	Z=68	Z=78	Z=88	Z=98	Z=108
Z=9	Z=19	Z=29	Z=39	Z=49	Z=59	Z=69	Z=79	Z=89	Z=99	Z=109

HF+BCS -> $\rho_{HF+BCS}(U)$

- Goriely Nucl. Phys. A605, (1996) 28.
- Demetriou and Goriely, Nucl. Phys. A695 (2001) 95.
- http://www-astro.ulb.ac.be/Html/nld.html

HFB+Combinatorial: $\rho(E_x, J, \pi)$

- S. Hilaire, J.P. Delaroche and A.J. Koning, Nucl. Phys. A632, 417 (1998).
- S. Hilaire, J.P. Delaroche and M. Girod, Eur. Phys. J. A12 (2001) 169.
- S. Hilaire and S. Goriely, Nucl. Phys. A779 (2006)

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- http://www-astro.ulb.ac.be/Html/nld_comb.html

SciDAC Scientific Discovery through Advanced Computing

Experimental Data

http://ocl.uio.no/compilation/

^{50}V, ^{51}V

^{56}Fe, ^{57}Fe

^{93}Mo, ^{94}Mo, ^{95}Mo, ^{96}Mo, ^{97}Mo, ^{98}Mo

^{148}Sm, ^{149}Sm

^{160}Dy, ^{161}Dy, ^{162}Dy

^{167}Er, ^{168}Er

^{170}Yb, ^{171}Yb, ^{172}Yb

http://inpp.ohiou.edu/~voinov/

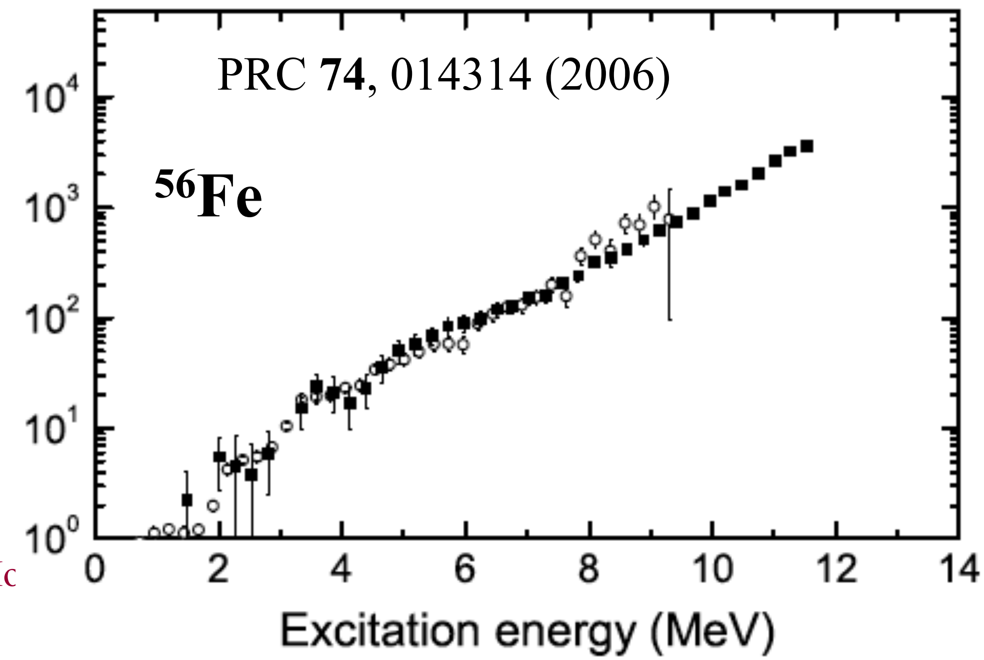
^{44}Sc

^{47}Ti

^{56}Fe, ^{57}Fe

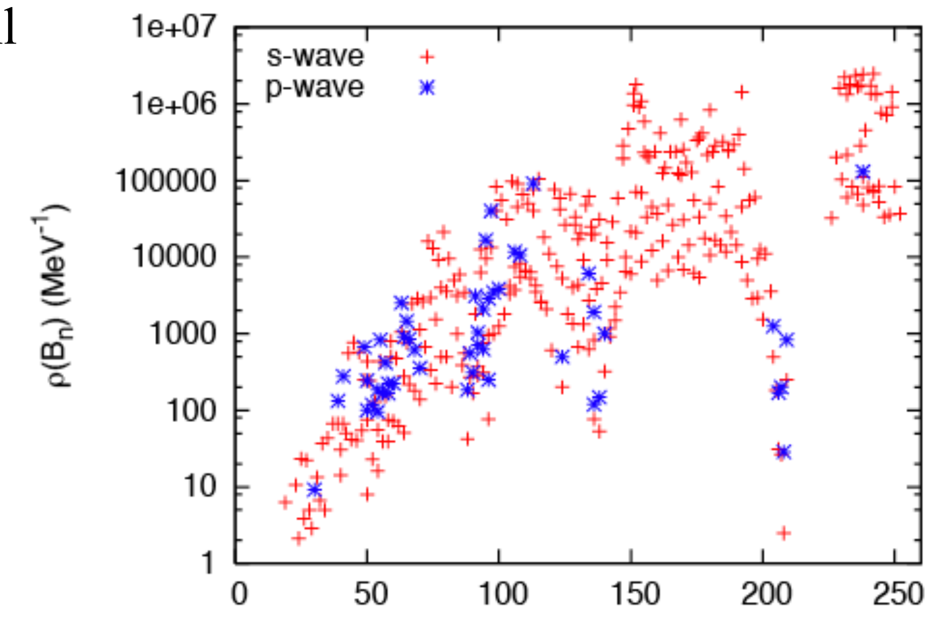
^{60}Ni,

^{60}Co



Experimental Data: Neutron Resonances

http://www-nds.iaea.org/ripl-2/densities.html

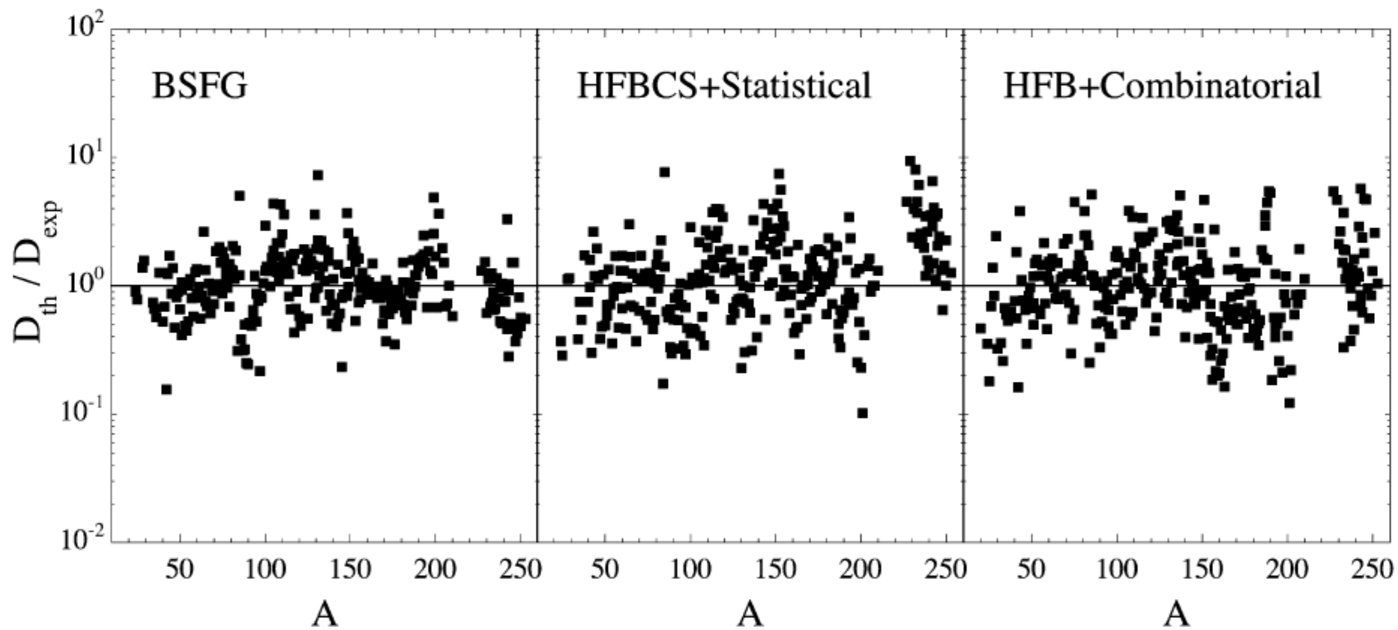


$$\rho(B_n) = \frac{1000}{D_0}$$

$$f_{\text{rms}} = \exp\left[\frac{1}{N_e}\sum_{i=1}^{N_e} \ln^2 \frac{D^i_{\text{th}}}{D^i_{\text{exp}}}\right]^{1/2}$$

$$f_{rms} \sim 2$$

Hilaire and Goriely, NPA 799, 63 (2006)



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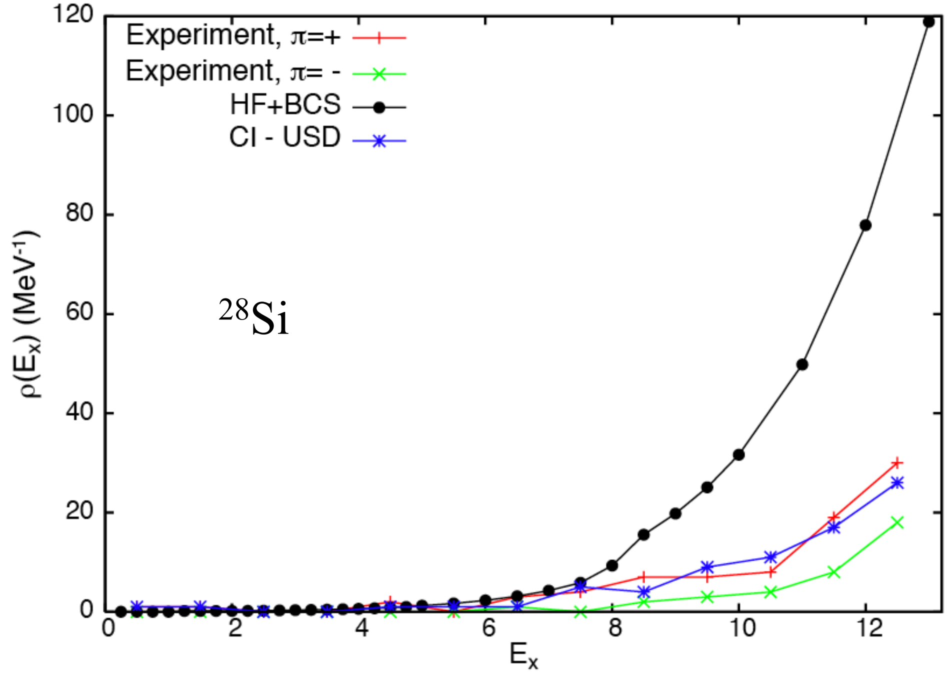
Accurate Nuclear Level Densities

Comparison of:

1. CI,
2. HF+BCS
   www-astro.ulb.ac.be/Html/nld.html
3. experimental data

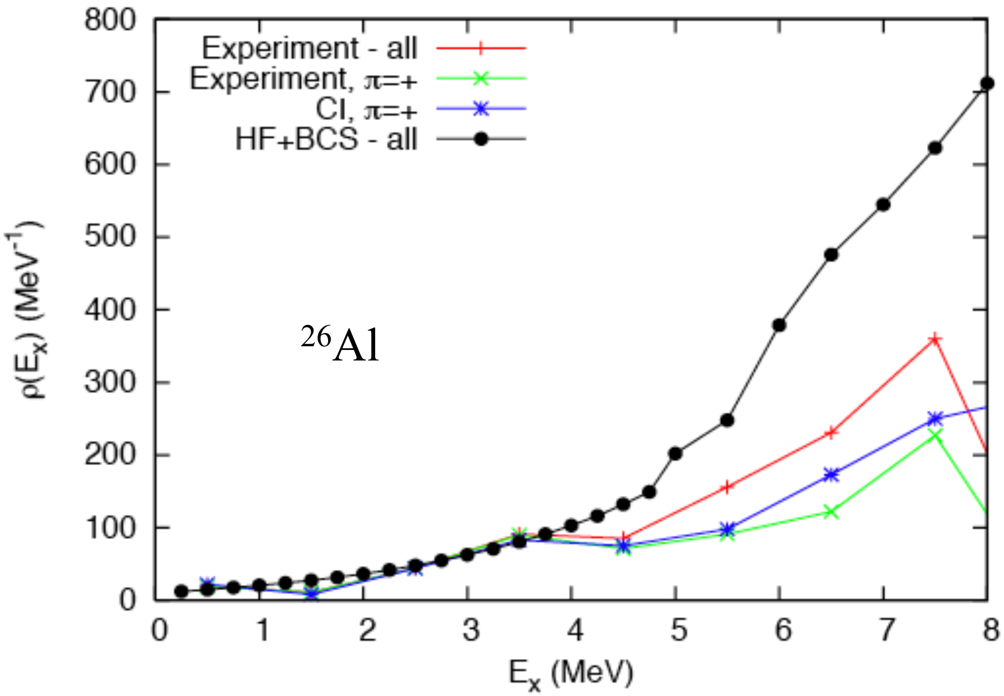


Complete spectroscopy: sd-shell nuclei

Conclusions:

- HF+BCS overestimates the data

- CI accurately describes the data



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NLD and Statistical Spectroscopy

M. Horoi et al. :

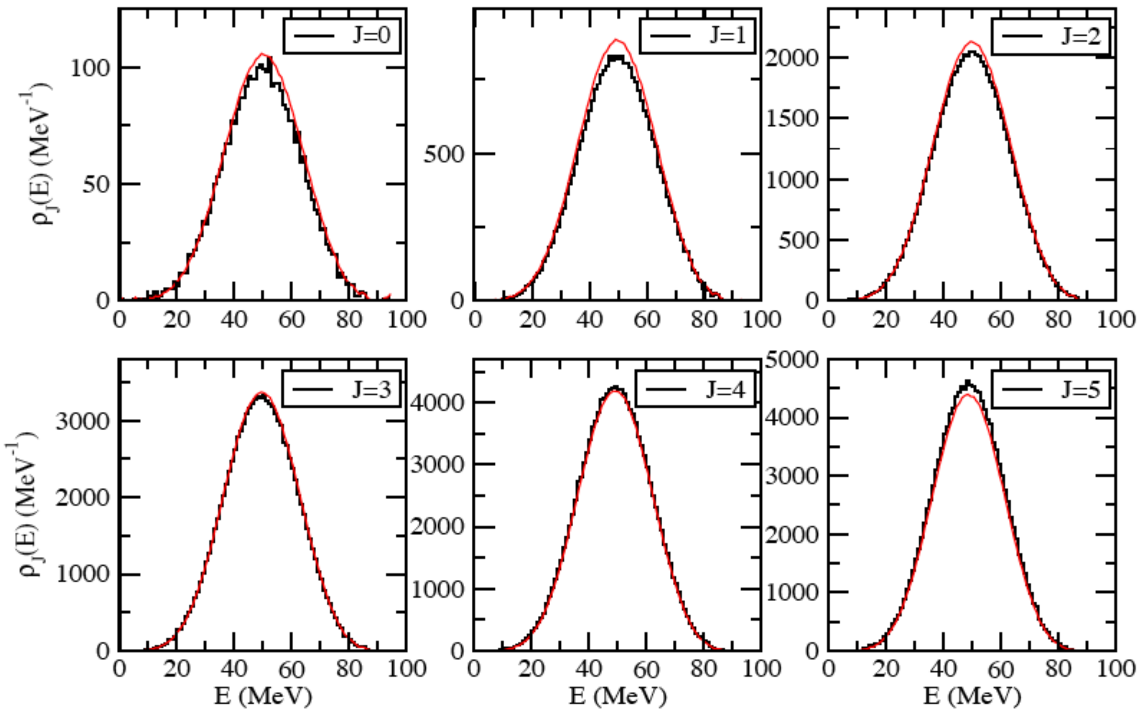
PRC **67**, 054309 (2003),

PRC **69**, 041307(R) (2004),

NPA **785**, 142 (2005).

PRL **98**, 265503 (2007)

^{28}Si $\pi = +$ staircase: CI, USD



Configurations: e.g. 4 particles in sd
d3 d5 s1
4 0 0
3 1 0
3 0 1 …
preserve rotational invariance and parity

$$\rho(E_x,J,\pi) = \sum_{c\in conf} D_c(J,\pi) G_{FR}\left(E, E_c(J), \sigma_c(J)\right)$$

$$E_c(J),\sigma_c(J) \leftarrow Tr_{SD_c} < M \mid H^q \mid M >_{SD_c}$$

$$E_x = E - E_{g.s.}$$

$E_{g.s.}$ from CI, PCI, Exponential Convergence Method (PRL **82**, 2064 (1999)), CC, etc.

$E_c(J)$, $\sigma_c(J)$: computational intensive

Configurations can be calculated in parallel

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Fixed J Configuration Centroids and Widths

PHYSICAL REVIEW C **69**, 041307(R) (2004)

Fixed spin and parity nuclear level density for restricted shell model configurations

Mihai Horoi,[1] Monica Ghita,[1] and Vladimir Zelevinsky[2,3]
[1]*Physics Department, Central Michigan University, Mount Pleasant, Michigan 48859, USA*
[2]*National Superconducting Cyclotron Laboratory, East Lansing, Michigan 48824, USA*
[3]*Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA*
(Received 14 January 2004; published 30 April 2004)

$$<< H >>_{\vec{m}nMT_z} = \sum_i \epsilon_i D^i(\vec{m}nMT_z) + \sum_{i<j} V_{ijij} D^{ij}(\vec{m}nMT_z)$$

$$\begin{aligned} << H^2 >>_{\vec{m}nMT_z} \; = \; & \sum_i \epsilon_i^2 D^i(\vec{m}nMT_z) + \\ & \sum_{i<j} \left[2\epsilon_i\epsilon_j + 2(\epsilon_i+\epsilon_j)V_{ijij} + \sum_{k<l} V_{ijkl}^2 \right] D^{ij}(\vec{m}nMT_z) + \\ & \sum_{(i<j)\neq l} \left[\sum_k (2V_{liik}V_{ljjk} - V_{ijkl}^2) + 2\epsilon_l V_{ijij} \right] D^{ijl}(\vec{m}nMT_z) + \\ & \sum_{(i<j)\neq(k<l)} \left[V_{ijkl}^2 + V_{ijij}V_{klkl} - 4V_{kiil}V_{kjjl} \right] D^{ijkl}(\vec{m}nMT_z) \end{aligned}$$

$$E_{\vec{m}}(J) = < \; H \; >_{\vec{m}nJT_z} = \left(<< H >>_{nM=JT_z} - << H >>_{\vec{m}nM=(J+1)T_z} \right) / D(\vec{m}nJT_z)$$

$$< \; H^2 \; >_{\vec{m}nJT_z} = \left(<< H^2 >>_{\vec{m}nM=JT_z} - << H^2 >>_{\vec{m}nM=(J+1)T_z} \right) / D(\vec{m}nJT_z)$$

$$\sigma_{\vec{m}nJT_z} = \sqrt{< \; H^2 \; >_{\vec{m}nJT_z} - < \; H \; >_{\vec{m}nJT_z}^2}$$

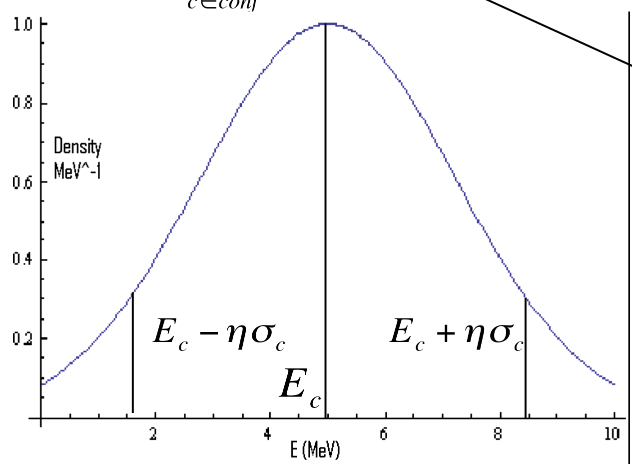
C. Jacquemin, Z. Phys. A **303**, 135 (1981)

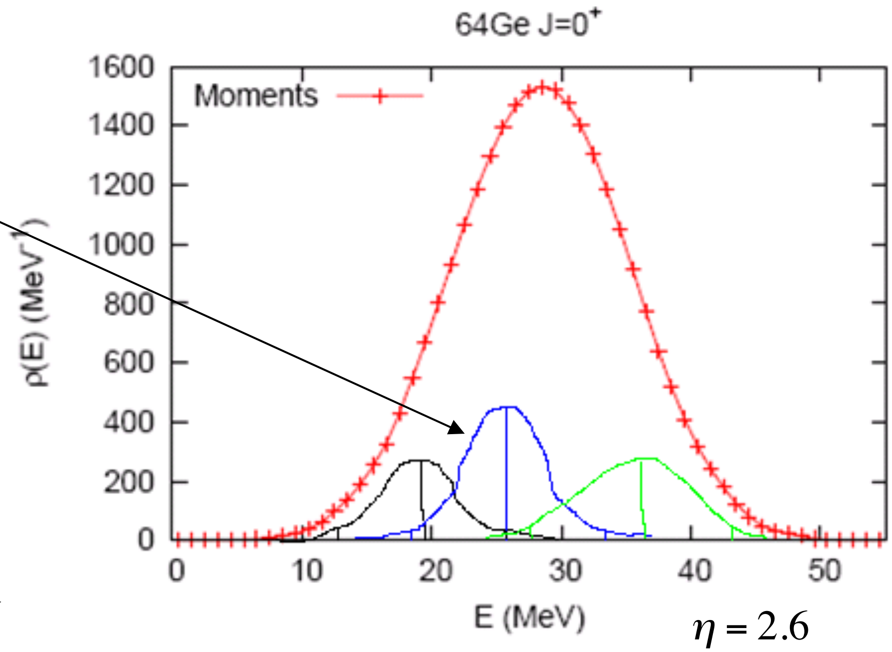
n - is the number of particles
$D^i(\vec{m}nMT_z)$ is the number of determinants in a partition $\vec{m}$ with nMT_z and state i occupied, etc.

$$D^{\vec{k}}(n\vec{m}M) = \sum_{k \le t \le n} (-1)^{t-k} \sum_{t_1+\cdots+t_k=t} D((n-t)(\vec{m}-t_1U_1-\cdots-t_kU_k)(M-t_1m_{k_1}-\cdots-t_km_{k_k}))$$

Study of Errors

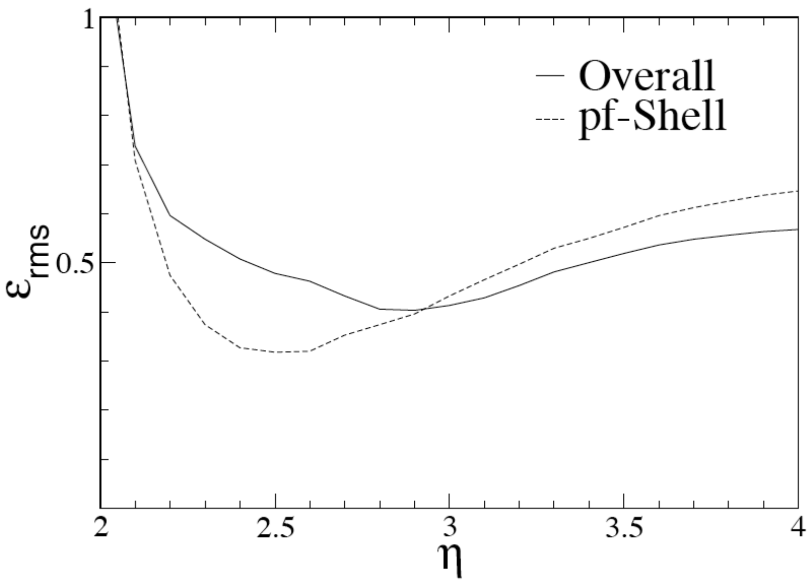
$$\rho(E_x, J, \pi) = \sum_{c \in conf} D_c(J,\pi)\, G_{FR}\big(E, E_c(J), \sigma_c(J)\big)$$

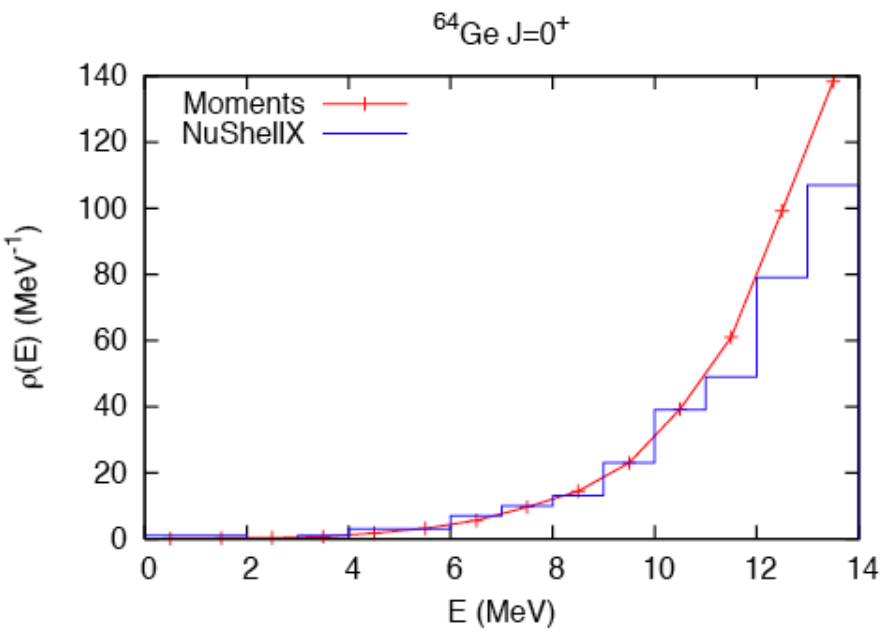




$\eta = 2.6$

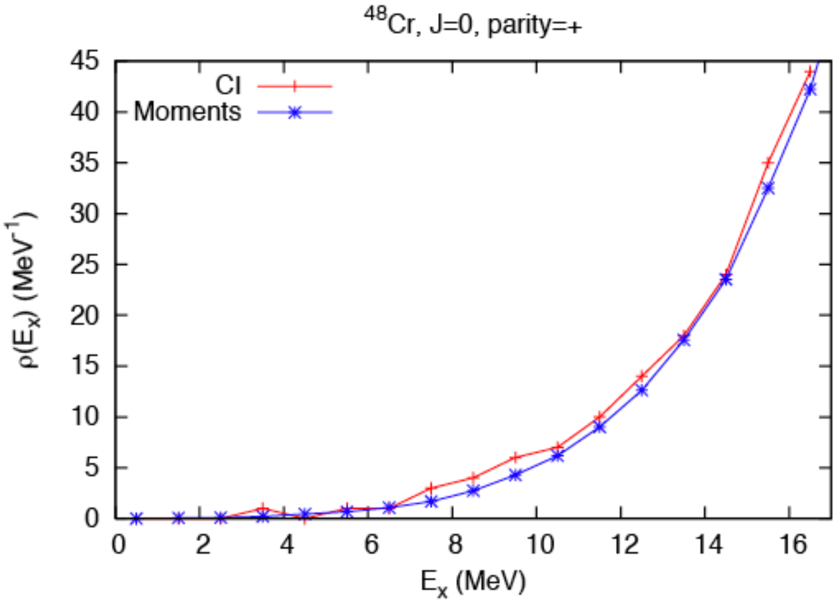
$$\varepsilon_{rms} = \exp\left[\sqrt{\frac{1}{N}\sum_{i}^{N}\left(\ln\frac{\rho_i^{MOM}}{\rho_i^{CI}}\right)^2}\right] - 1 \quad \textit{error relative to CI}$$

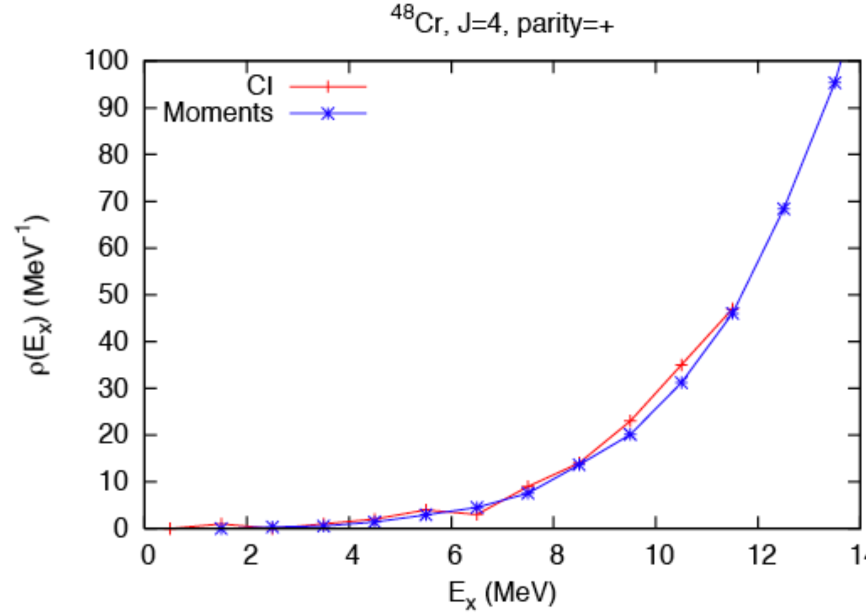


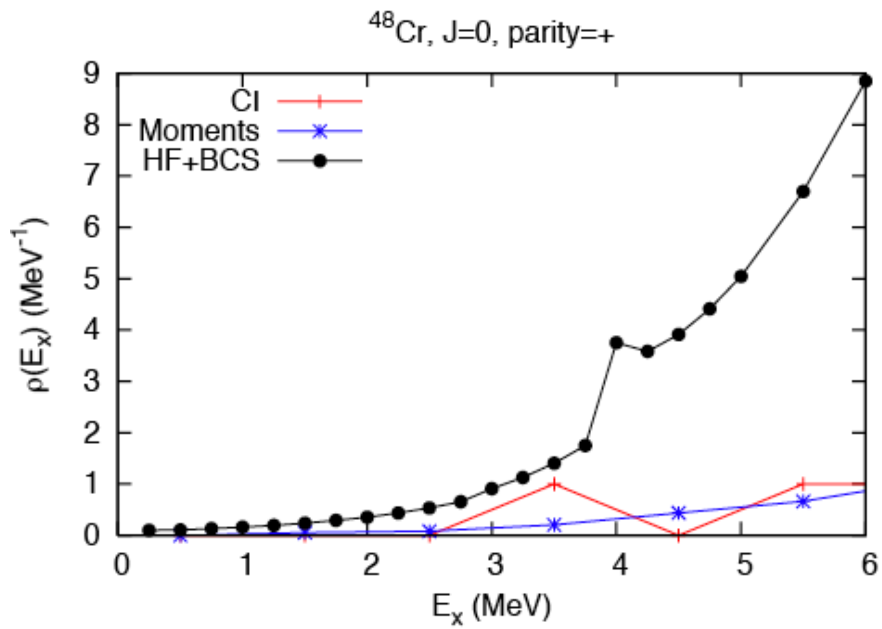


M. Horoi CI

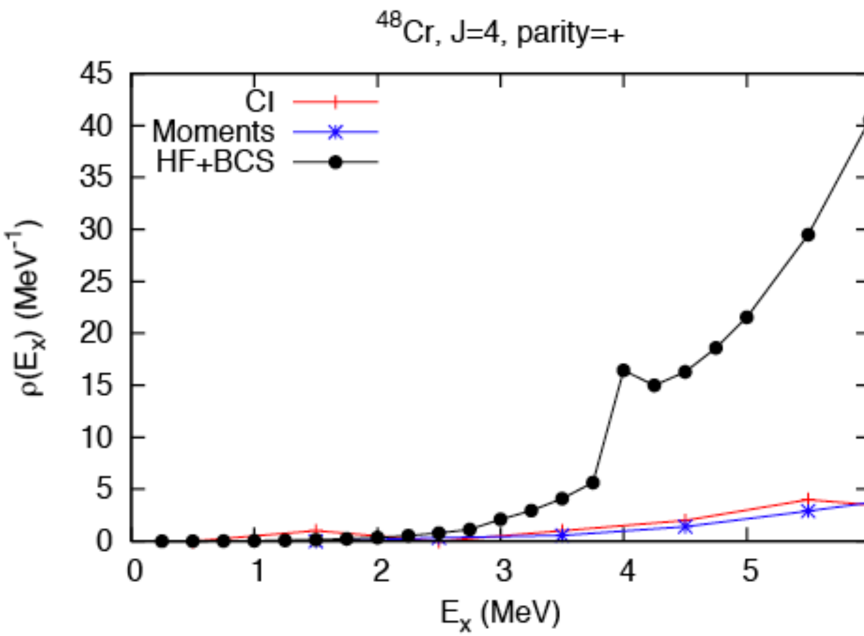
NLD Comparison: CI, Moments, HF+BCS



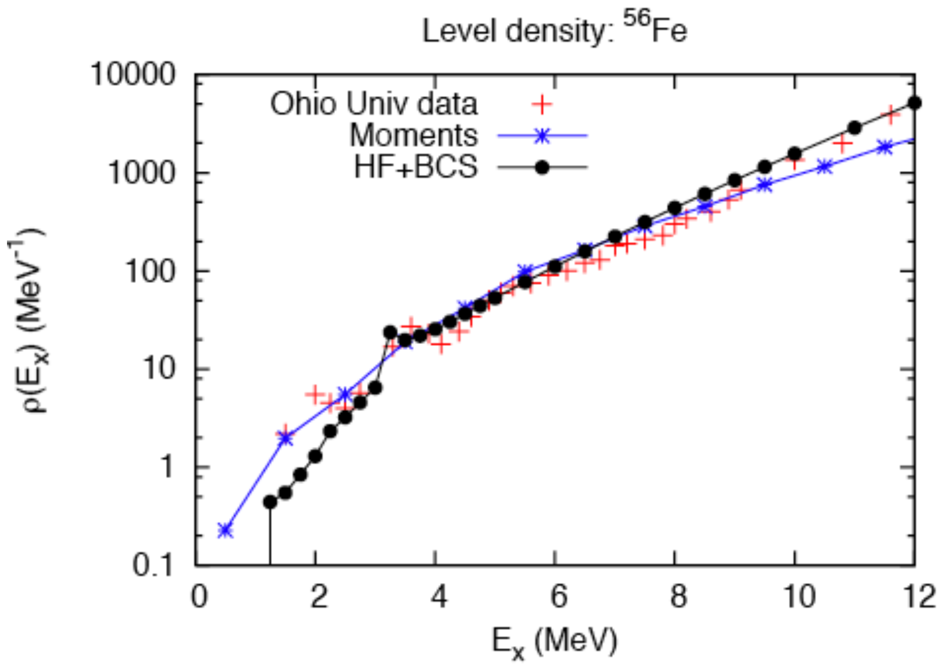


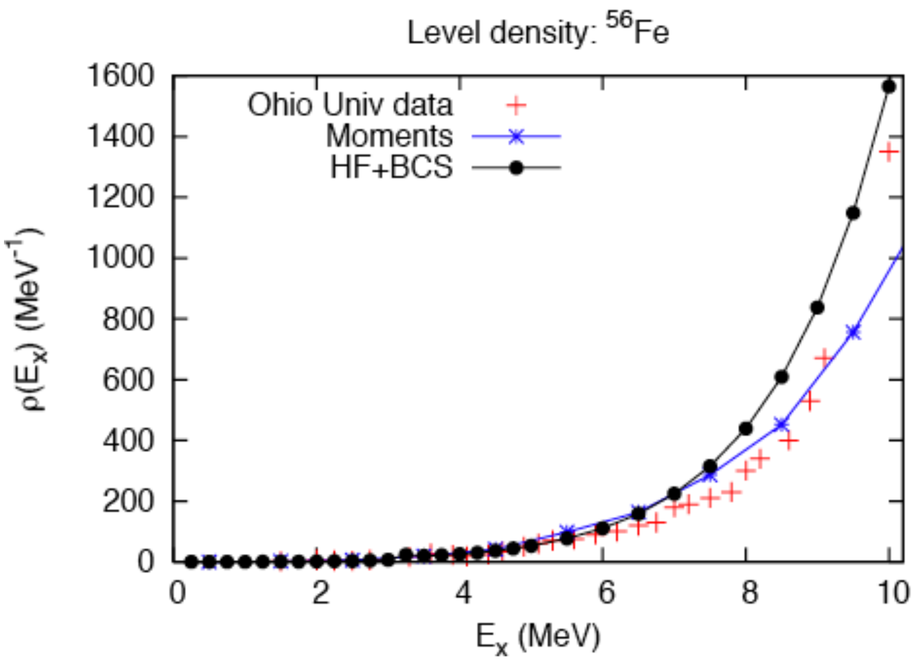


roi

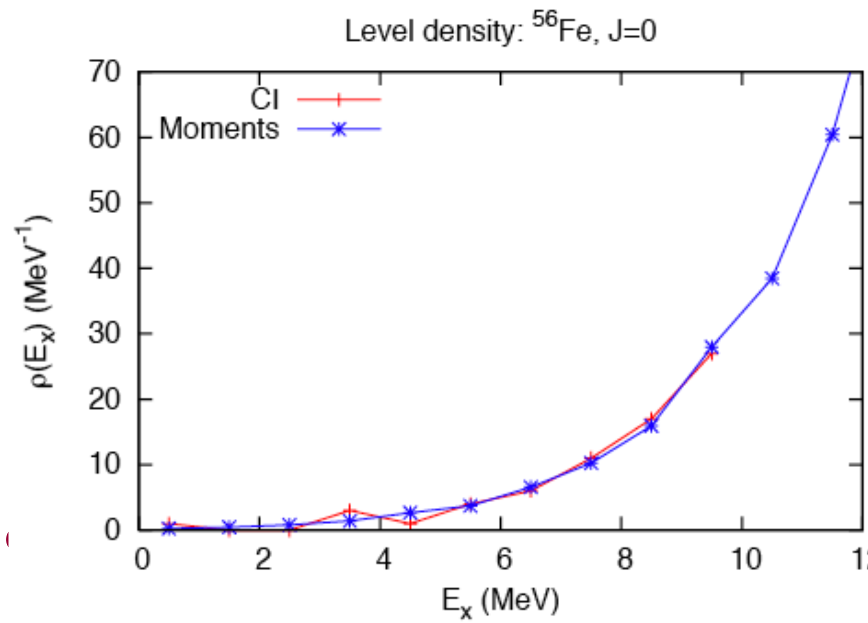


NLD of ^{56}Fe: CI, Moments, HF+BCS





Ohio data: PRC **74**, 014314 (2006)



Theory: *pf* model space,

GXPF1A interaction

Ratio of unnatural to natural NLD of different parities at low energies

$$\rho(E_x, J, \pi) = (1/2)\ \mathcal{F}(U, J)\ \rho_{FG}(U)$$

$$U = E_x - \Delta$$

Equal contribution to both parities

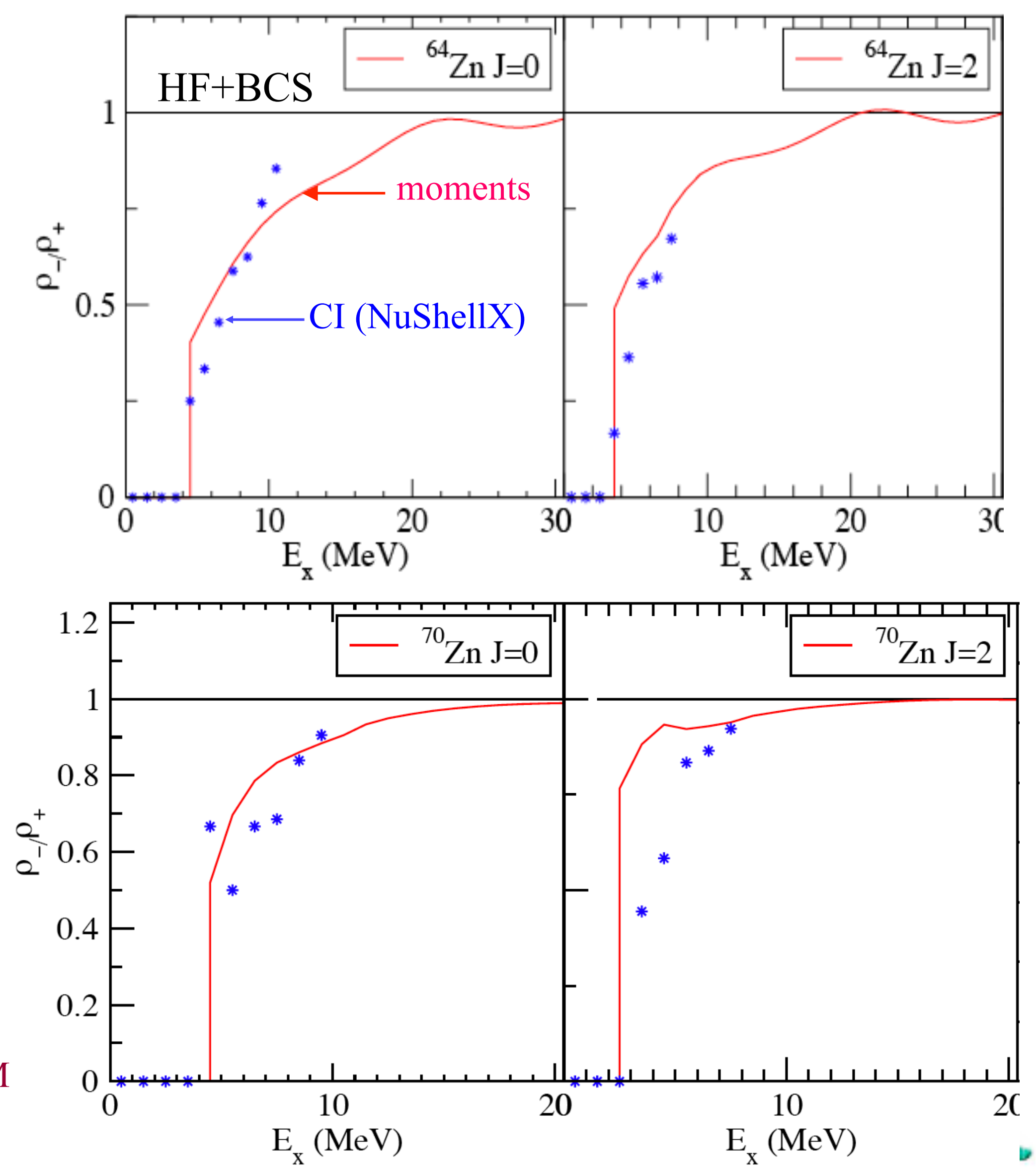
Remedy by Alhassid, Bertsch, Liu, Nakada, PRL 84, 4313 (2000) + Basel group (Rauscher)

Configurations: e.g. 4 particles in fpg

f5	p3	p1	g9	π
4	0	0	0	+
3	1	0	0	+
3	0	1	0	+
3	0	0	1	-

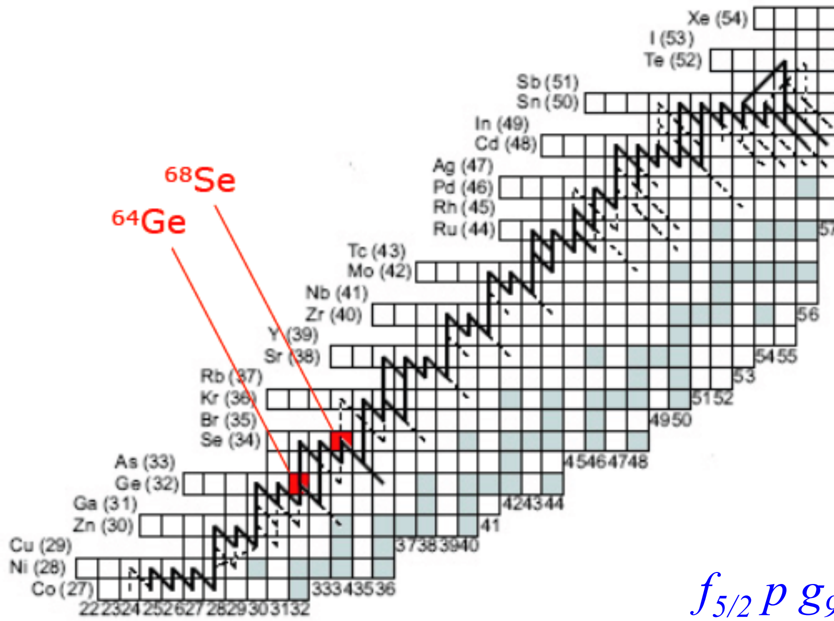
…

preserve rotational invariance and parity



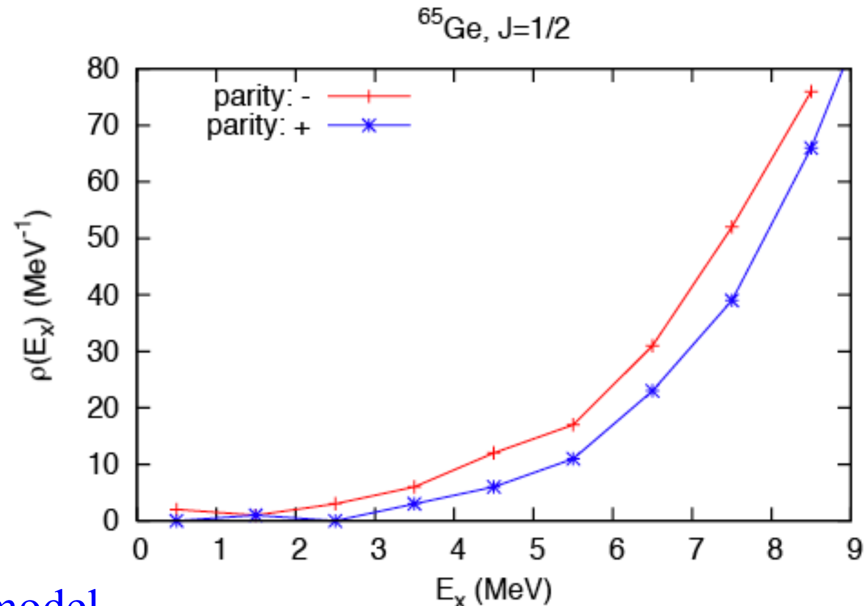
NLD for the rp-process

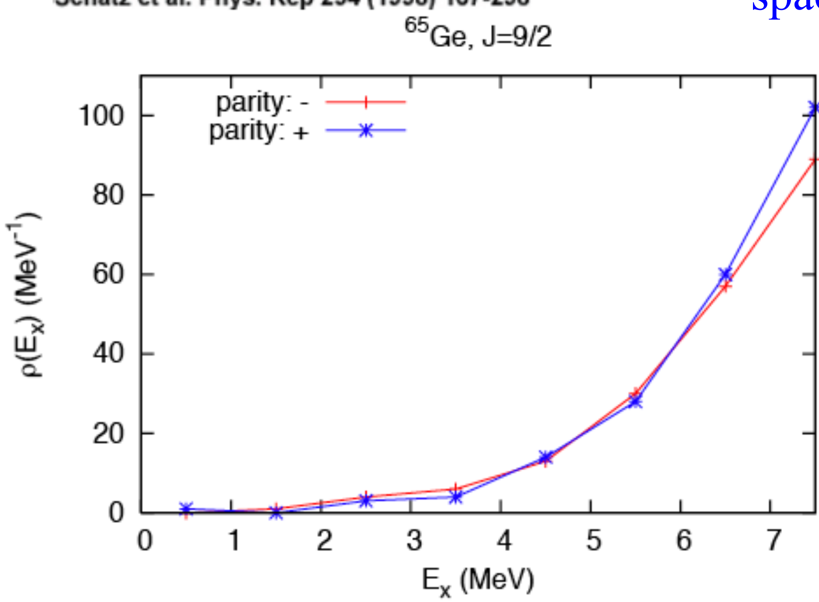
the rp-process path

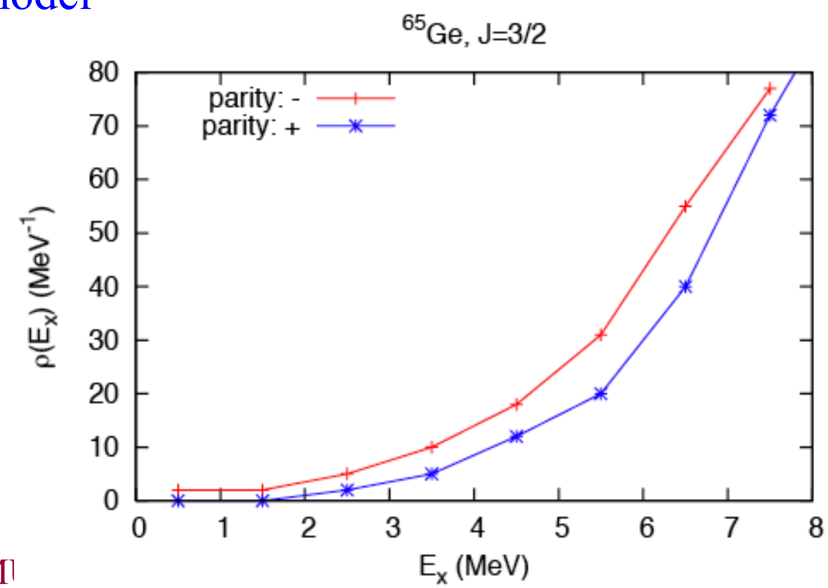


Schatz et al. Phys. Rep 294 (1998) 167-298

$f_{5/2}\, p\, g_{9/2}$ model space







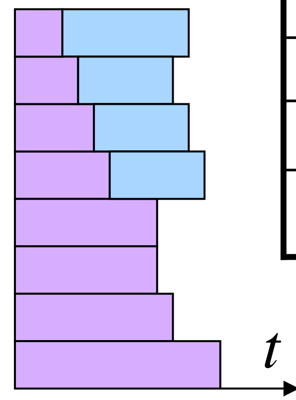
Scaling of the MPI JMOMENTS Code

Domain decomposition: many-body configurations

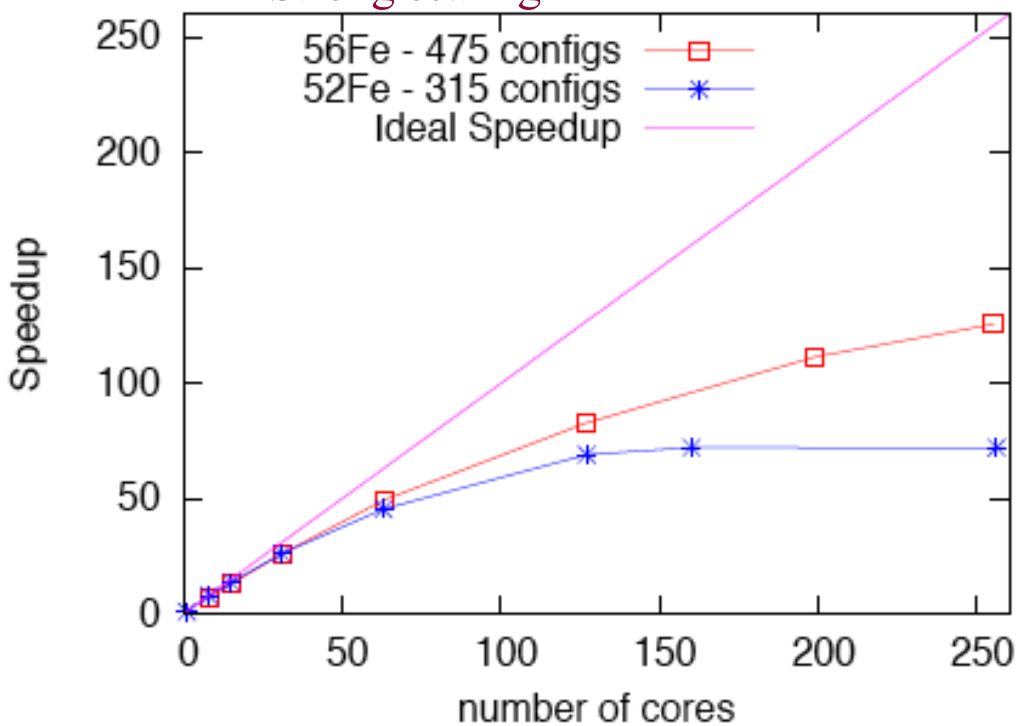
Algorithm: Dynamical Load Balancing

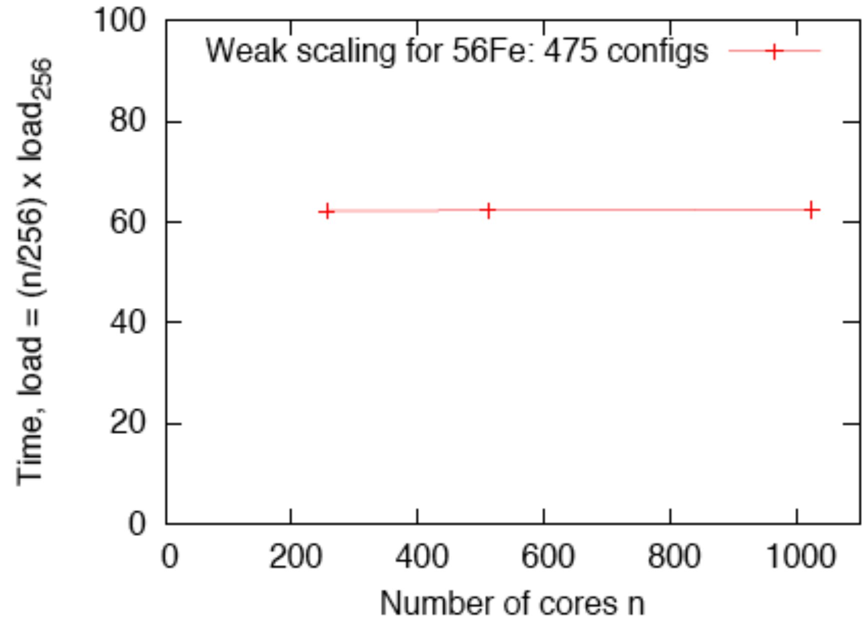
Machine: Franklin/NERSC

Nucleus / model space	Isospin configs	PN - configs
52Fe/pf	315	22028
56Fe/pf	475	51174
64Ge/pfg9/2	3749	510544



Strong scaling





NLD and Statistical Spectroscopy: PN Formalism

M. Horoi et al. :

PRC **67**, 054309 (2003),

PRC **69**, 041307(R) (2004),

NPA **785**, 142 (2005).

PRL **98**, 265503 (2007)

Configurations: e.g. 4P and 4N in *pf* model space

Pf7	Pp3	Pf5	Pp1	Nf7	Np3	Nf5	Np1
4	0	0	0	4	0	0	0
3	1	0	0	4	0	0	0
4	0	0	0	3	1	0	0
…							

preserve rotational invariance and parity

$$\rho(E_x,J,\pi) = \sum_{c\in conf} D_c(J,\pi) G_{FR}\left(E,E_c(J),\sigma_c(J)\right)$$

$$E_c(J),\sigma_c(J) \leftarrow Tr_{SD_c} < M \mid H^q \mid M >_{SD_c}$$

$$E_x = E - E_{g.s.}$$

$E_{g.s.}$ from CI, PCI, Exponential Convergence Method (PRL **82**, 2064 (1999)), CC, etc, **or determined**.

$E_c(J)$, $\sigma_c(J)$: computational intensive

Many more configurations, which can be more efficiently be calculated in parallel

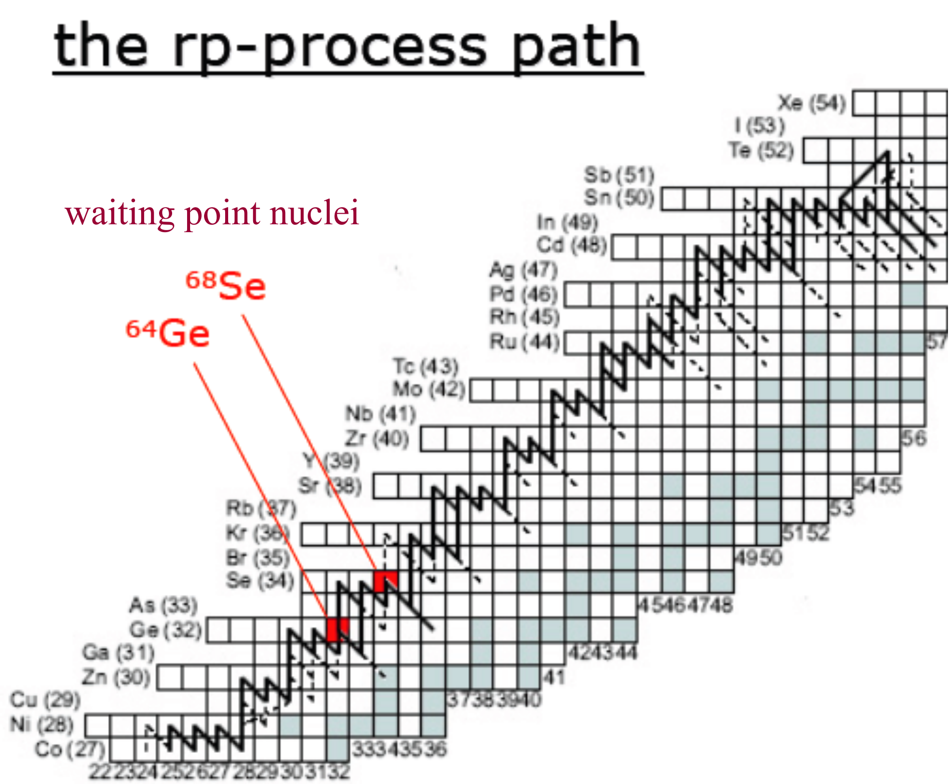
$$D^{\vec{k}}(PN\vec{m}M) = \sum_{M_P+M_N=M} D^{\vec{k}_P}(P\vec{m}M_P) D^{\vec{k}_N}(N\vec{m}M_N)$$

JMOMENTS PN Code for Nuclear Level Density

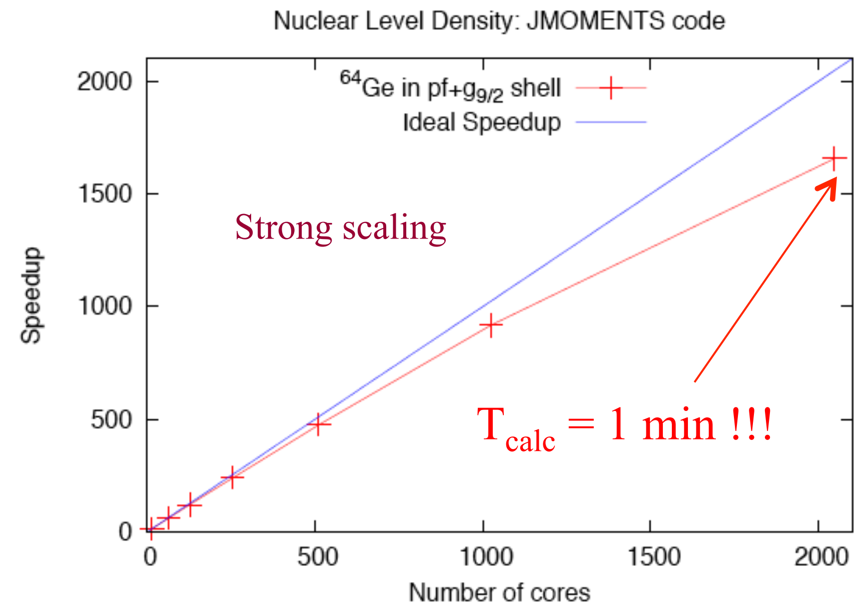
Domain decomposition: many-body configurations

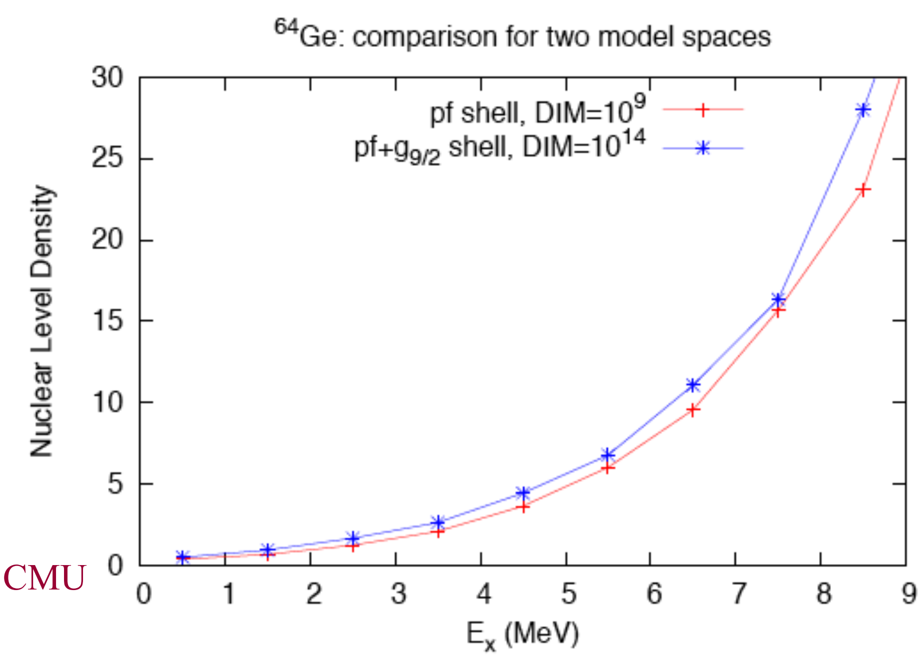
Algorithm: Dynamical Load Balancing

Machine: Franklin/NERSC



Schatz et al. Phys. Rep 294 (1998) 167-298



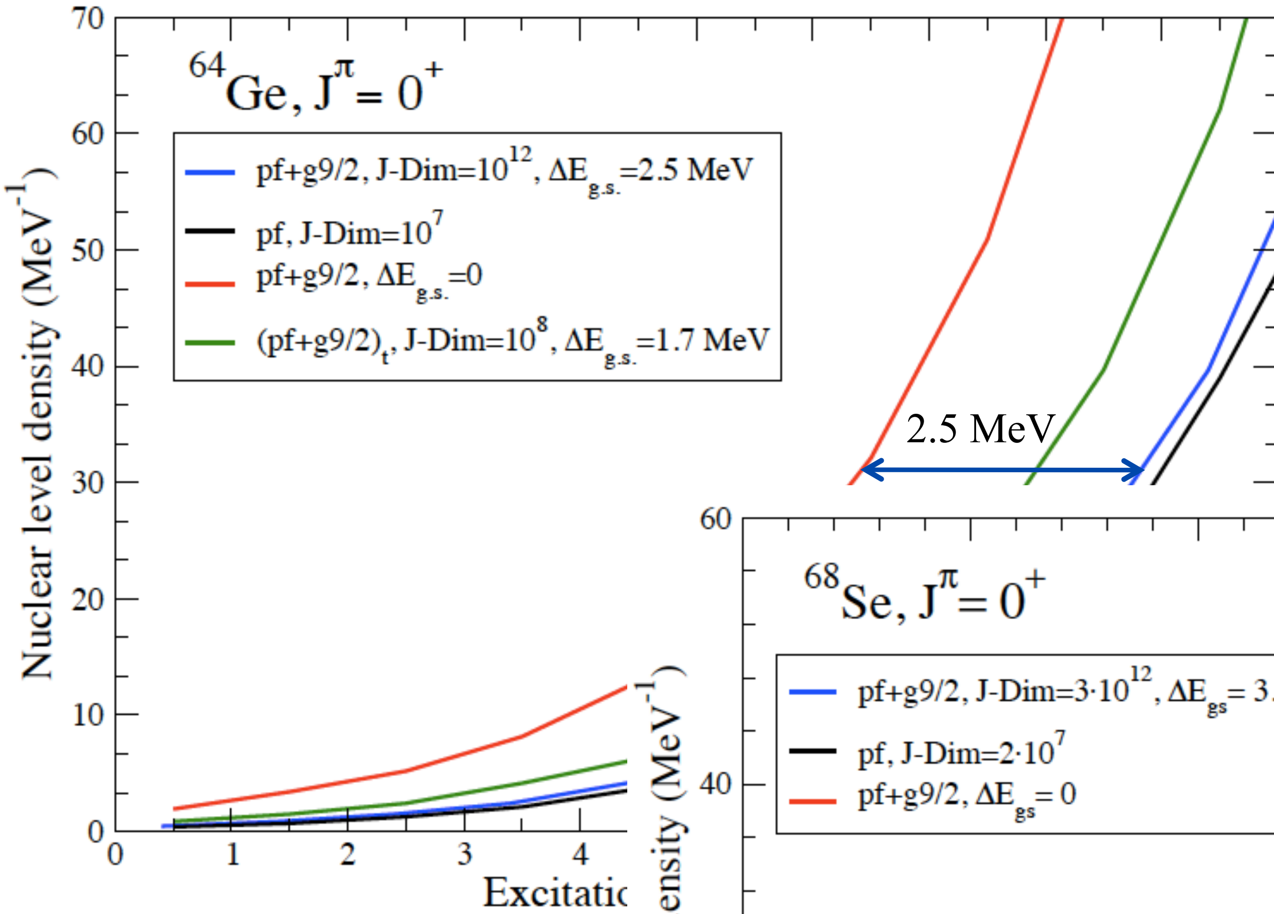


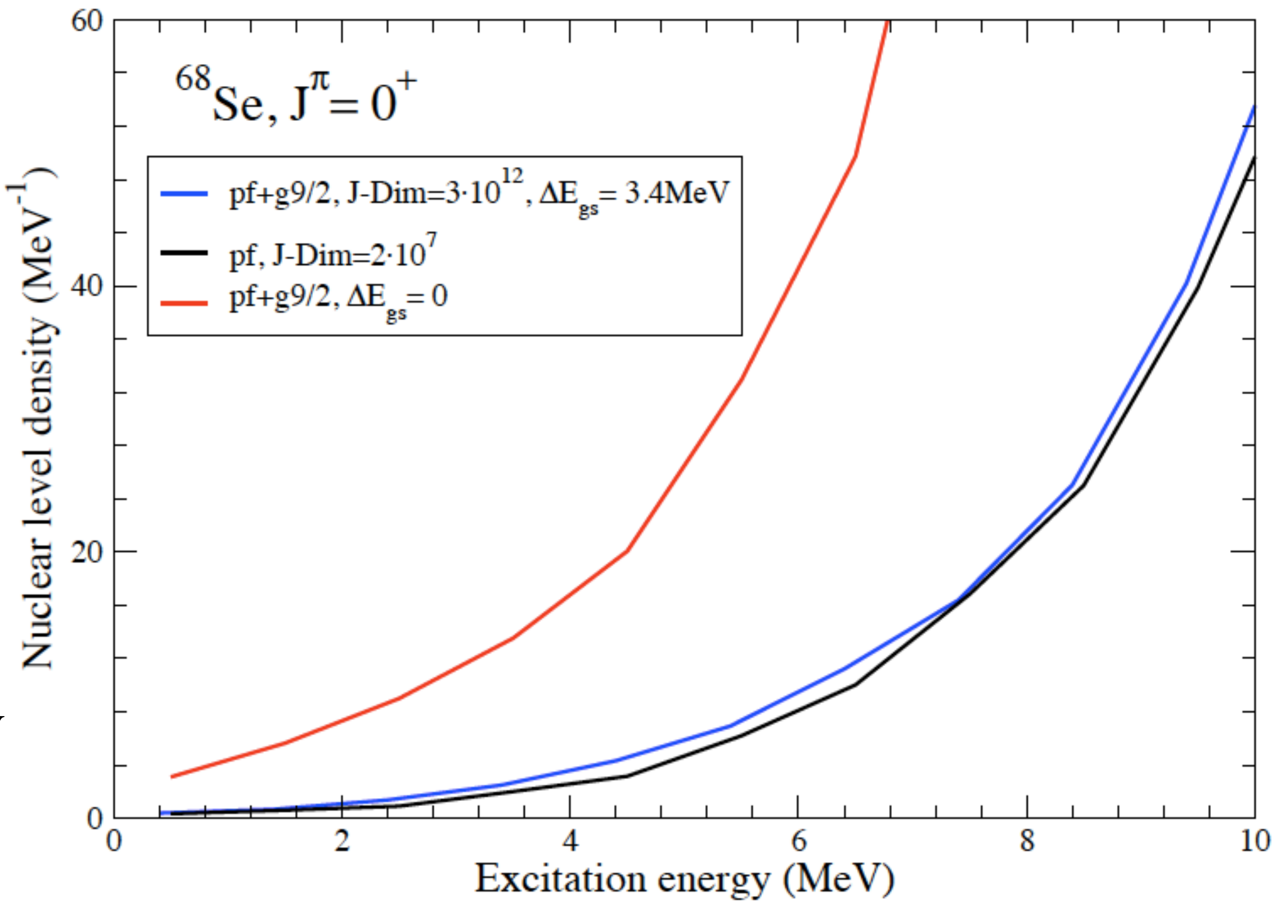
Results

$E_{gs}(pf) = -304.25$ MeV

$E_{gs}(pf+g9/2)_t = -305.95$ MeV

$E_{gs}(pf+g9/2)_s = -306.75$ MeV



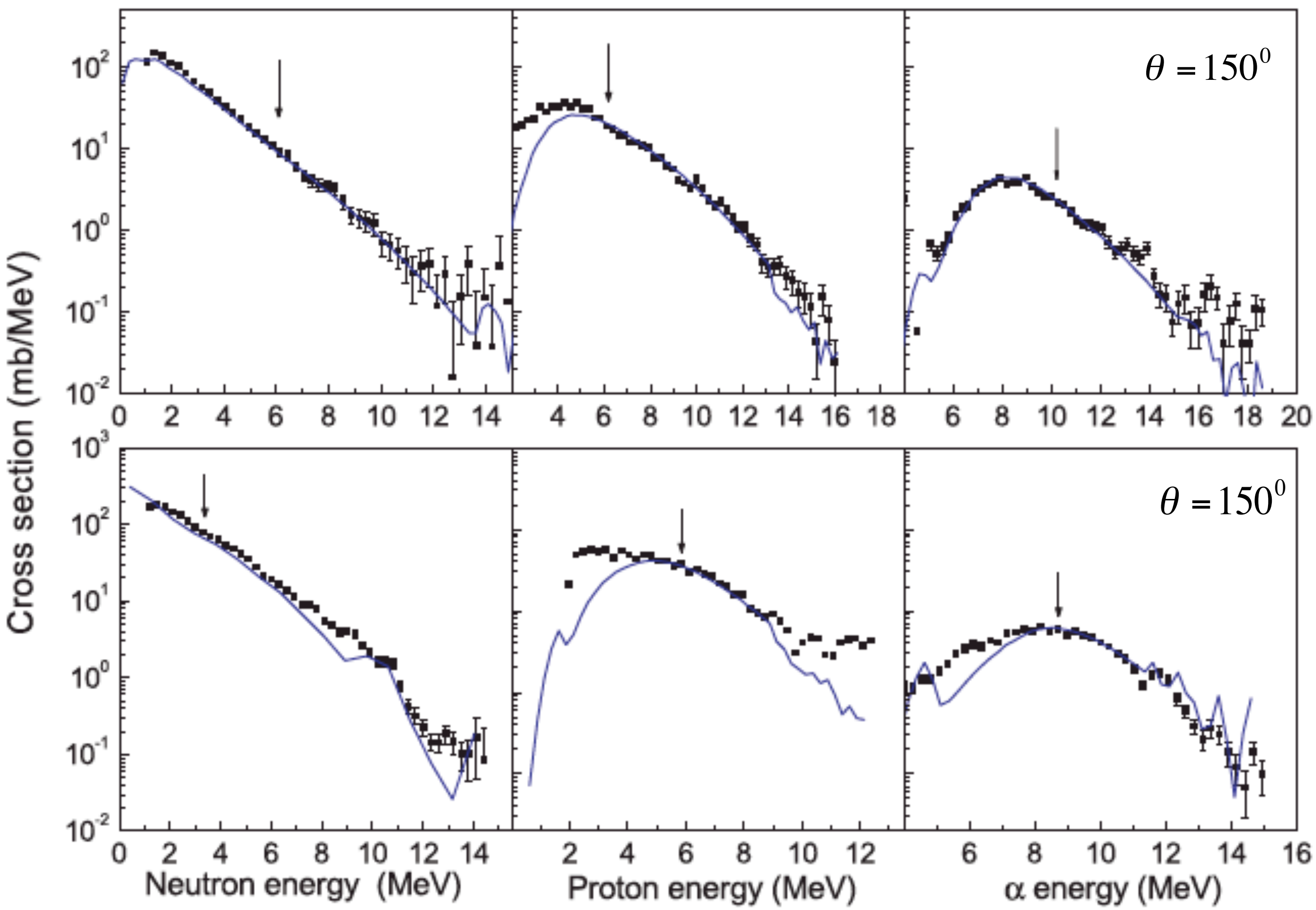


$E_{gs}(pf) = -353.1$ MeV

$E_{gs}(pf+g9/2)_s = -356.6$ MeV

NLD and Hauser-Feshbach

From A. Voinov et al., PRC **76**, 044602 (2007)



$\leftarrow\ ^3He + ^{58}Fe$

$E_{^3He} = 10\,MeV$

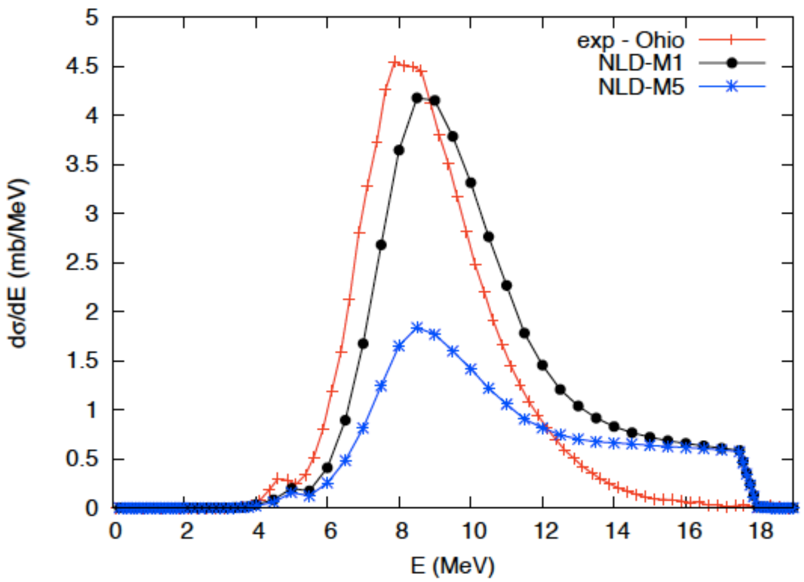
$^{61}Ni^*$ compund

$\leftarrow\ d + ^{59}Co$

$E_d = 7.5\,MeV$

NLD and Hauser-Feshbach

talys 1.2 : www.talys.eu



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

$\theta = 150^0$

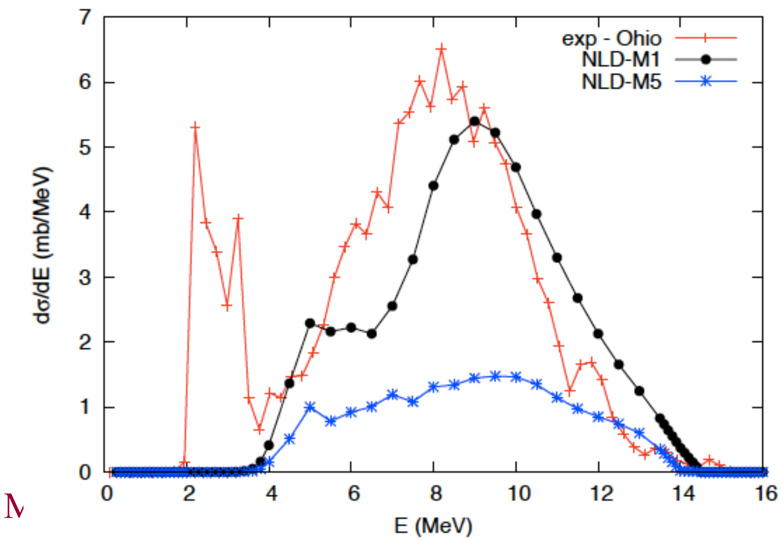
ldmodel 1: Constant temperature + Fermi gas model

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



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

$\theta = 150^0$

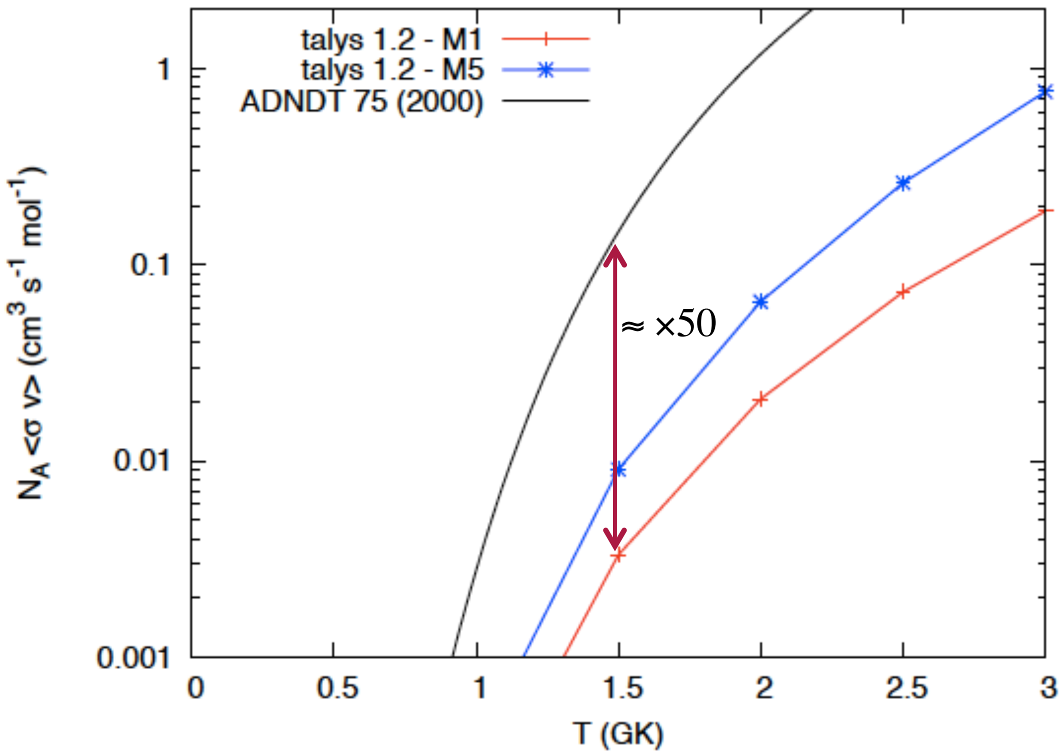
NLD: reaction rates

talys 1.2 : www.talys.eu

Rauscher & Thielemann ADNDT **75**, 1 (2000)

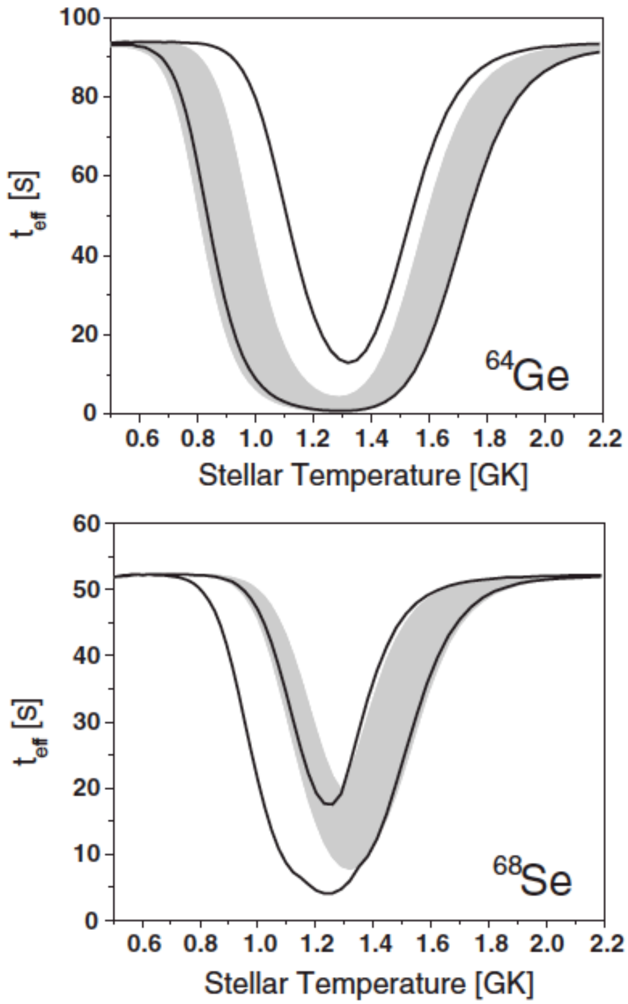
$$N_A\langle\sigma v\rangle^*_{\alpha\alpha'}(T) = \left(\frac{8}{\pi m}\right)^{1/2}\frac{N_A}{(kT)^{3/2}\,G(T)}\int_0^\infty\sum_\mu\frac{(2I^\mu+1)}{(2I^0+1)}\times \sigma^\mu_{\alpha\alpha'}(E)E\exp\left(-\frac{E+E^\mu_x}{kT}\right)dE,$$

$$G(T) = \sum_\mu (2I^\mu+1)/(2I^0+1)e^{-E_x^\mu/kT} \rightarrow \sum_{I,\pi}\int (2I^\pi+1)/(2I^0+1)\rho(E_x,I,\pi)e^{-E_x/kT}$$



NLD: rp-process

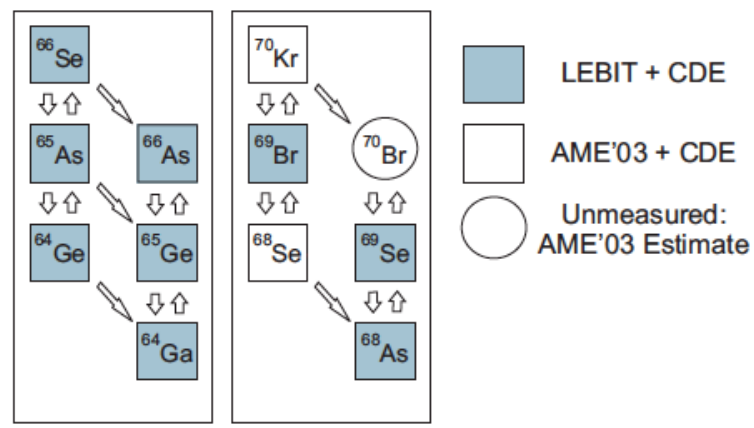
See also PRC 75, 032801(R) (2007)



From. P. Shury et al., PRC 75, 055801 (2007)

TABLE VI. Reaction Q-values derived from mass measurements and Coulomb displacement energies reported herein and derived from AME'03 [31]. All values in keV.

Reaction	This work	AME'03
^{64}Ge(p,γ)^{65}As	−255(104)	−354(172)[a]
^{65}As(p,γ)^{66}Se	2350(200)	2433(246)
^{68}Se(p,γ)^{69}Br	−679(119)[b]	−463(129)[b]
^{69}Br(p,γ)^{70}Kr	2450(216)	2234(227)



Rauscher & Thielemann ADNDT **75**, 1 (2000)

Removal of Spurious Center-of-Mass Excitations

$\rho(E, J, 0+2)$: total density in a model space including all $0+2$ h.o. excitations

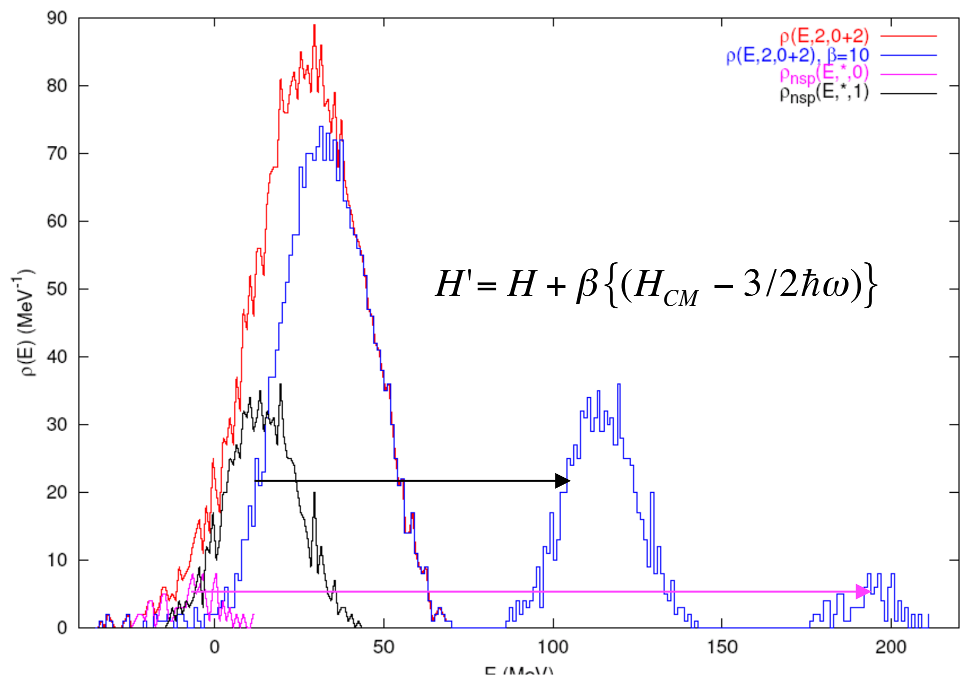
$\rho_{nsp}(E, J, 0+2)$: center-of-mass excitations removed

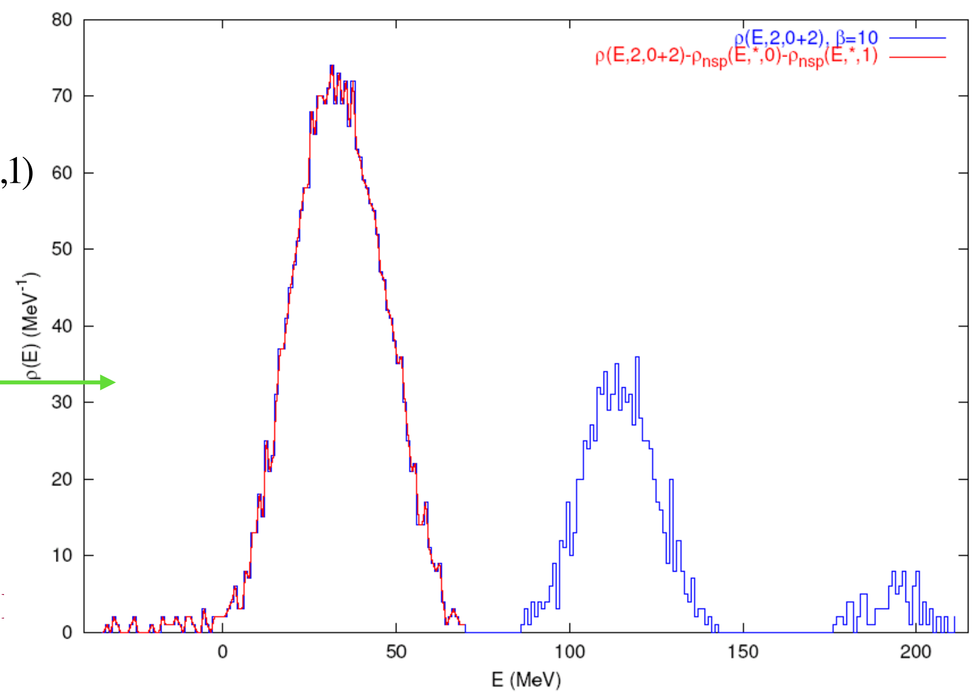
$$\rho_{nsp}(E, J=2, 0+2) =$$

$$\rho(E,2,0+2) - \sum_{\substack{J_K=0 \\ step\ 2}}^{2} \sum_{J'=|2-J_K|}^{2+J_K} \rho_{nsp}(E,J',0) - \sum_{J'=1}^{3} \rho_{nsp}(E,J',1)$$

^{10}B: 10 particles in *s-p-sd-pf* shell model space

Horoi and Zelevinsky, PRL **98**, 265503 (2007)





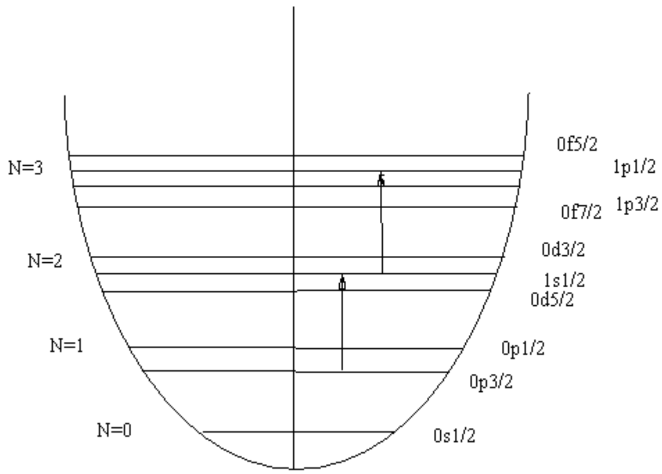
Fixed J Restricted Configuration Widths

PHYSICAL REVIEW C 69, 041307(R) (2004)

[redacted]

Fixed spin and parity nuclear level density for restricted shell model configurations

Mihai Horoi,[1] Monica Ghita,[1] and Vladimir Zelevinsky[2,3]
[1]*Physics Department, Central Michigan University, Mount Pleasant, Michigan 48859, USA*
[2]*National Superconducting Cyclotron Laboratory, East Lansing, Michigan 48824, USA*
[3]*Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA*
(Received 14 January 2004; published 30 April 2004)



$$
\begin{aligned}
<< H^2 >>_{\vec{m}nMT_z}(m' = m) &\equiv << H|m >< m|H >> \\
&= \sum_i \epsilon_i^2 D^i(\vec{m}nMT_z) + \\
&\sum_{i<j} \left[2\epsilon_i\epsilon_j + 2(\epsilon_i + \epsilon_j)V_{ijij} + V_{ijij}^2\right] D^{ij}(\vec{m}nMT_z) + \\
&\sum_{(i<j)\neq l} \left[2V_{liil}V_{ljjl} + 2\epsilon_l V_{ijij}\right] D^{ijl}(\vec{m}nMT_z) + \\
&\sum_{(i<j)\neq(k<l)} \left[V_{ijij}V_{klkl}\right] D^{ijkl}(\vec{m}nMT_z)
\end{aligned}
$$

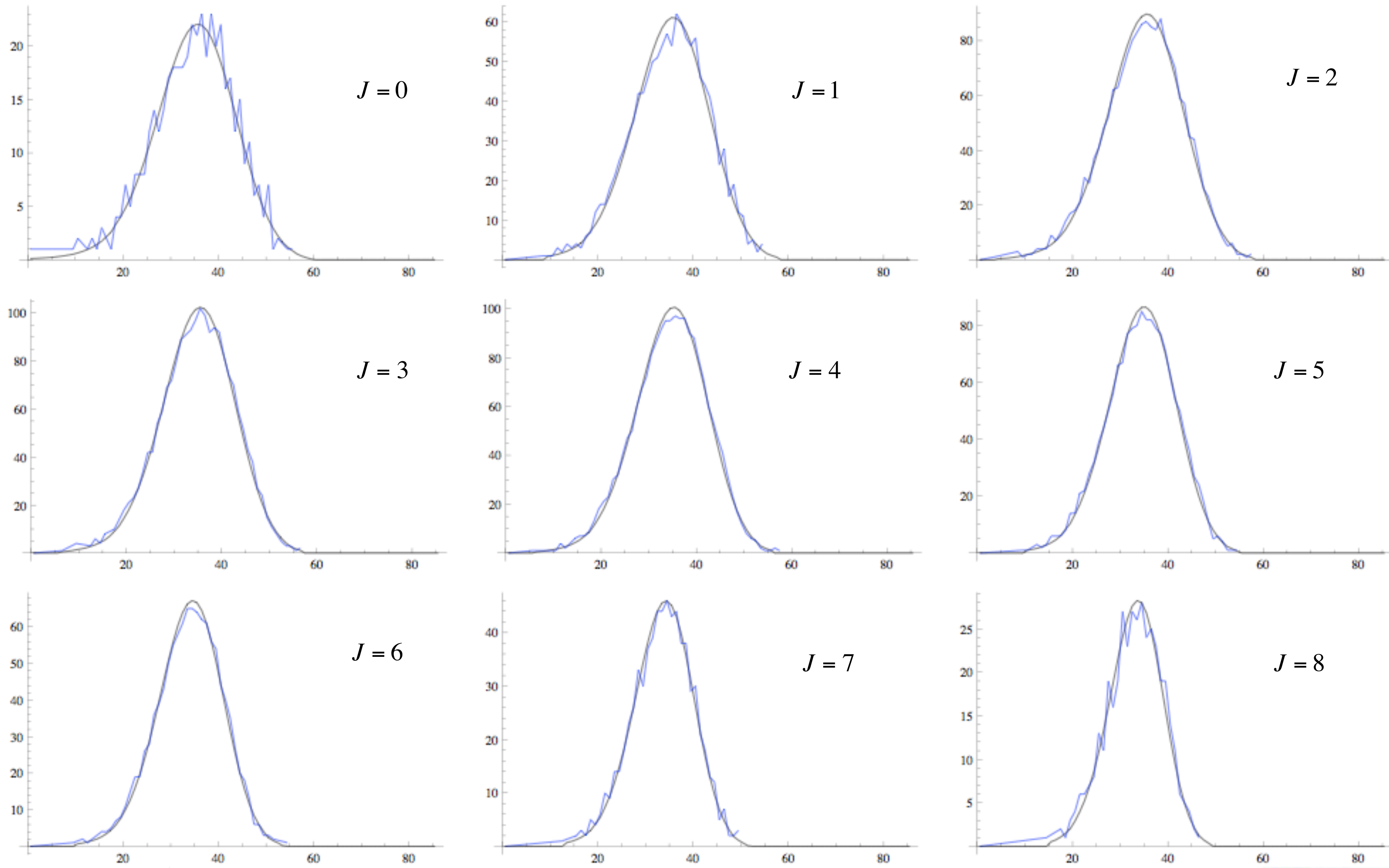
$$
\begin{aligned}
H^2 >>_{\vec{m}nMT_z}(\vec{m}' = \vec{m} : r^{-1}s^{+1}) = &\sum_i V_{riis}^2 D^{ir}(\vec{m}nMT_z) - \\
&\sum_i V_{riis}^2 D^{irs}(\vec{m}nMT_z) + \\
&\sum_{i\neq j} V_{riis}V_{rjjs} D^{ijs}(\vec{m}nMT_z) - \\
&\sum_{i\neq j} V_{riis}V_{rjjs} D^{ijrs}(\vec{m}nMT_z)
\end{aligned}
$$

$$
\begin{aligned}
<< H^2 >>_{\vec{m}nMT_z}(\vec{m}' = \vec{m} : r^{-1}s^{-1}t^{+1}u^{+1}) = &V_{rstu}^2 D^{rs}(\vec{m}nMT_z) - \\
&V_{rstu}^2 D^{rst}(\vec{m}nMT_z) - \\
&V_{rstu}^2 D^{rsu}(\vec{m}nMT_z) + \\
&V_{rstu}^2 D^{rstu}(\vec{m}nMT_z)
\end{aligned}
$$

$$D^{ij}, D^{ijr}, D^{ijrs}$$

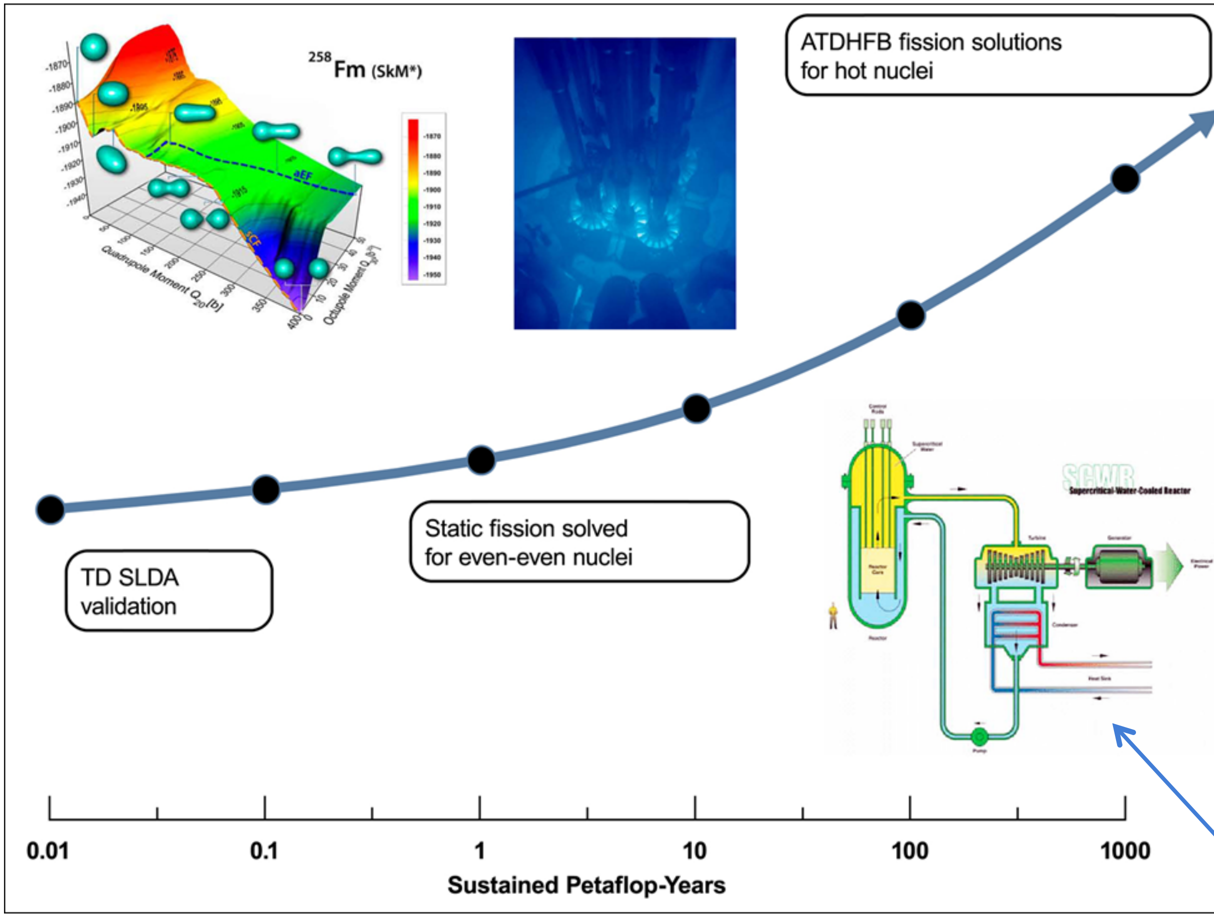
Moments method with restricted configurations

Si in sd model space: only 4p-4p configurations included



Extreme Computing Goals

http://extremecomputing.labworks.org/nuclearphysics/report.stm



Reaction DB TENDL-2009: www.talys.eu → MCNPX: mcnpx.lanl.gov

Summary and Outlook

- ✓ Shell model techniques describe and predict a large number of data in medium and heavy nuclei.
- ✓ BSFG and mean-field models describe the existing data within a factor of 10 (average 2), but they can calculate NLD for all nuclei.
- ✓ CI J-dependent NLD seem to be more accurate, but can only be obtained for a limited number of nuclei.
- ✓ J-dependent **moments** method reproduces very well the CI J-dependent NLD and could provide accurate NLD for a much larger class of nuclei.
- ✓ Work to integrated SM NLD with reaction codes is in progress.