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Interface Between Shell Model Nuclear Level Densities and Nuclear Reaction Code

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Overview

- The interactive shell model and effective Hamiltonians
- Spin and parity moments method and nuclear level density
- Removal of center-of-mass spurious states
- Applications to reaction rates
- Interface with TALYS code
- Summary and Outlook

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Nuclear Configuration Interaction

$0\hbar\omega$

$1\hbar\omega$

$(0+2)\hbar\omega$

$(1+3)\hbar\omega$

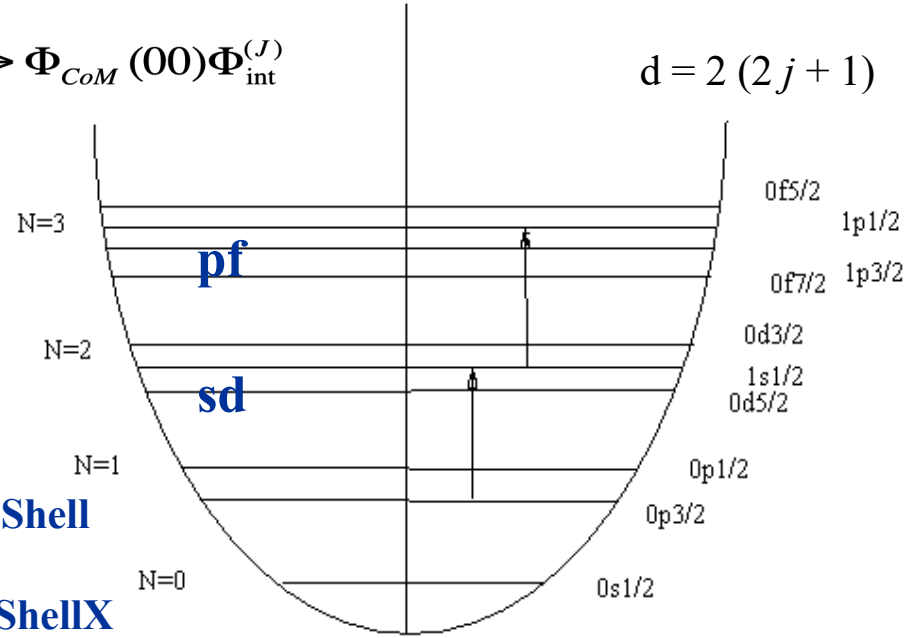
$$H' = H + \beta(H_{CoM} - 3/2\hbar\omega)$$

Center-of-mass spurious states

$$\Psi^{(J)} = [\Phi_{CoM}(NL)\Phi^{(J')}_{\text{int}}]^{(J)} \rightarrow \Phi_{CoM}(00)\Phi^{(J)}_{\text{int}}$$

$d = 2(2j+1)$

N_{max}



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

$$|\alpha> = \sum_i C_i^\alpha \, |i(JT)>$$ **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, …**

Limits: 10^{10} – 10^{11} m-scheme basis states, about 50 s.p. valence states (p+n)

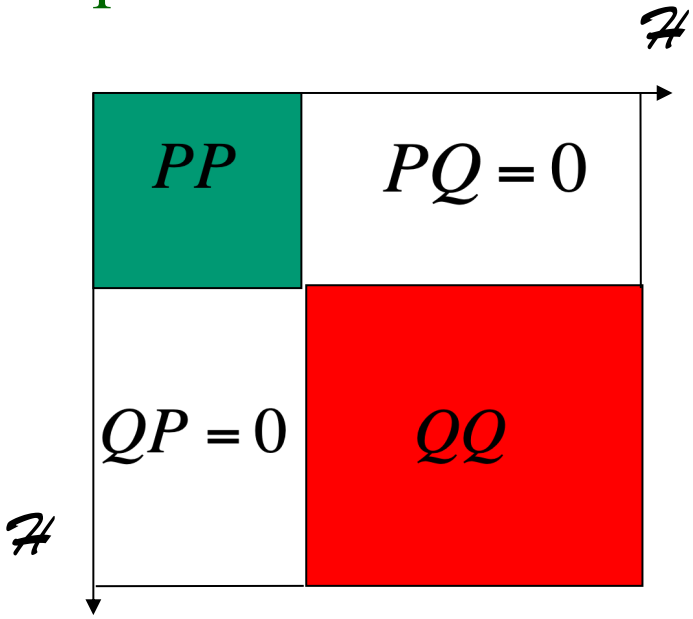
$$\sum_j <i|H|j> C_j^\alpha = E_\alpha C_i^\alpha$$

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

Effective Hamiltonians for Large N $\hbar\omega$ Excitation Model Spaces

Renormalization methods:

- G-matrix: Physics Reports 261, 125 (1995)
- Lee-Suzuki (NCSM): PRC 61, 044001 (2000)
- $V_{low\ k}$: PRC 65, 051301(R) (2002)
- Unitary Correlation Operator: PRC 72, 034002 (2004)
- Similarity Renormalization Group (SRG): PRL 103, 082501 (2009)



"Bare" Nucleon-Nucleon Potentials:

- Argonne V18: PRC 56, 1720 (1997)
- CD-Bonn 2000: PRC 63, 024001 (2000)
- N^{3}LO: PRC 68, 041001 (2003)
- INOY: PRC 69, 054001 (2004)

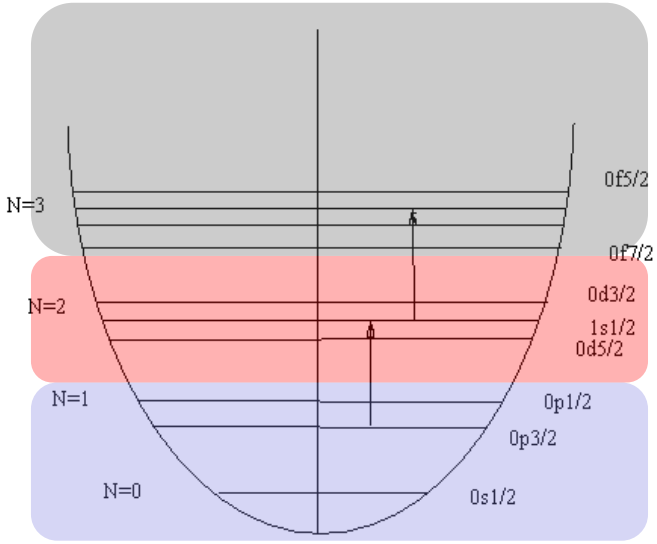
$$H = T + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \cdots$$

$$\Psi_{\mathcal{H}} \rightarrow \Psi_P \quad P\Psi_{\mathcal{H}}$$

$$\mathcal{H} = U\,H U^{+} = \mathcal{H}_2 + \mathcal{H}_3 + \mathcal{H}_4 + \ldots$$

$$O \rightarrow U\,O\,U^{+}$$

Shell Model Effective Hamiltonians



$g_A \sigma\tau \xrightarrow{quenched} g_A\, 0.77 \sigma\tau$

empty

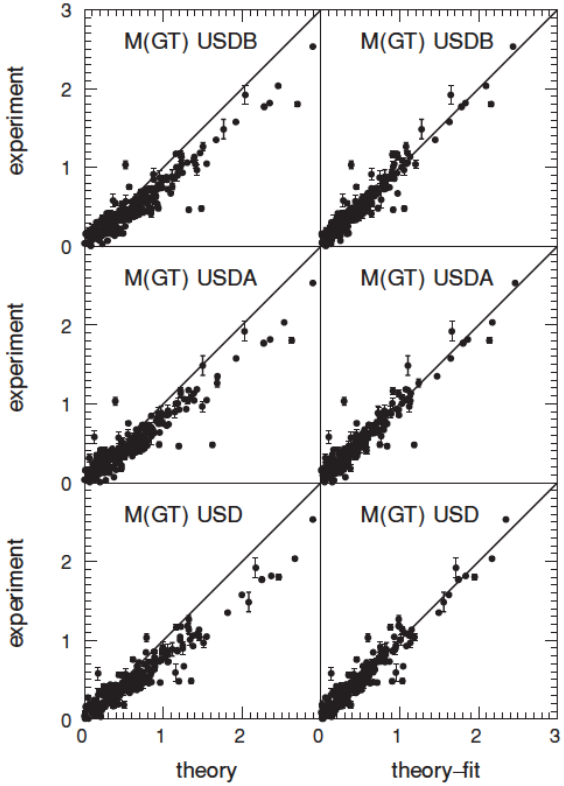
valence

frozen core

$H_{valence} = H_{2-body}$

can describe most correlations around the Fermi surface!

$H_{valence}\Psi = E_n\Psi$

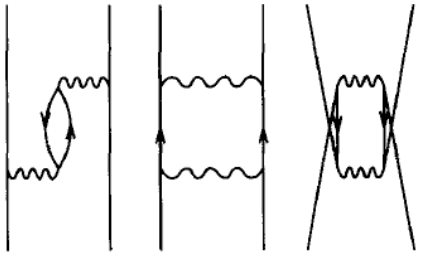


$\mathcal{H}$

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

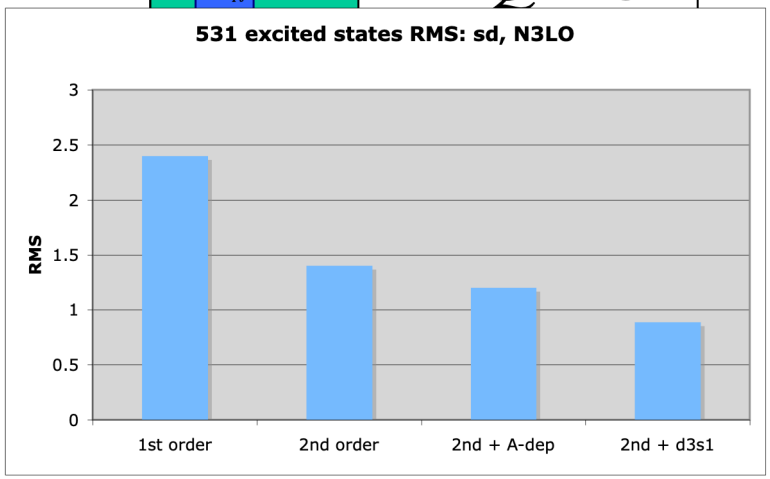


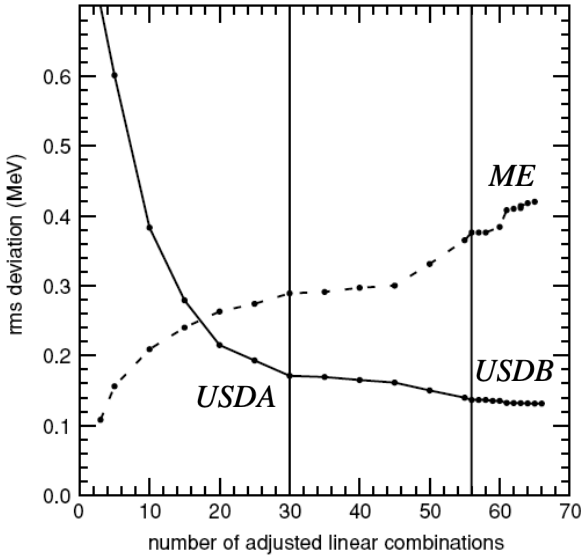
core polarization: Phys.Rep. **261**, 125 (1995)





$PQ = 0$



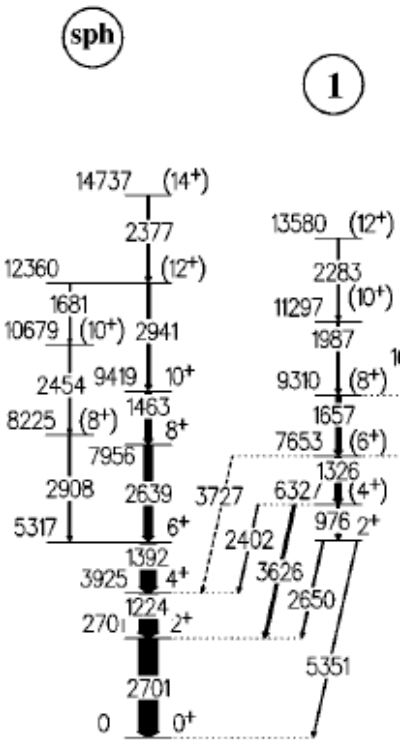


FRIB July 2, 2026

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

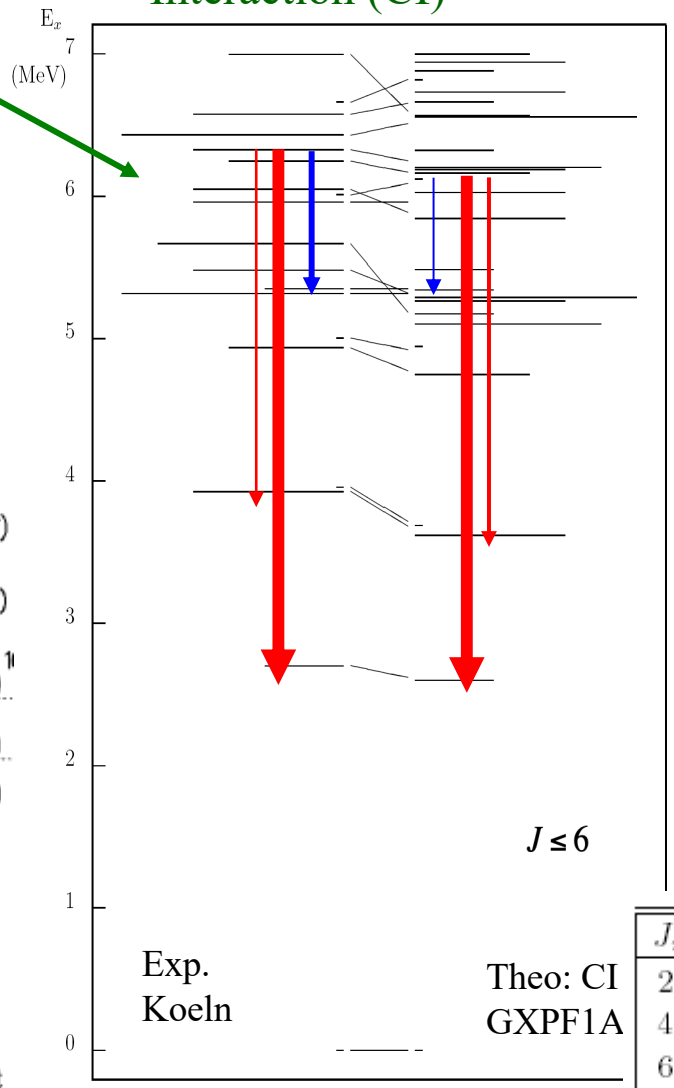
$^{56}_{28}Ni_{28}$



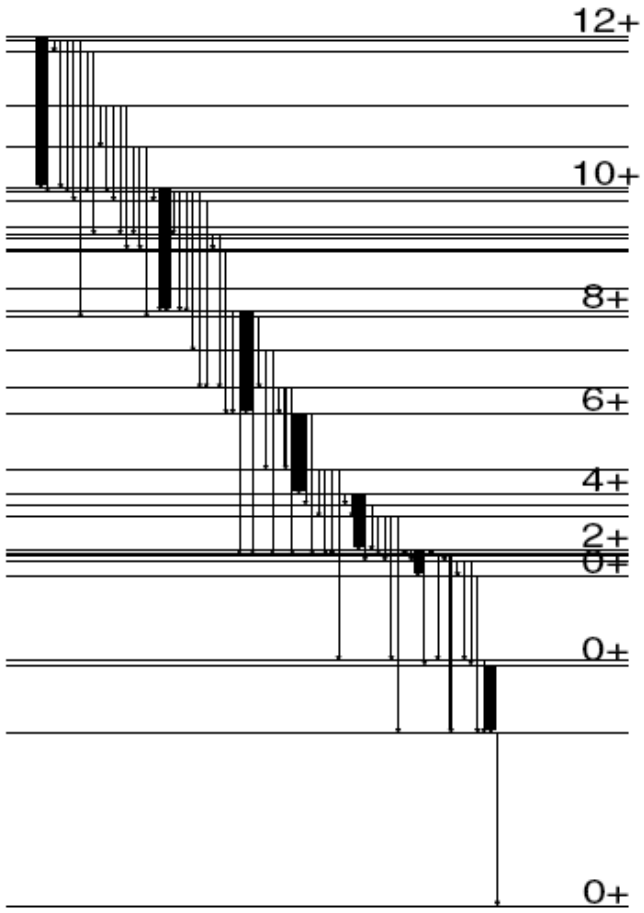
LBNL high spin **experiment**

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

Configuration Interaction (CI)



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



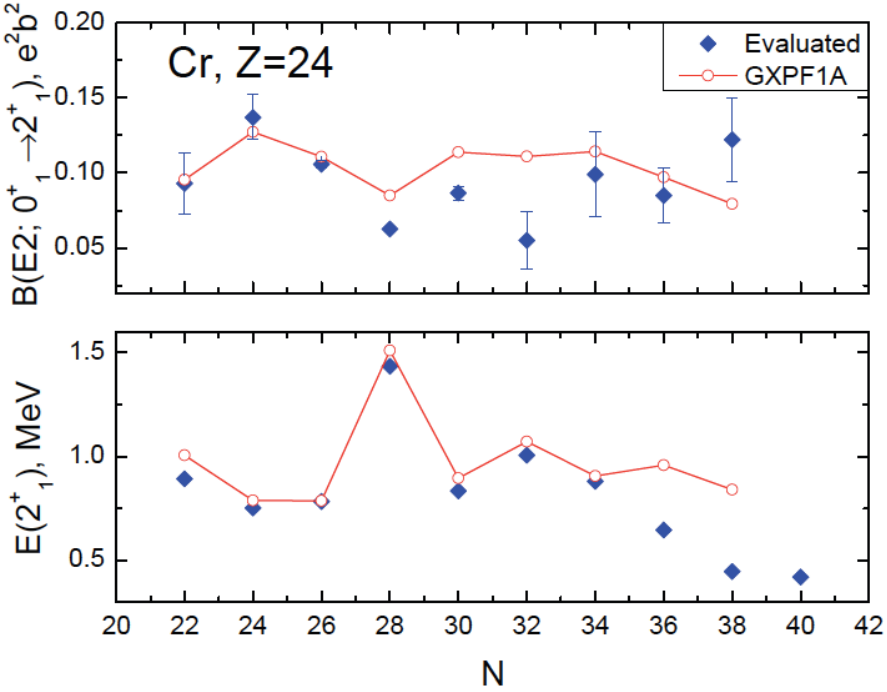
J_n	E_x (MeV)	$< Q >_{J0}$	$(Q_0)_{sp}$	B(E2; $J \rightarrow J-2$)	$\mid Q_0 \mid_{tr}$
2_3	5.342	-41.6	+145.3	413.2	144.1
4_5	6.027	-55.2	+151.9	598.0	143.8
6_3	7.556	-56.2	+140.6	609.3	139.5
8_4	9.300	-47.2	+112.2	558.4	130.5
10_6	10.782	-63.9	+147.0	591.1	132.5
12_5	13.071	-62.7	+141.1	612.3	133.7

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

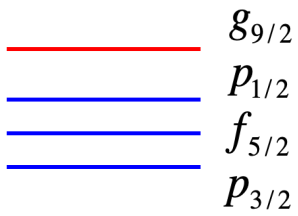
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B. Pritycenko, J. Choquette, M. Horoi, B. Karamy, B. Singh, Atomic Data and Nuclear Data Tables, **107**, 1 (2016)

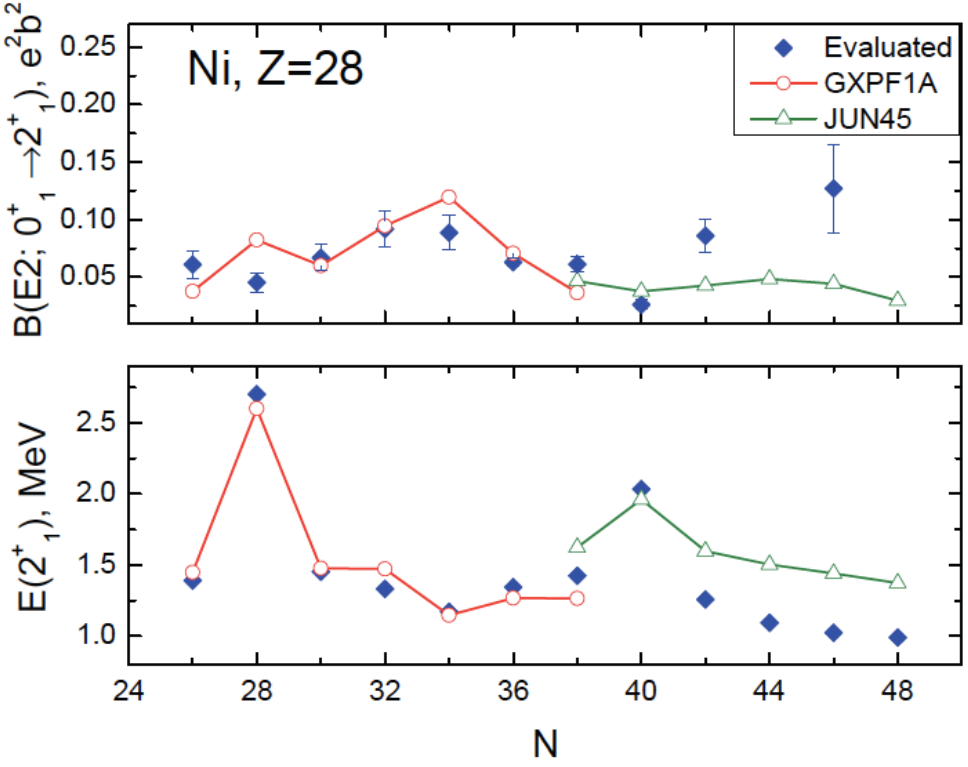
Shell-model Calculations

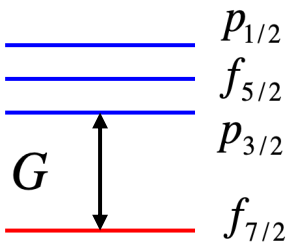


e been
GXPF1A and
$e^{p}_{eff} = 1.5 \quad e^{n}_{eff} = 0.5$

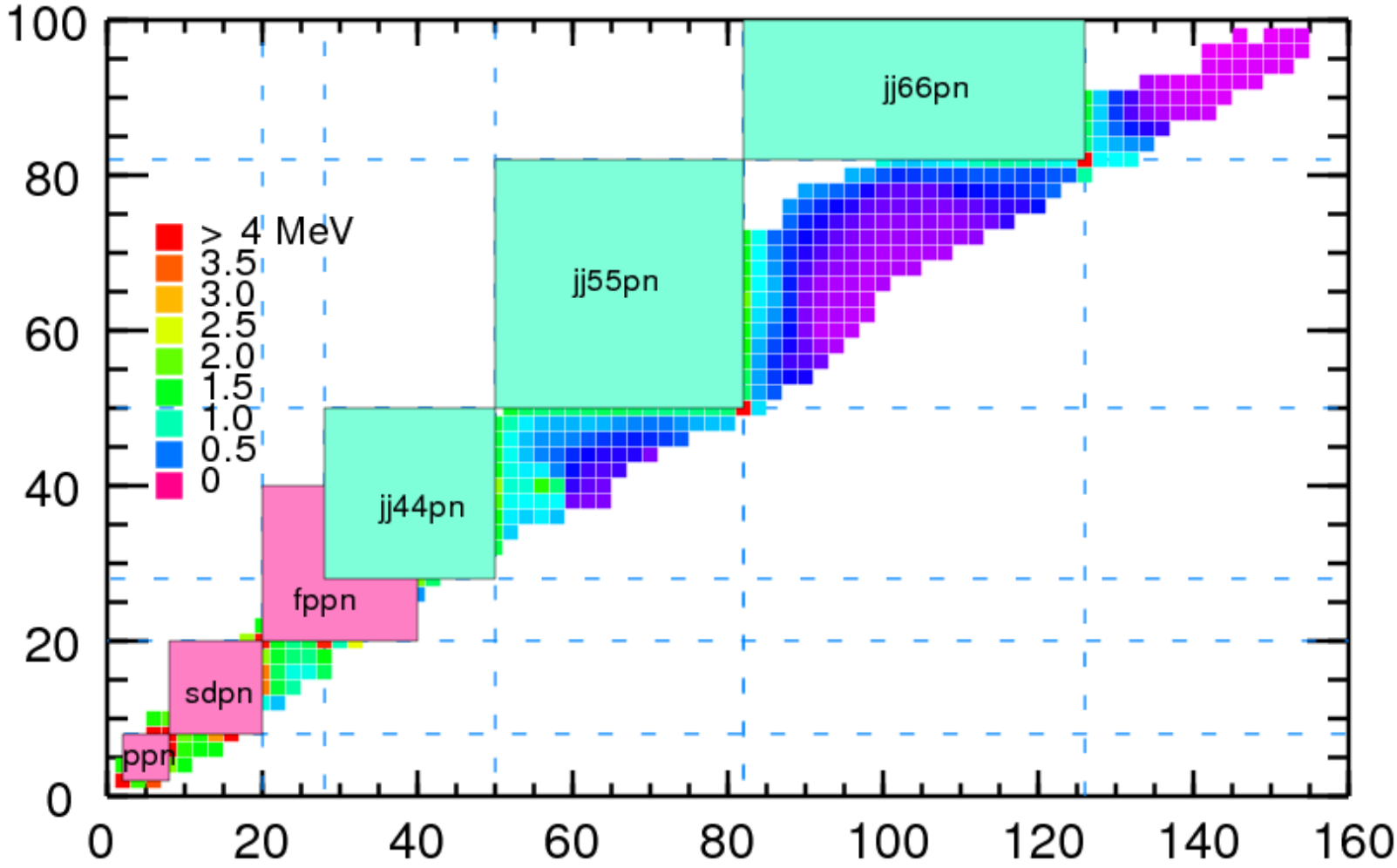


*JUN*45





*GXPF*1*A*


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

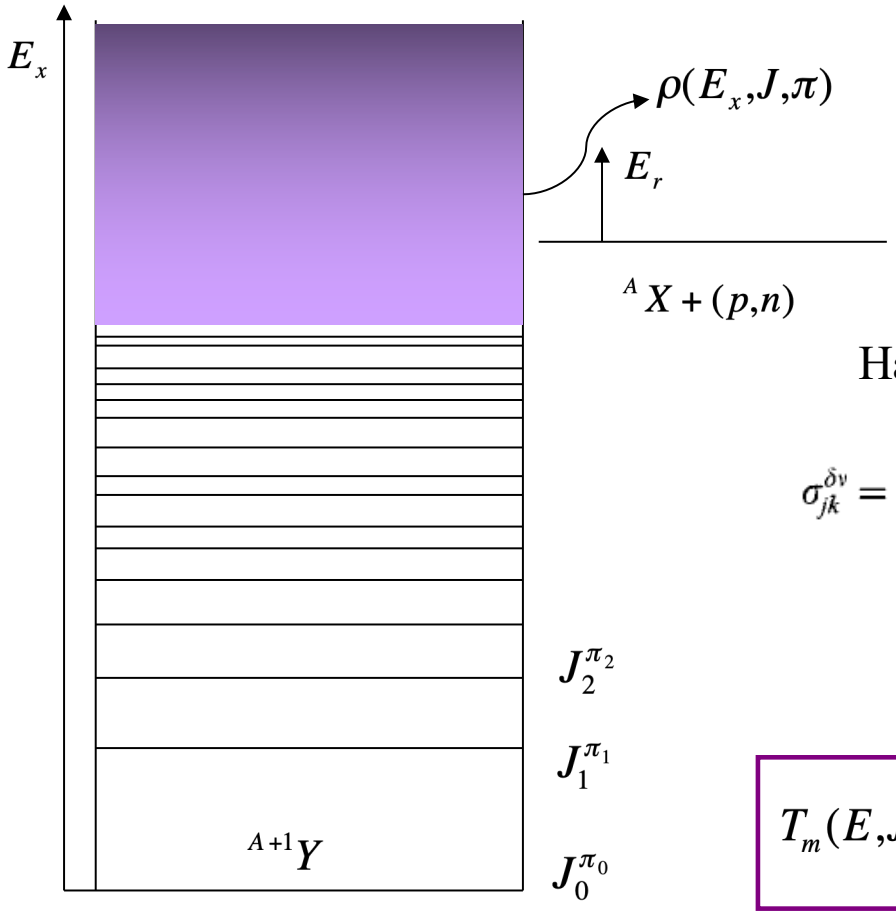
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Shell Model: Gold Standard of Nuclear Structure

- ✓ Shell model techniques **describe** and **predict** a large amount of data in light, medium, and heavy nuclei:
  - ✓ Energies and quantum numbers
  - ✓ Electromagnetic transition probabilities
  - ✓ Spectroscopic amplitudes
  - ✓ Nuclear level densities
  - ✓ Beta decay probabilities and charge exchange strength functions
  - ✓ 2ν/0ν Double-beta decay matrix elements

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Nuclear Level Densities (NLD)



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

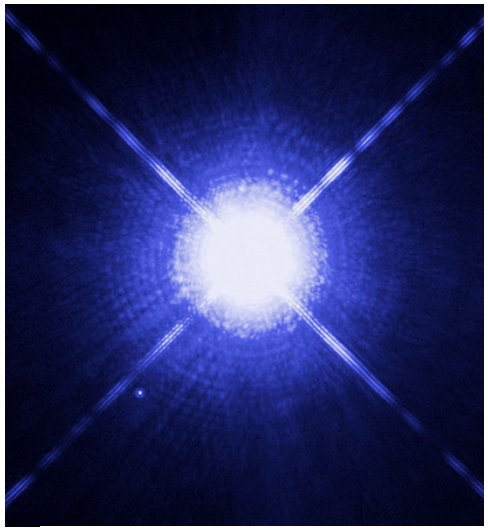
Hauser and Feshbach, Phys. Rev **87**, 366 (1952)

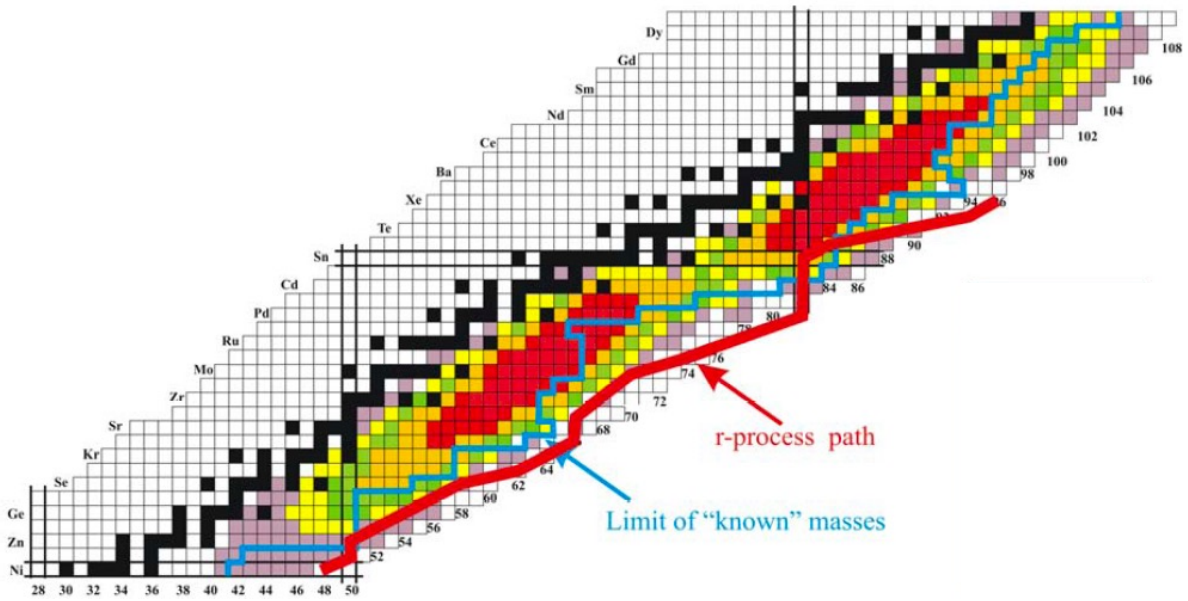
$$\sigma_{jk}^{\delta\nu} = \frac{\pi\hbar^2}{2\mu_{ij}E_{ij}}\frac{1}{(2J_i^{\delta}+1)(2J_j+1)} \times \sum_{J,\pi}(2J+1)\frac{T_j^{\delta}(E,J,\pi,E_j^{\delta},J_j^{\delta},\pi_j^{\delta})\,T_k^{\nu}(E,J,\pi,E_k^{\nu},J_k^{\nu},\pi_k^{\nu})}{\sum_m T_m(E,J,\pi)}$$

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

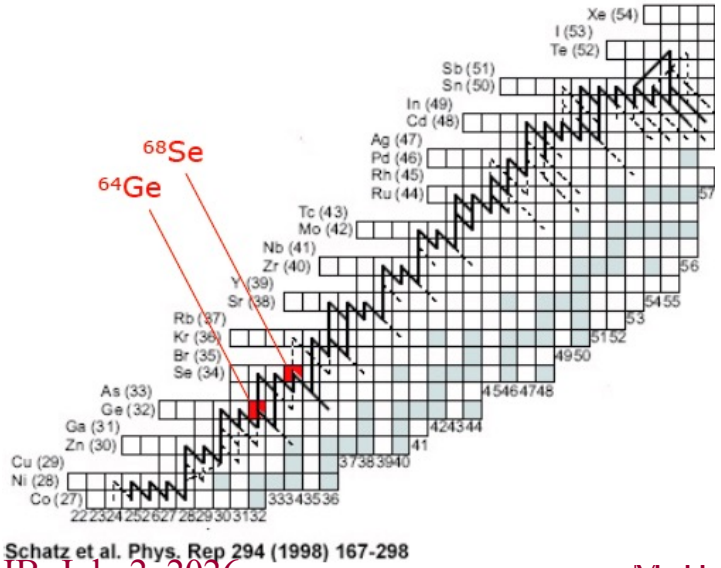
Where are NLD Needed: Nuclear Astrophysics

Binary stars XRB: Sirius





the rp-process path



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

SN 1987 A



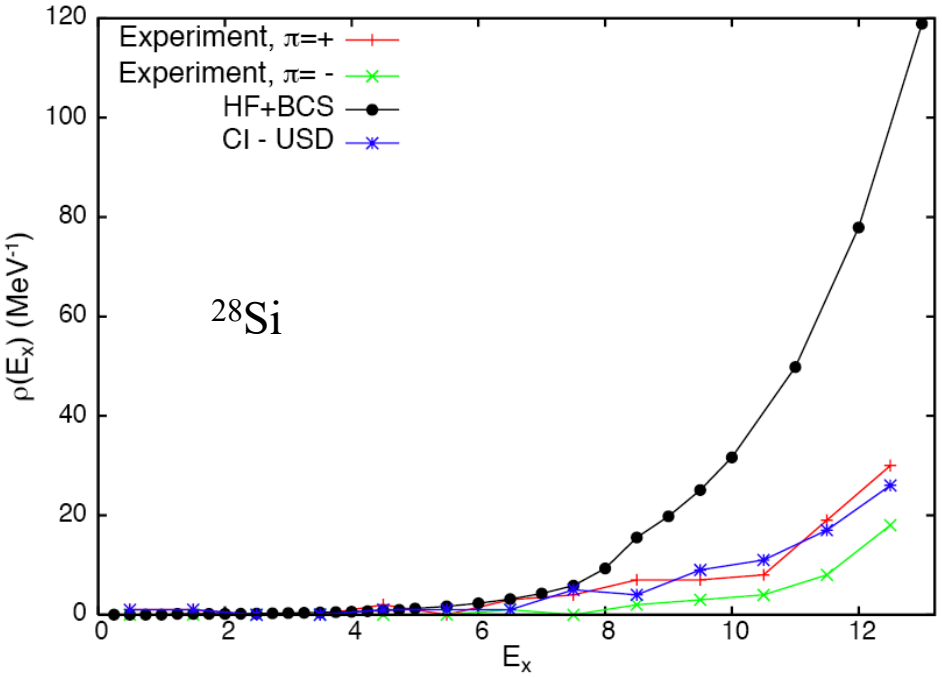
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Accurate Nuclear Level Densities

Comparison of:

1. CI
2. HF+BCS

   www-astro.ulb.ac.be/Html/nld.html
3. experimental data

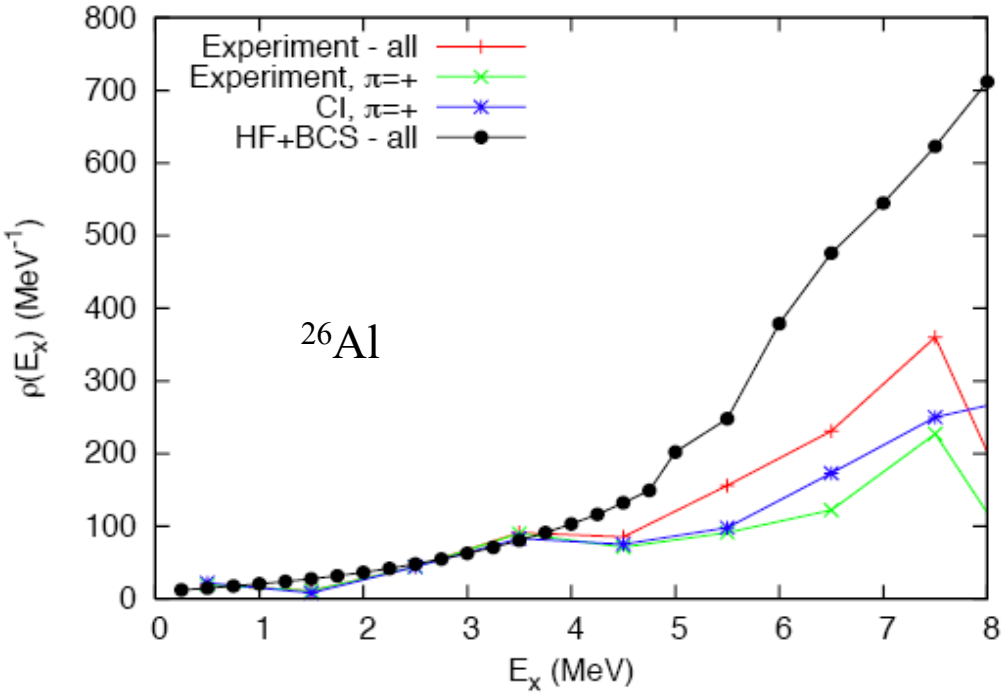


Complete spectroscopy: sd-shell nuclei

Conclusions:

- HF+BCS seems to overestimate the data

- CI seem to accurately describe the data



RGY Science

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NLD and Statistical Spectroscopy

M. Horoi et al. :

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

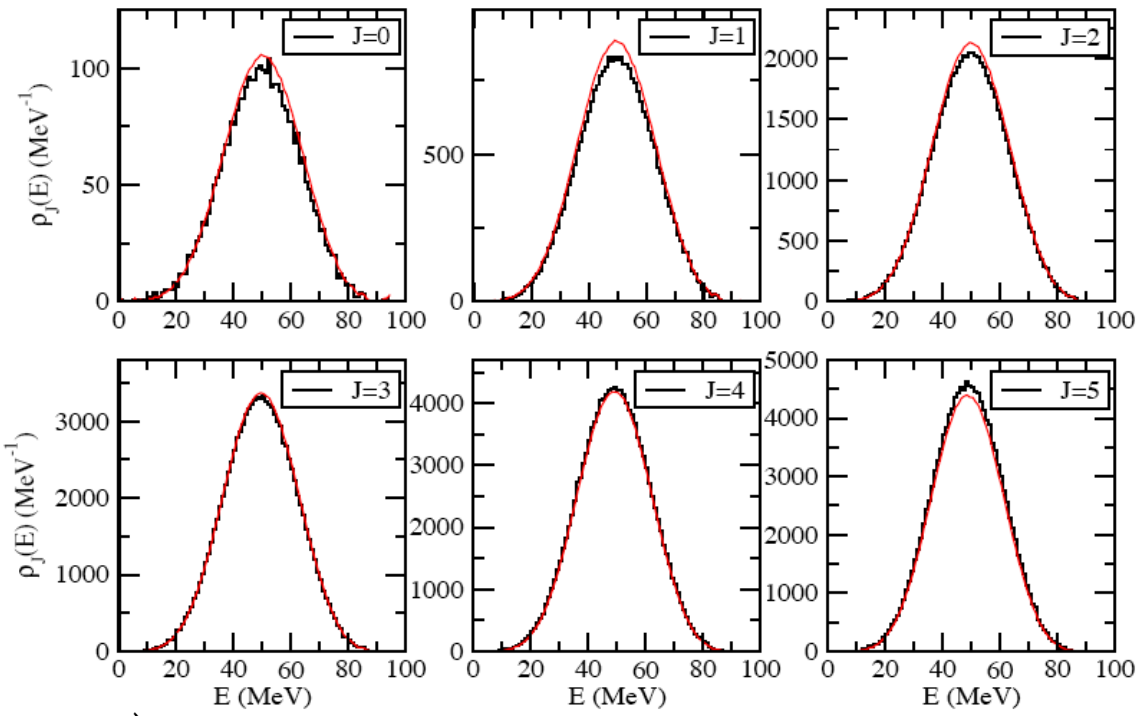
PRC **69**, 041307(R) (2004),

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

PRL **98**, 265503 (2007)

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

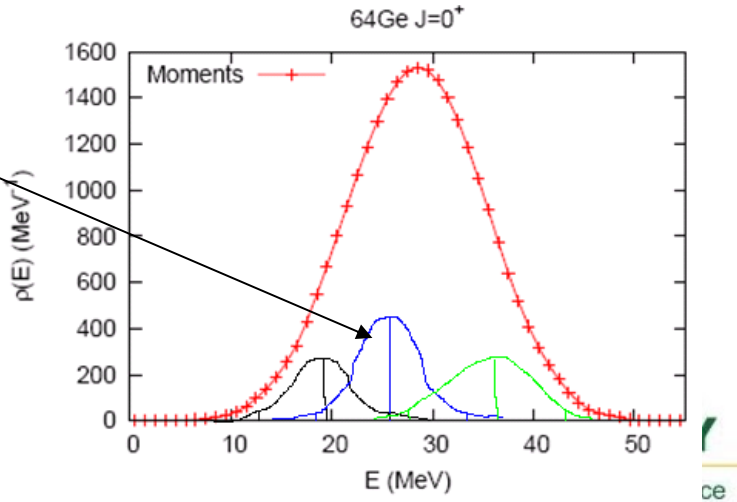
^{28}Si $\pi = +$ staircase: CI, USD



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

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

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



$E_{g.s.}$ from CI, ECM (PRL **82**, 2064 (1999)), CC, etc.

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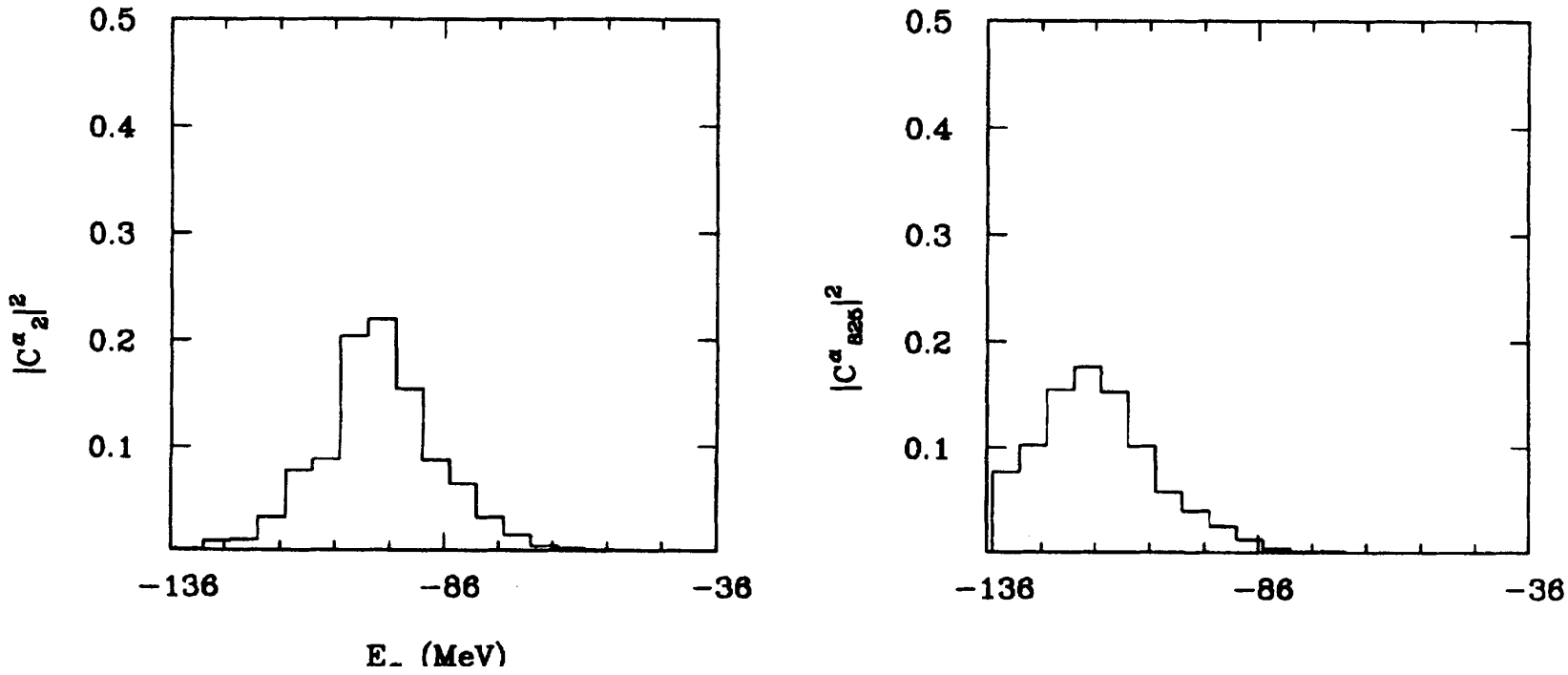
Moments

PHYSICAL REVIEW C VOLUME 50, NUMBER 5 NOVEMBER 1994

Truncation method for shell model calculations

M. Horoi,[1,2] B. A. Brown,[1] and V. Zelevinsky[1,3]

^{28}Si



$$\bar{E}_k \equiv \sum_\alpha |C_k^\alpha|^2 E_\alpha = H_{k,k}$$

$$\sigma_k \equiv \sqrt{\sum_\alpha |C_k^\alpha|^2 E_\alpha^2 - \bar{E}_k^2} = \sqrt{\sum_{k' \neq k} H_{k',k}^2}.$$

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NLD and Statistical Spectroscopy

M. Horoi et al. :

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

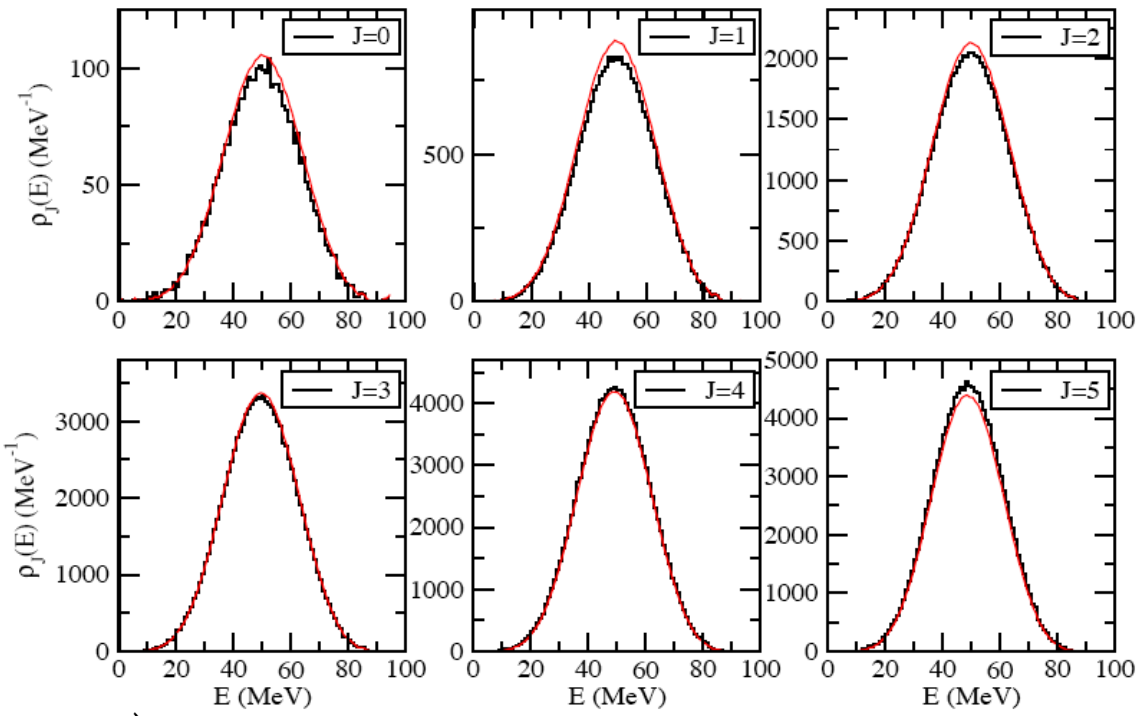
PRC **69**, 041307(R) (2004),

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

PRL **98**, 265503 (2007)

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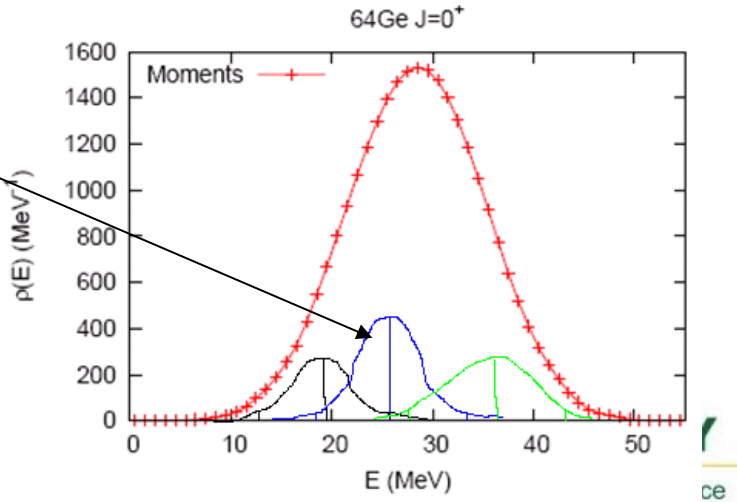
^{28}Si $\pi = +$ staircase: CI, USD



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



$E_{g.s.}$ from CI, ECM (PRL **82**, 2064 (1999)), CC, etc.

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Shell model moments method: pro and con

- ✓ Pro
  - ✓ Spin and parity dependent centroids take into account the s.p. energy shifting due the monopoles (tensor interaction)
  - ✓ Spin and parity dependent widths take into account more realistic spreading, beyond that of pairing
  - ✓ No need to consider rotational/vibrational amplifications
- ✓ Con
  - ✓ Relatively small number of s.p. orbitals in the valence space: natural parity favored (unique)
  - ✓ Reliable Hamiltonians hard to obtain
  - ✓ Energy of the g.s. could be a problem (but there are some solutions)
  - ✓ The configuration distribution could be asymmetric (some solutions here as well)

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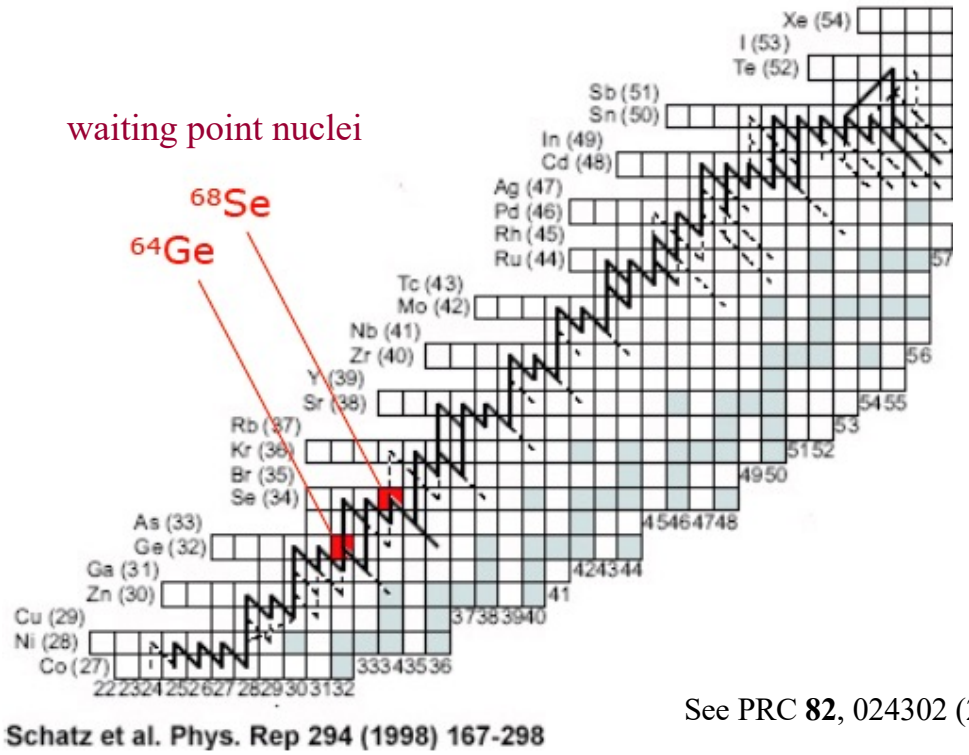
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JMOMENTS Proton-Neutron Code for NLD

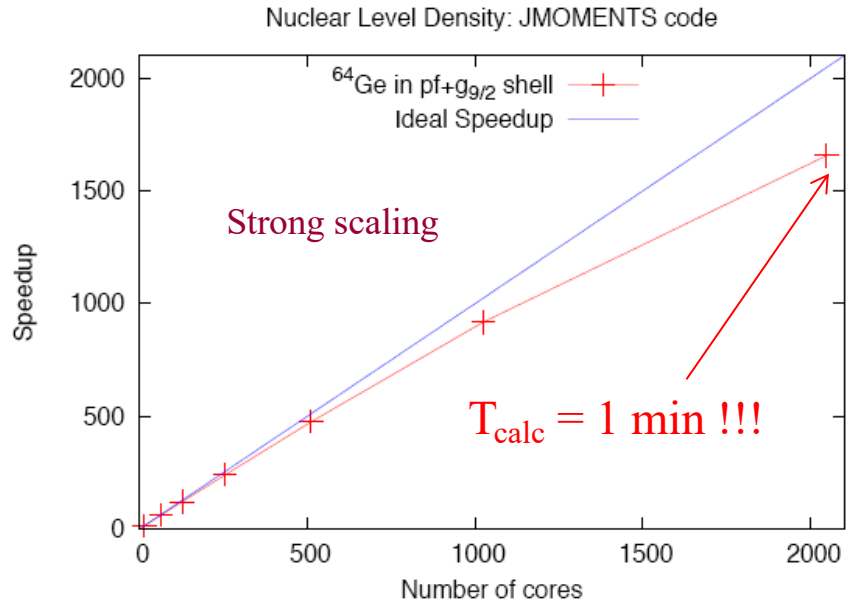
Domain decomposition: many-body configurations

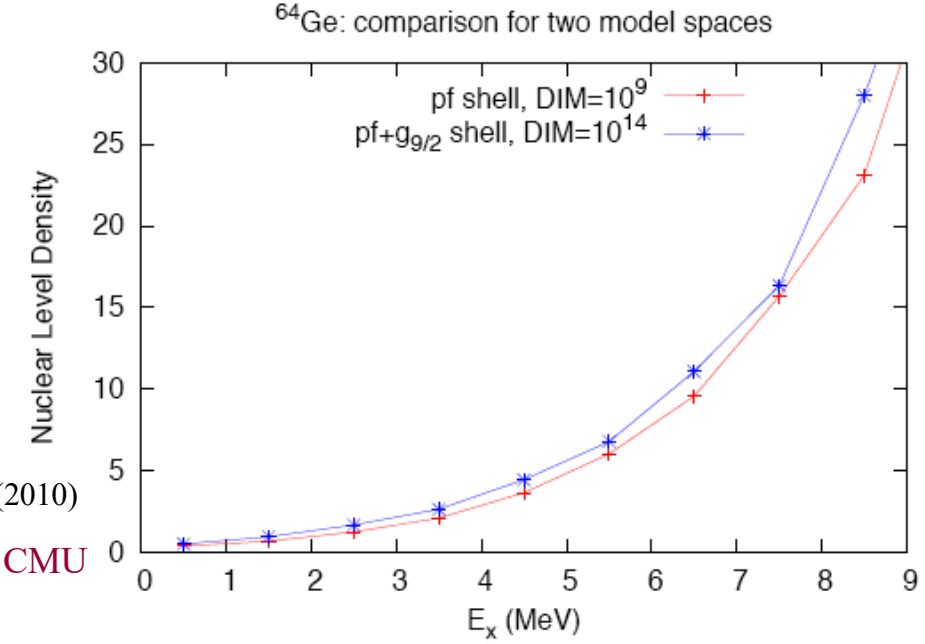
Algorithm: Dynamical Load Balancing

Where: NERSC



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

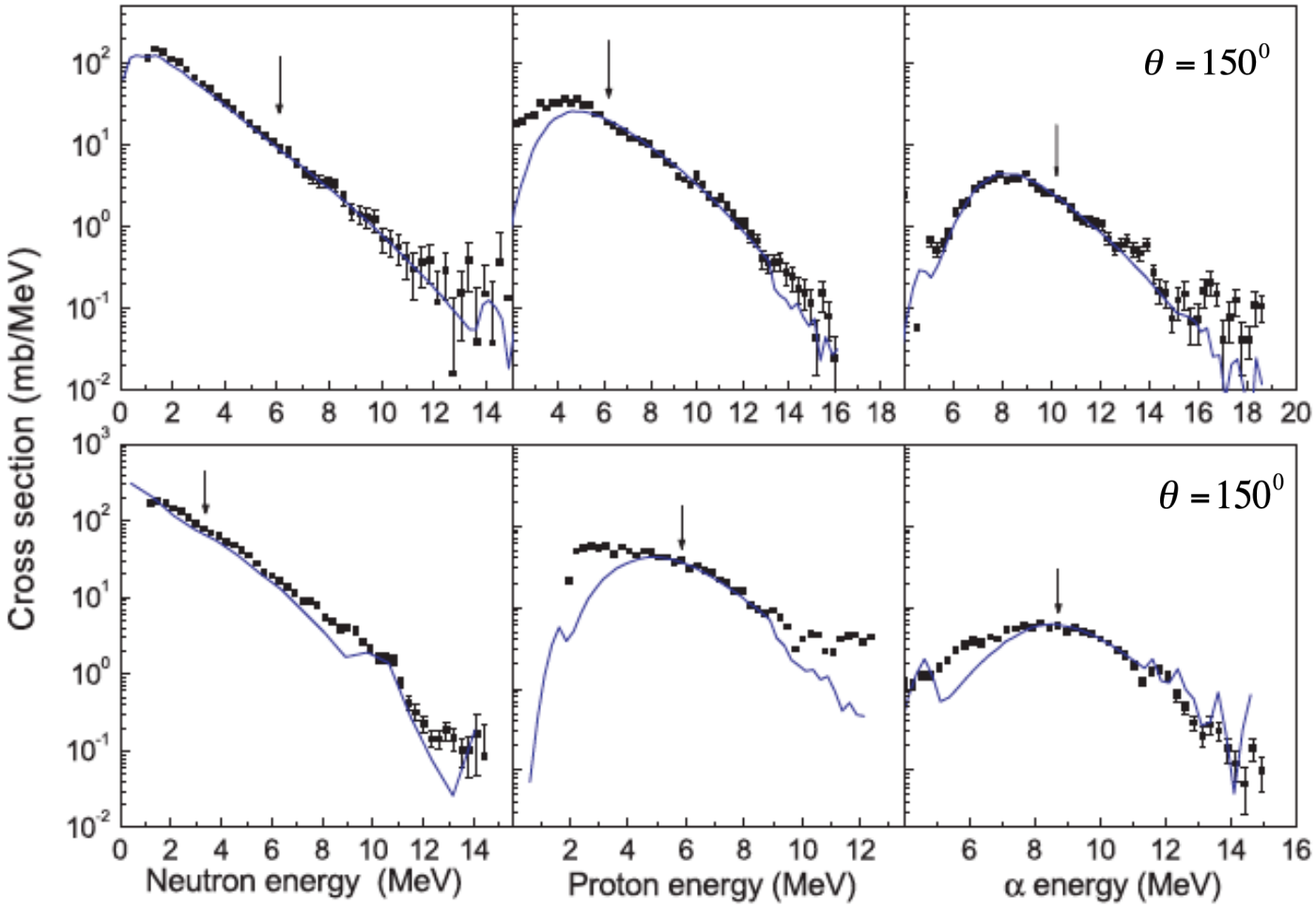




See PRC **82**, 024302 (2010)

NLD and Hauser-Feshbach Cross-Sections

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



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

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

$^{61}Ni^{*}\ compund$

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

$E_{d} = 7.5\,MeV$

Comparison with Moments Densities

talys : www.talys.eu

NLD-M1

ldmodel 1: Constant temperature + Fermi gas model

ldmodel 2: Back-shifted Fermi gas model

ldmodel 3: Generalised superfluid model

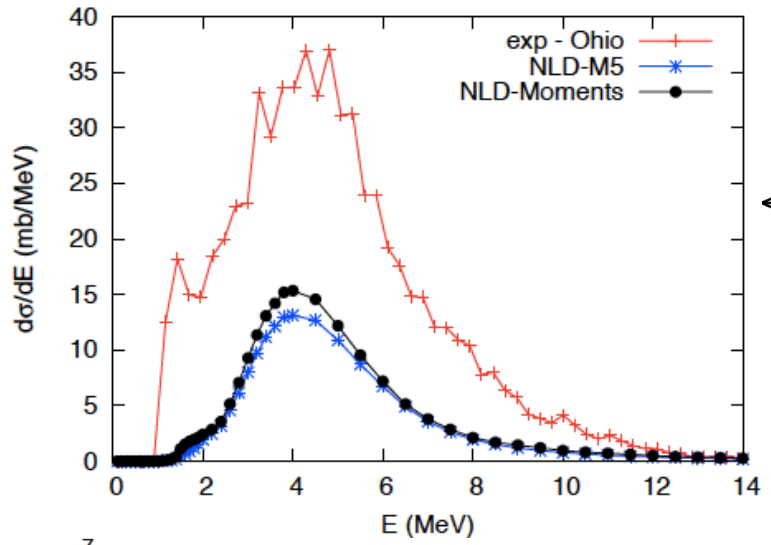
ldmodel 4: Microscopic level densities from Goriely's table

ldmodel 5: Microscopic level densities from Hilaire's table

NLD-M5

Interface:

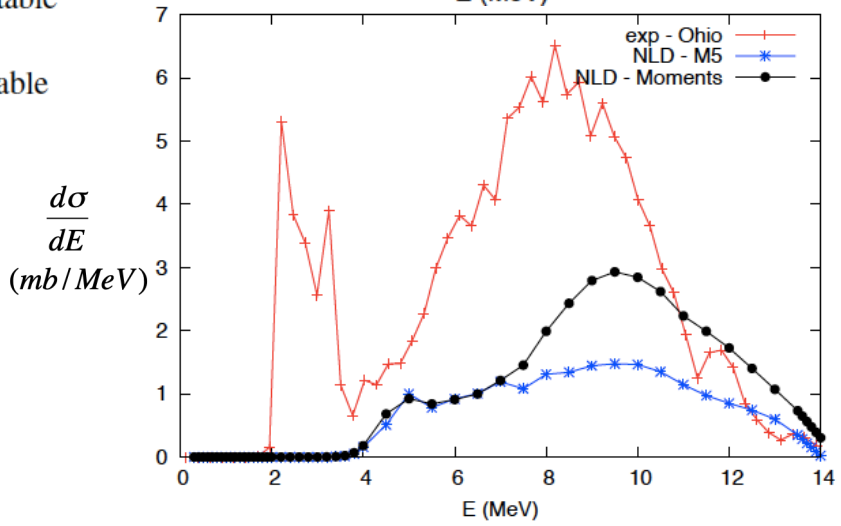
Moments table -> Hilaire's table



$\leftarrow {}^{58}Fe\left({}^{3}He, p\right){}^{60}Co$

$\theta = 150^{0}$

$E_{{}^{3}He} = 10.0\ MeV$



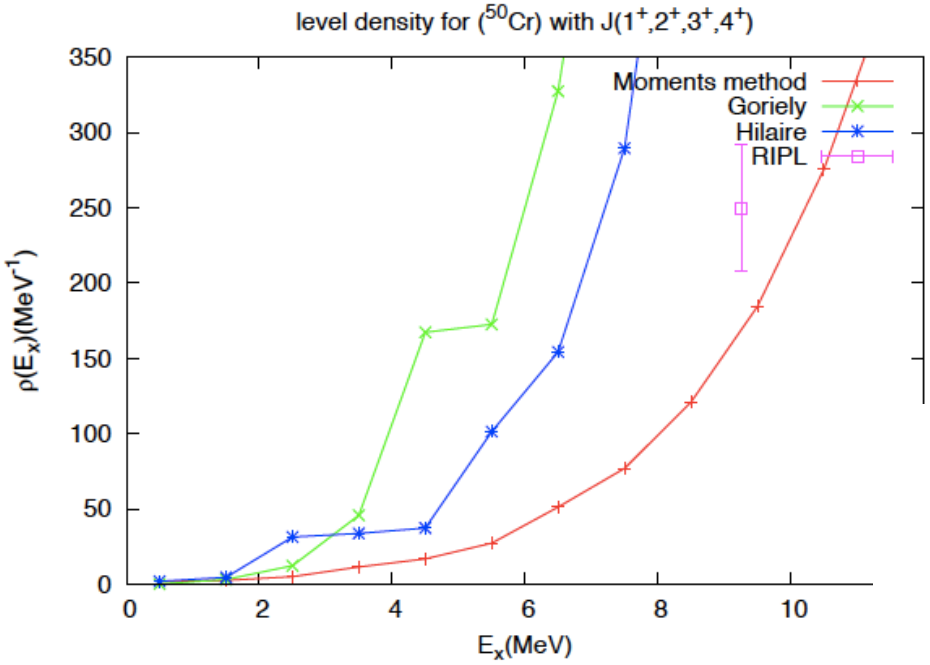
$\leftarrow {}^{59}Co\left(d, \alpha\right){}^{57}Fe$

$\theta = 150^{0}$

$E_{d} = 7.5\ MeV$

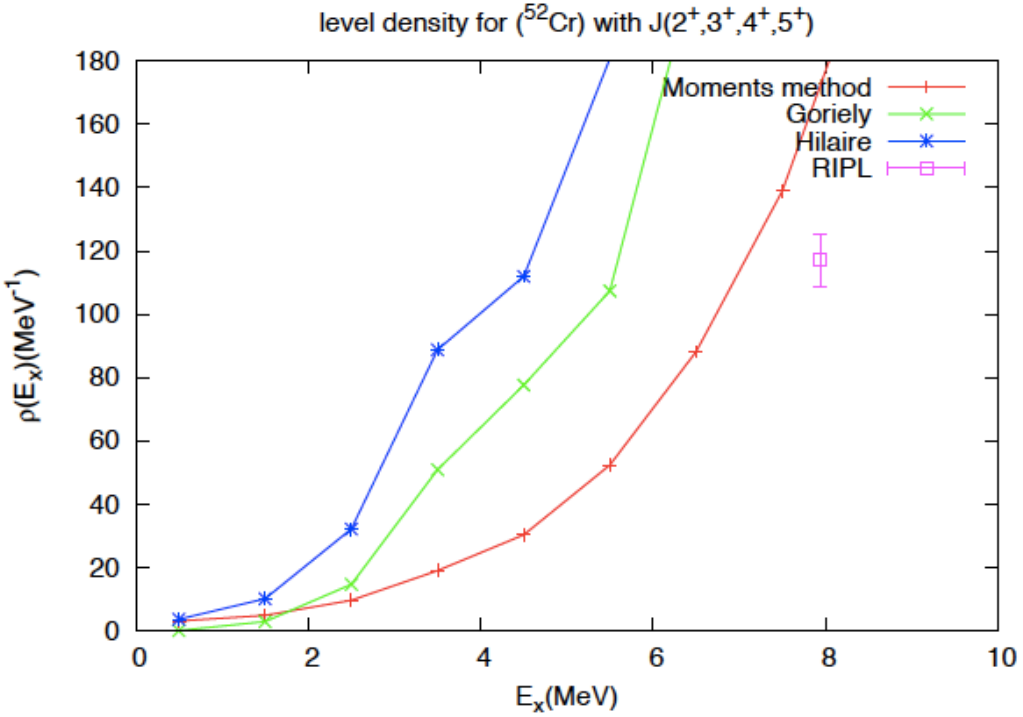
Exp – Ohio: A. Voinov et al., PRC **76**, 044602 (2007)

Comparison with RIPL-3 p-waves neutron resonances data



$^{49}Cr(5/2^-) + n(l=1, s=1/2) \rightarrow ^{50} Cr(J^\pi = 1^+, 2^+, 3^+, 4^+)$

$^{51}Cr(7/2^-) + n(l=1, s=1/2) \rightarrow ^{52} Cr(J^\pi = 2^+, 3^+, 4^+, 5^+)$



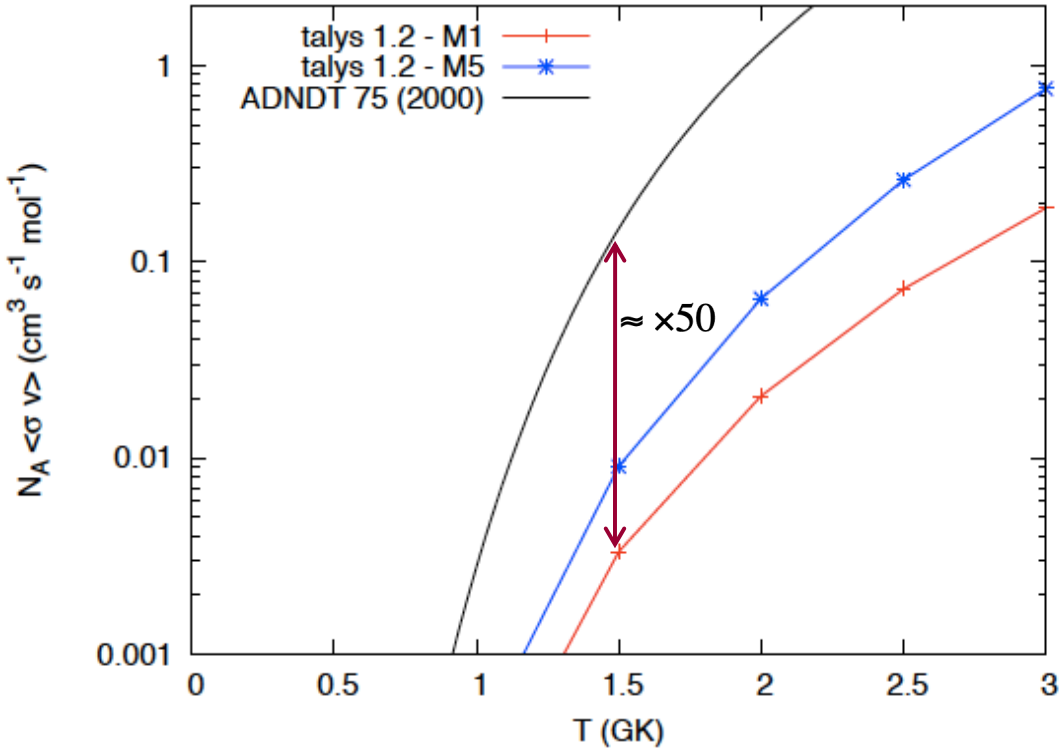
NLD: reaction rates

talys 1.2 : www.talys.eu

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

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

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



$^{64}Ge(p,\gamma)$

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

R.Senkov, M.Horoi and V.Zelevinsky,Phys.Lett B 702,413 (2011)

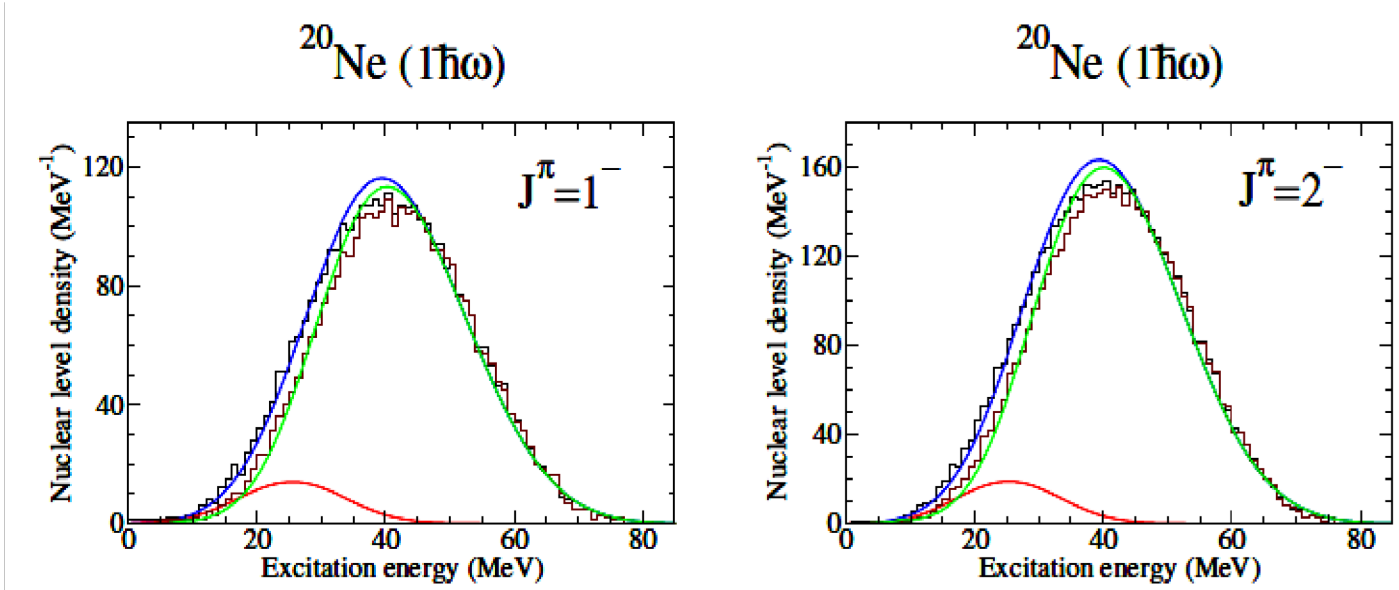
Removal of CoM Spurious States

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

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

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

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



—, — are shell model calculations with $\beta = 0$ and $\beta = 4$,

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

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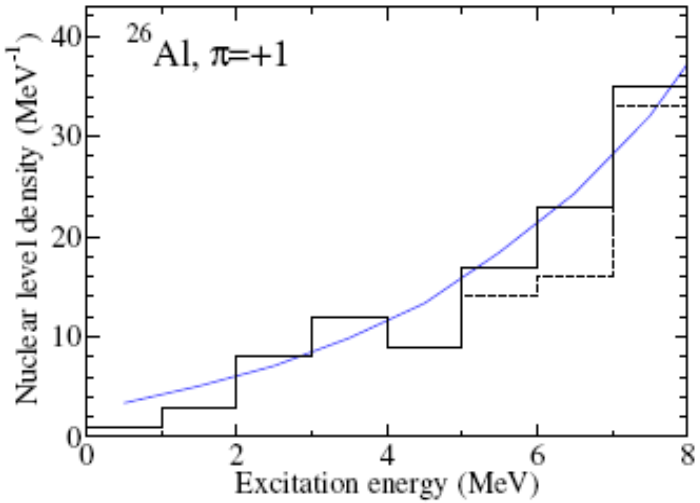
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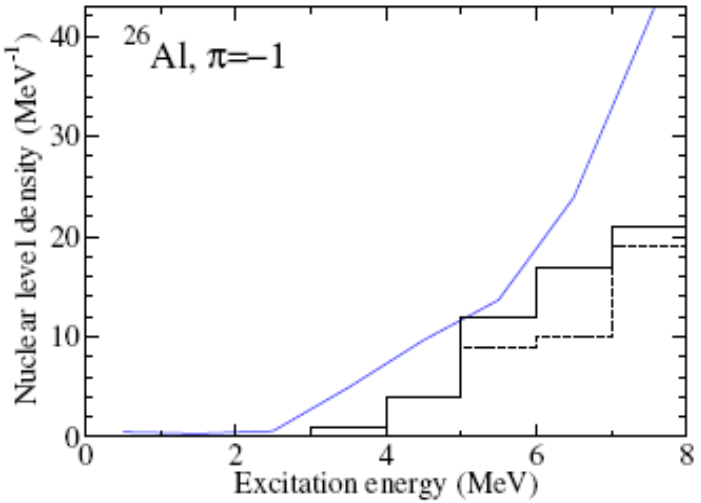
Experiment Vs Moments method

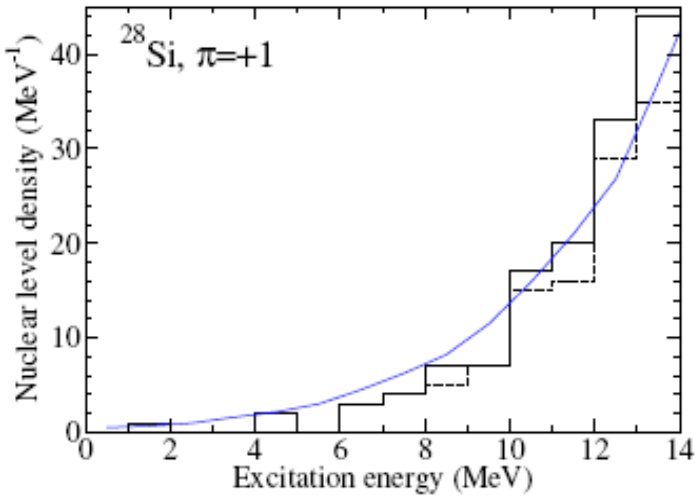
Nuclear level density for ^{26}Al & ^{28}Si with both parities for all J

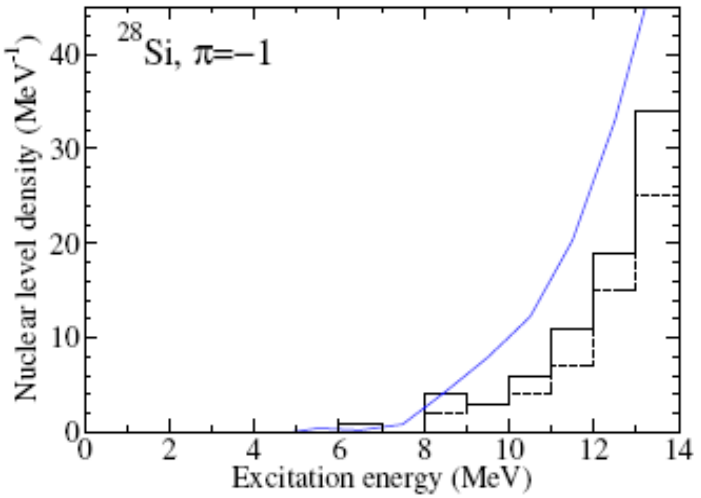
Model Space-(*s-p-sd-pf*)

Interaction-*WBT*







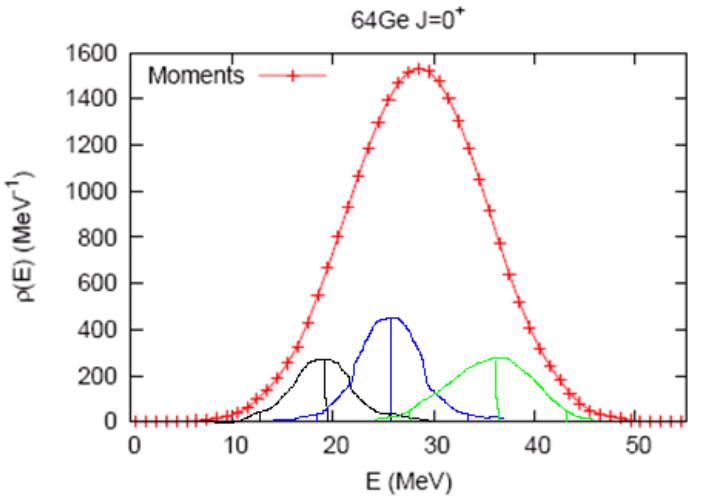


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Problems with SM NLD:

- Hard to define "enough complexity": how many valence nucleons in a valence space can provide a "sufficient" number of low-lying levels.
- Domain of reliability: until what excitation energy the number of missing states is small/negligible?
- Moment's method has a cutoff parameter that can change the low-energy shape.

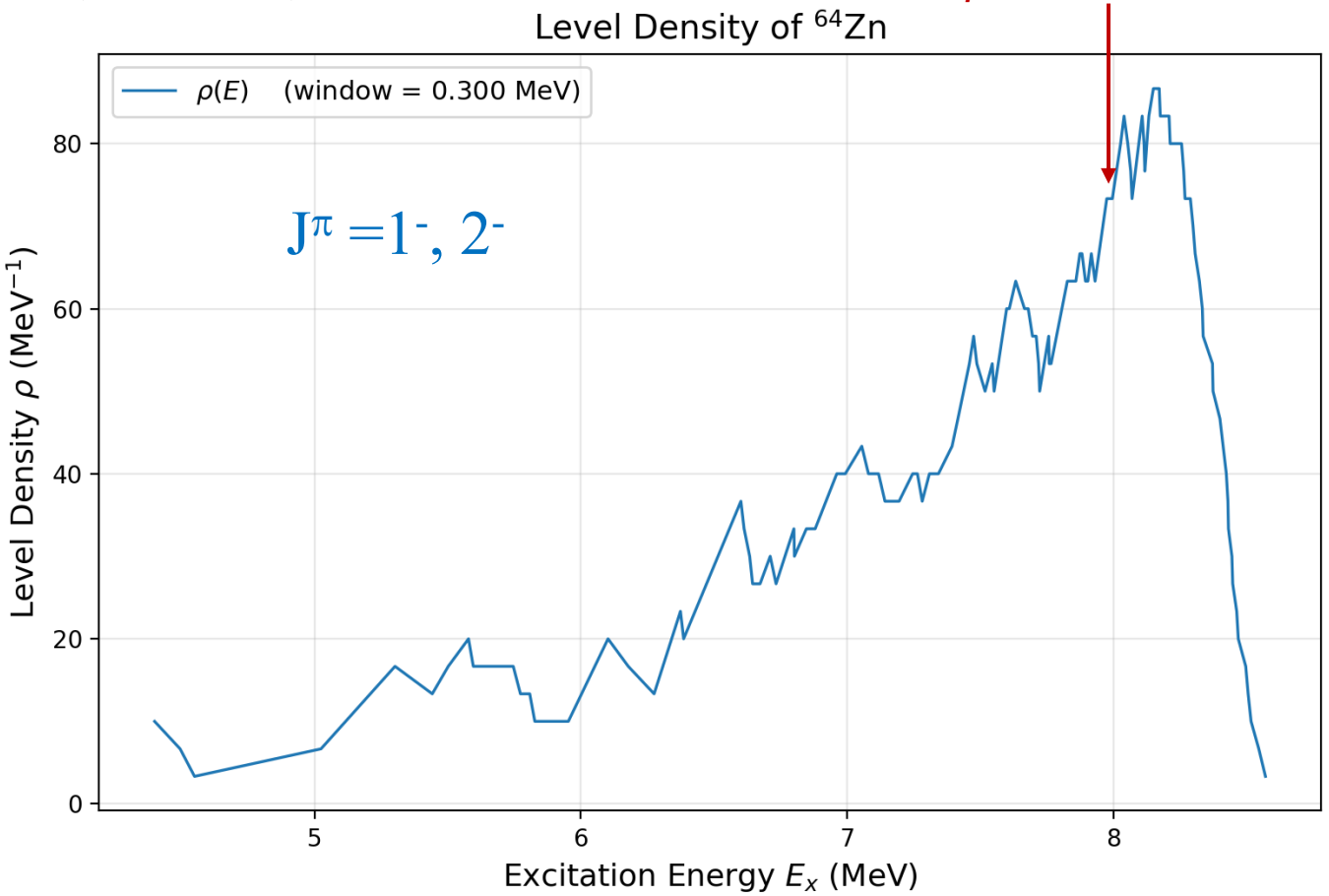


^{64}Zn: 8 nucleons in jj44

Neutron resonances: s-wave, RIPL3

$\rho = 435 \pm 50\ MeV^{-1}$

^{63}Zn($J^{\pi} = 1.5^{-}$)

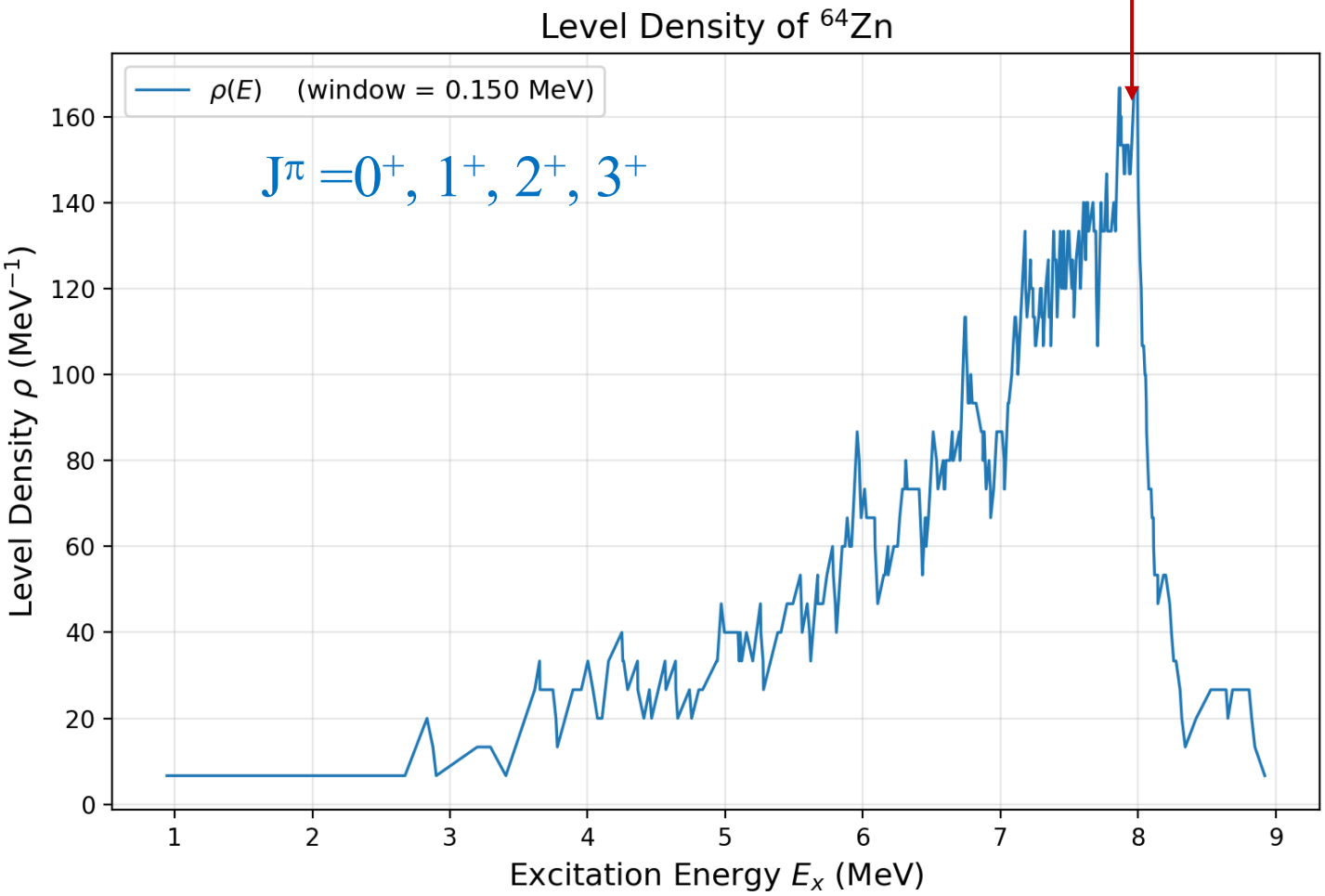


^{64}Zn: 8 nucleons in jj44

^{63}Zn($J^\pi = 1.5^-$)

Neutron resonances: p-wave, RIPL3

$\rho = 909 \pm 84\ MeV^{-1}$



$\rho(7.9\ MeV) \approx 150\ MeV^{-1}$

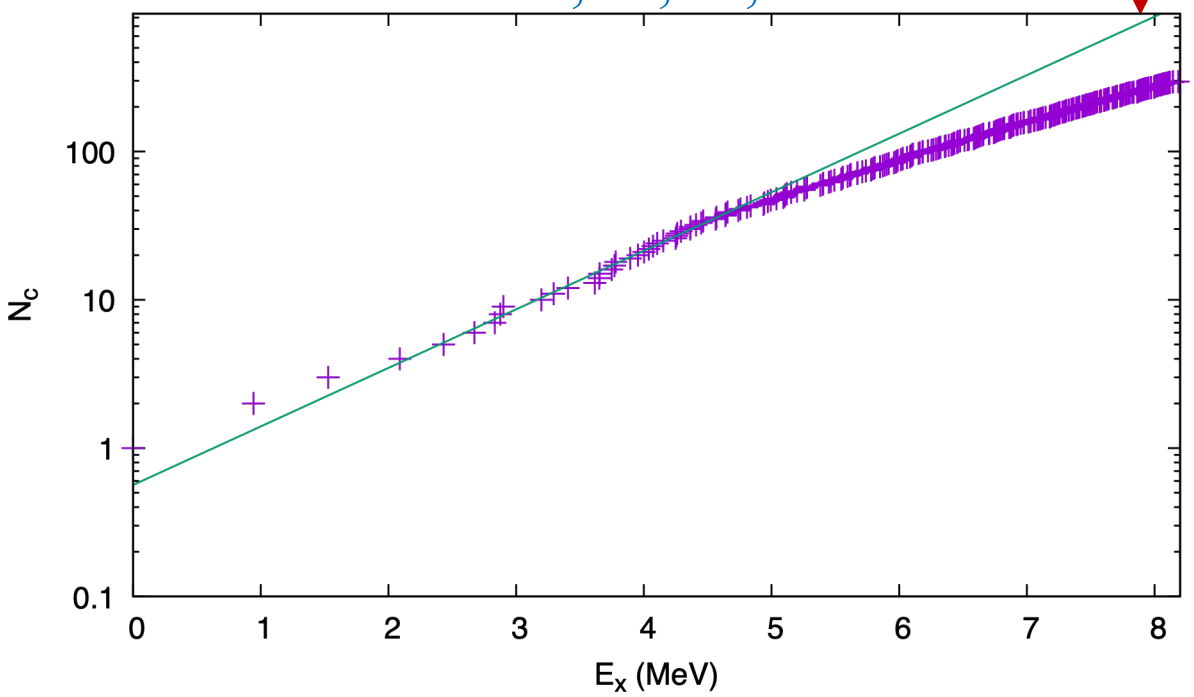
^{64}Zn: 8 nucleons in jj44

Neutron resonances: p-wave, RIPL3

$\rho = 909 \pm 84\ MeV^{-1}$

^{63}Zn($J^\pi = 1.5^-$)

$J^\pi = 0^+, 1^+, 2^+, 3^+$



$$N_c(E_x) = \exp(\frac{E_x - E_0}{T})$$

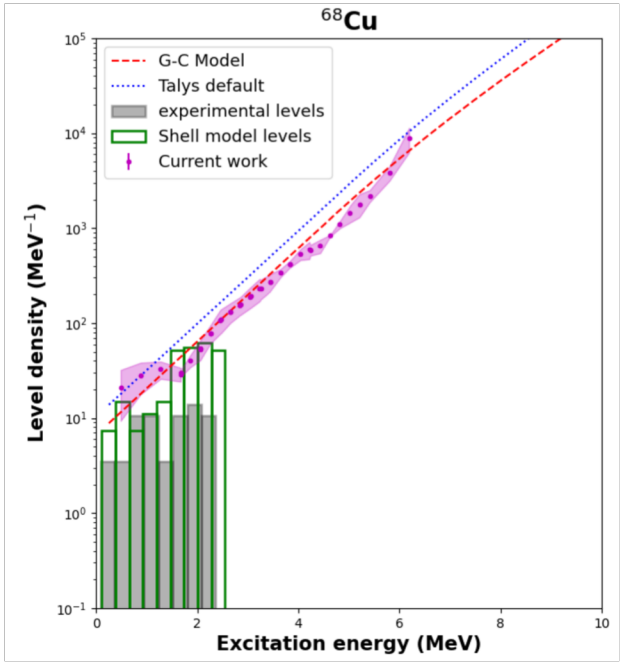
$$\rho(E_x) = \frac{1}{\mathrm{T}} \exp(\frac{E_x - E_0}{T})$$

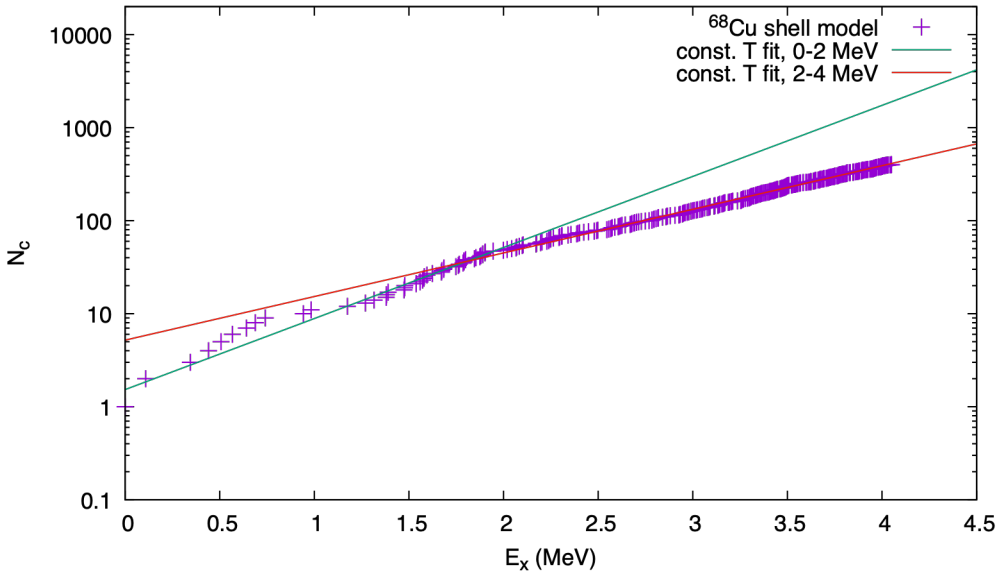
$$N_c(E_x) = \exp(\frac{E_x - 0.63}{1.1})$$

$$\rho(7.98\ MeV) = 740\ MeV^{-1}$$

Extension of low-energy NLD

$^{68}Zn(n,p)^{68}Cu$





Low energy: constant temperature $N_c(E_x) = e^{(E_x - E_{0g})/T_g}$

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Fix for TALYS: LECTND

Constant temperature (low energy) + Fermi gas

$$\rho_T^{\rm tot}(E_x) = \frac{dN(E_x)}{dE_x} = \frac{1}{T}\exp(\frac{E_x - E_0}{T})$$

$$\rho_F(E_x, J, \Pi) = \frac{1}{2}\frac{2J+1}{2\sqrt{2\pi}\sigma^3}\exp\left[-\frac{(J+\frac{1}{2})^2}{2\sigma^2}\right]\frac{\sqrt{\pi}}{12}\frac{\exp\left[2\sqrt{aU}\right]}{a^{1/4}U^{5/4}}$$

$$U = E_x - \Delta^{\rm CTM} \qquad \Delta^{CTM} = \chi\frac{12}{\sqrt{A}}$$

$$\sigma^2 = \left(0.83A^{0.26}\right)^2$$

a from neutron resonances

Constraints to find E_M, E_0, T:

1. $\rho_T^{\rm tot}(E_M) = \rho_F^{\rm tot}(E_M)$

2. $\frac{d\rho_T^{\rm tot}}{dE_x}(E_M) = \frac{d\rho_F^{\rm tot}}{dE_x}(E_M)$

3. Use low energy levels: $N_U = N_L + \int_{E_L}^{E_U} dE_x \rho^{\rm tot}(E_x)$

$$N_U = N_L + \left(\exp[\frac{E_U}{T}] - \exp[\frac{E_L}{T}]\right)\exp[\frac{-E_0}{T}]$$

Use shell model low energy levels for range consistent with CT.

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Projected Shell Model (PSM) NLD

PHYSICAL REVIEW C **111**, 034324 (2025) ^{163}Dy

$$\hat{H} = \hat{H}_0 - \frac{1}{2}\chi_{QQ}\sum_{\mu}\hat{Q}^{\dagger}_{2\mu}\hat{Q}_{2\mu} - G_M\hat{P}^{\dagger}\hat{P} - G_Q\sum_{\mu}\hat{P}^{\dagger}_{2\mu}\hat{P}_{2\mu}$$

$$\{a^{\dagger}_{\nu_i}|\phi\rangle, a^{\dagger}_{\nu_i}a^{\dagger}_{\nu_j}a^{\dagger}_{\nu_k}|\phi\rangle, a^{\dagger}_{\nu_i}a^{\dagger}_{\pi_j}a^{\dagger}_{\pi_k}|\phi\rangle, a^{\dagger}_{\nu_i}a^{\dagger}_{\nu_j}a^{\dagger}_{\nu_k}a^{\dagger}_{\pi_l}a^{\dagger}_{\pi_m}|\phi\rangle, \dots\}$$

for even-odd nuclei,

$$\{a^{\dagger}_{\pi_i}|\phi\rangle, a^{\dagger}_{\pi_i}a^{\dagger}_{\pi_j}a^{\dagger}_{\pi_k}|\phi\rangle, a^{\dagger}_{\nu_i}a^{\dagger}_{\nu_j}a^{\dagger}_{\pi_k}|\phi\rangle, a^{\dagger}_{\nu_i}a^{\dagger}_{\nu_j}a^{\dagger}_{\pi_k}a^{\dagger}_{\pi_l}a^{\dagger}_{\pi_m}|\phi\rangle, \dots\}$$

for odd-even nuclei.

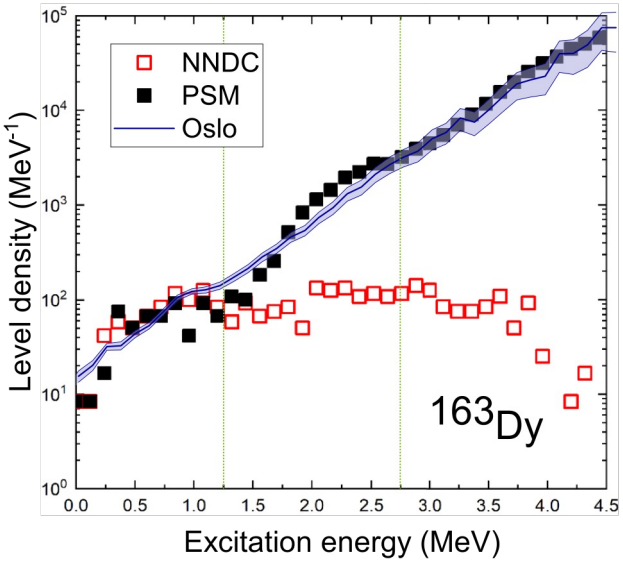
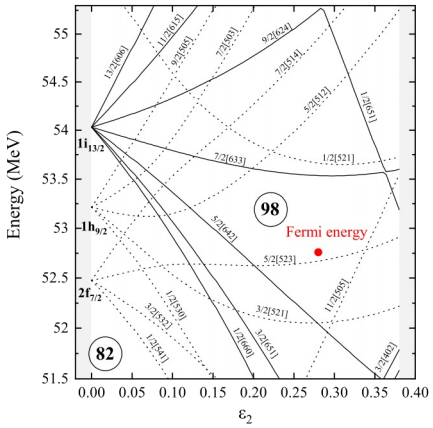


FIG. 5. Level densities (filled squares) in the excitation energy

PHYSICAL REVIEW C **108**, 034309 (2023) ^{164}Dy



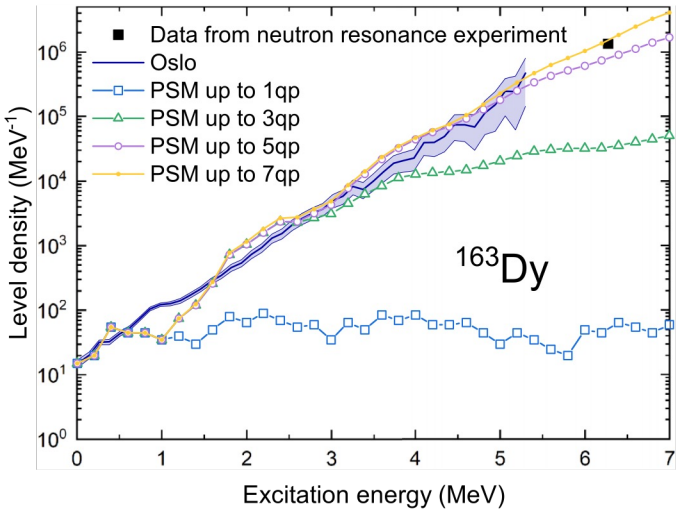


FIG. 6. Unmixed NLDs (see text for definition) in the excitation

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Summary and Outlook

- ✓ Shell model techniques **describe** and **predict** a large amount of data in light, medium, and heavy nuclei:
  - ✓ Energies and quantum numbers
  - ✓ Electromagnetic transition probabilities
  - ✓ Spectroscopic amplitudes
  - ✓ Spin and parity dependent nuclear level densities
  - ✓ Beta decay, charge exchange, 2ν/0ν double-beta decay
- ✓ These observables are essential, but:
  - ✓ There is a clear need to obtain accurate effective Hamiltonians for enlarged, but tractable valence spaces.
  - ✓ There is need to obtain accurate effective operators in tractable valence spaces
  - ✓ Skewness and excess of the moments may be needed: they became affordable
  - ✓ Effective truncation scheme for configurations (partitions)
- ✓ Practical use for nuclear reactions in TALYS: Use shell model low energy levels for the energy range consistent with constant temperature NLD

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