Impact of Nuclear Level Densities and Gamma-ray Strength Functions on Astrophysical Reaction Rates for Neutron Capture Processes

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Outline

1. Astrophysical reaction rates with realistic nuclear level densities
   - Introductions
   - Employed models and results
   - Summary

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Introduction

- Radiative neutron capture processes are crucial for complete understanding of nuclear astrophysical network calculations like, r-process, s-process.
- All such data are not accessible in the accelerator-based experiments, and one needs to rely on theoretical estimates.
- Within a statistical framework, the radiative neutron capture cross-sections and relevant reaction rates calculations require- (i) neutron-nucleus optical model potential (OMP), (ii) γ-ray strength function (γSF), and (iii) nuclear level density (NLD).
- we have used realistic NLDs obtained from the spectral distribution method followed by an appropriate parity equilibration scheme for *pf*-model space to calculate the neutron capture reaction cross sections and astrophysical reaction rates.

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- Various methods have been employed: From simple phenomenological models based on non-interacting degenerate Fermi gas to more complex mean-field descriptions.

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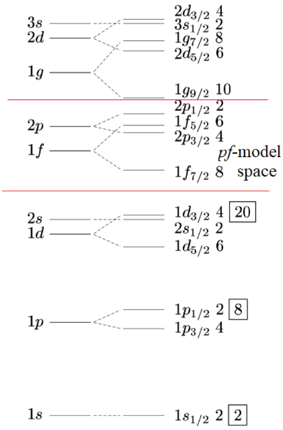
- Problems:Interaction is not properly considered, fitting to the experimental data is required for collective excitations.
- In a shell-model approach Hamiltonian may be constructed starting from a realistic NN potential. This naturally accounts for the collective excitations which gives more complete description of sevaral nuclear properties.

Shell model approach

- Total Hamiltonian,
  $\hat{H} = \hat{T} + \hat{V}$, where $\hat{T} = \sum_i \hat{t}_i$; $\hat{V} = \sum_{i<j} \hat{V}_{ij}$
  $\hat{H} = (\hat{T} + \hat{U}) + (\hat{V} - \hat{U}) = \hat{H}_0 + V_{res}$
- In the shell model, the configuration mixing through the residual interaction naturally accounts for the collective excitations.
- Problem: Huge dimension matrix needs to be diagonalized.
- There are few different approaches to calculate the NLDs within the framework of shell model. One of them is based on the spectral distribution method (SDM) for many-body shell model Hamiltonian in full configuration space, which avoids the diagonalization of huge dimensional matrices.



Outline

Spectral distribution method (SDM)

- For a given isotope (Z, N), the valence nucleons can be distributed in many ways over available orbitals. Each of these configurations is known as partition, p which contains $D_{\alpha p}$ many-body states with exact quantum numbers α. For each partition, the statistical average of an operator $\hat{O}$,

$$\langle \hat{O} \rangle = \frac{1}{D_{\alpha p}} Tr^{\alpha p} \hat{O} \tag{1}$$

- First moment of the Hamiltonian,

$$E_{\alpha p} = \frac{1}{D_{\alpha p}} Tr^{\alpha p} \hat{H} \tag{2}$$

- The second moment of the Hamiltonian,

$$\sigma^2_{\alpha p} = \langle H^2 \rangle_{\alpha p} - E^2_{\alpha p} = \frac{1}{D_{\alpha p}} Tr^{\alpha p} H^2 - E^2_{\alpha p} \tag{3}$$

Spectral distribution method (SDM)

- The actual distributions are close to the Gaussians. Finally, the level density $\rho(E;\alpha)$ is found by summing the Gaussians weighted over their dimensions for all partitions at given energy E and with quantum numbers α,

$$\rho(E;\alpha) = \sum_{p} D_{\alpha p} G_{\alpha p}(E) \tag{4}$$

where,

$$G_{\alpha p}(E) = G(E - E_{\alpha p} + E_{\mathrm{g.s.}}; \sigma_{\alpha p}) \tag{5}$$

- The ground state energies $E_{\mathrm{g.s.}}$ appearing in Eq. (5) must be calculated using full Hamiltonian matrix in order to be consistent with the first and second moments.

Ground state energy ($E_{\mathrm{g.s.}}$) calculation

- The calculation of $E_{\mathrm{g.s.}}$ turns out to be difficult in few cases due to large dimension corresponding to full model space (N_{full}) of the Hamiltonian matrix.
- In such cases, ($N_{full} \geq 5 \times 10^6$) we have used exponential convergence method. The ground state energies obtained for several restricted model spaces are fitted to the exponential function of the form $a + be^{-cN}$.

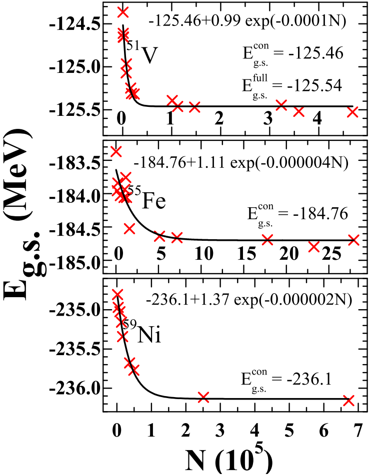


Figure: Phys. Rev. C 105, 044320 (2022)

Cross-sections for (n, γ) processes using *pf* model space

- we have calculated the reaction cross-sections for $^{50}V(n,\gamma)^{51}V$, $^{54}Fe(n,\gamma)^{55}Fe$, and $^{58}Ni(n,\gamma)^{59}Ni$ processes.

	$^{50}V(n,\gamma)^{51}V$			$^{54}Fe(n,\gamma)^{55}Fe$			$^{58}Ni(n,\gamma)^{59}Ni$		
Channels	Nucleus	N_{full}	$E_{g.s.}$	Nucleus	N_{full}	$E_{g.s.}$	Nucleus	N_{full}	$E_{g.s.}$
(n,γ)	^{51}V	1242538	-125.54	^{55}Fe	25743302	-184.76	^{59}Ni	76528736	-236.37
(n,n)	^{50}V	795219	-114.79	^{54}Fe	5220621	-175.73	^{58}Ni	21977271	-227.59
(n,p)	^{50}Ti	39899	-109.86	^{54}Mn	17069465	-167.40	^{58}Co	37534140	-218.90
$(n,2n)$	^{49}V	422870	-105.63	^{53}Fe	21131892	-162.56	^{57}Ni	76528736	-215.55
(n,np)	^{49}Ti	150632	-99.24	^{53}Mn	14123745	-158.51	^{57}Co	90369789	-210.34
$(n,2p)$	^{49}Sc	28603	-90.41	^{53}Cr	3776746	-151.70	^{57}Fe	13436903	-203.30

- The *pf*-model space can yield the NLDs only for a single parity for a given nucleus. In even-A nuclei, it will correspond to only positive parity states and those for odd-A nuclei to the negative parity states.

s-wave neutron resonance spacings

- The cross-sections and reaction rates, relevant to the astrophysical process are predominantly governed by the NLDs corresponding to spin and parity which determines the level spacings D_0 for s-wave neutron resonance.

$$D_0 = \begin{cases} \frac{1}{\rho(S_n, J_t+1/2, \pi_t) + \rho(S_n, J_t-1/2, \pi_t)} & \text{for} \quad J_t \neq 0, \\ \frac{1}{\rho(S_n, 1/2, \pi_t)} & \text{for} \quad J_t = 0 \end{cases} \tag{6}$$

Nucleus	$J_t^{\pi_t}$	S_n (MeV)	D_0 (keV) Exp.	HFB-u	HFB	BSFG	GSM	SDM	SDM*
^{49}Ti	0^+	8.142	18.3 ± 2.9	24.6	18.6	19.1	15.2	174.4	104.9
^{50}Ti	$\frac{7}{2}^-$	10.939	4 ± 0.8	1.1	4	4.1	5.2	19.6	10.8
^{51}V	6^+	11.051	2.3 ± 0.6	0.9	1.5	2.8	4.8	6.2	3.5
^{53}Cr	0^+	7.939	43.4 ± 4.4	30.1	47.7	43	79	66.2	38.4
^{55}Fe	0^+	9.298	18 ± 2.4	5.5	15.9	16.3	104	31.7	18.4
^{57}Fe	0^+	7.646	25.4 ± 2.2	22	26.4	24.5	54.2	34.8	21.2
^{59}Ni	0^+	8.999	13.4 ± 0.9	6.1	12.8	14.1	95.7	23.8	13.9

Nuclear level densities (NLDs)

- Nuclear level densities as a function of excitation energies (E_x) for ^{51}V, ^{55}Fe and ^{59}Ni nuclei obtained from SDM in *pf*-model space by considering parity equilibration scheme at $E_0 = S_n$ and $0.8 S_n$ labelled as SDM and SDM*, respectively.

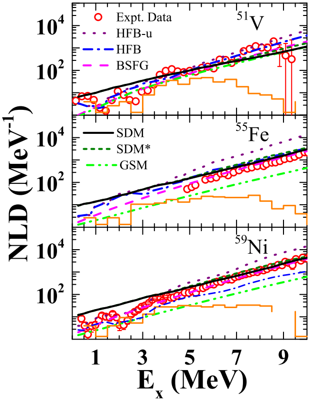


Figure: Nuclear level densities as a function of excitation energies (E_x). [Phys. Rev. C 105, 044320 (2022)]

Cross-sections for (n, γ) processes

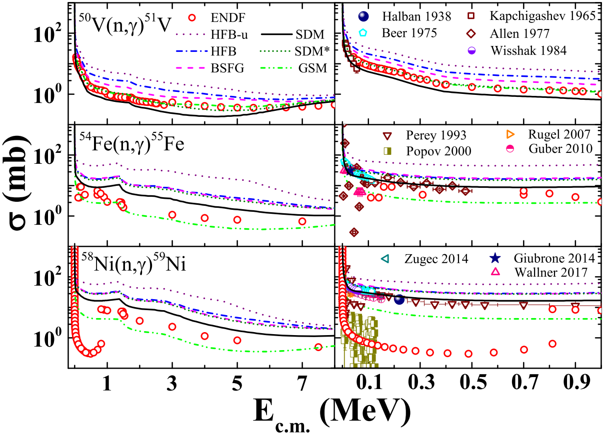
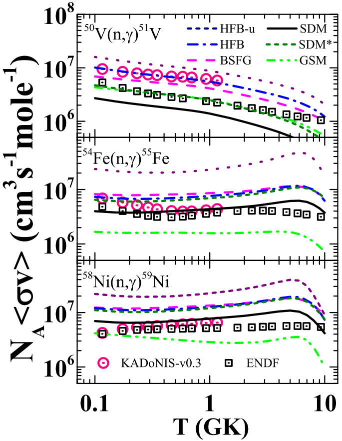


Figure: Cross-sections for (n, γ) processes as a function of incident neutron energies in center-of-mass frame ($E_{\text{c.m.}}$) calculated using NLDs from SDM and SDM* compared with those obtained from other models and experimental data [Phys. Rev. C 105, 044320 (2022)]

The astrophysical reaction rates

- The astrophysical reaction rates as a function of temperature using NLDs from SDM and SDM* compared with those obtained for other models. For comparison, the recommended values from ENDF and 'KADoNiS v0.3' are shown. [Phys. Rev. C 105, 044320 (2022)]



Calculations for *sd*-nuclei using full *sd*-*pf* model space

- Calculations for NLDs and D_0 for ^{24}Na, ^{25,26,27}Mg using SDM in *sd*-*pf* model space has been performed.
- The shell model ground state energies E_{gs} obtained for (0,2)$\hbar\omega$ and (0,4)$\hbar\omega$ excitations to *pf*-shell.

Nucleus	J^π	E_{gs} (MeV)		
		(0,2)	(0,4)	full
^{24}Na	4^+	-82.24	-82.61	-82.61
^{25}Mg	$5/2^+$	-100.94	-101.97	-102.01
^{26}Mg	0^+	-112.76	-114.02	-
^{27}Mg	$1/2^+$	-118.59	-119.61	-

NLDs for ^{24}Na, ^{25,26,27}Mg

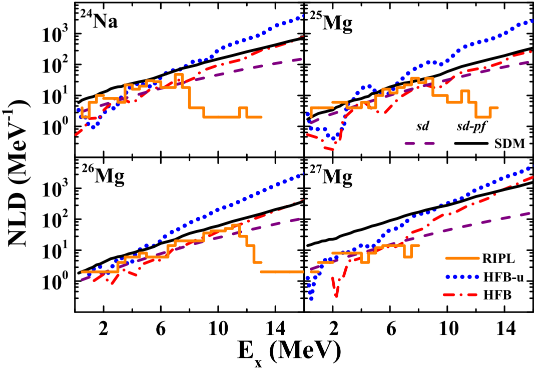


Figure: Excitation energy (E_x) dependence of NLDs for ^{24}Na and ^{25,26,27}Mg obtained by employing SDM within *sd-pf* model space. For comparison, we also show SDM results using *sd* model space [?] along with those for the mean-field models, HFB-u (un-normalized) and HFB (normalized) [?]. Histograms represent the NLDs obtained from low-lying discrete levels [?].

D_0 for ^{24}Na, ^{25,26,27}Mg

Table: The s-wave neutron resonances spacing (D_0) obtained from the NLDs for *sd* [**?**] and *sd-pf* model spaces using SDM. The experimental data [**?**] and those obtained for mean-field models [**?**] are also presented for the comparison.

Nucleus	$J_t^{\pi_t}$	S_n (MeV)	D_0 (keV) Expt.	HFB-u	HFB	SD	SDPF
^{24}Na	$\frac{3}{2}^+$	6.96	100 ± 20	54.0	122.3	149.7	86.6
^{25}Mg	0^+	7.33	480 ± 70	99.6	379.5	696.4	486.2
^{26}Mg	$\frac{5}{2}^+$	11.09	50 ± 10	8.7	46.1	78.9	53.0
^{27}Mg	0^+	6.45	210 ± 80	136.4	319.8	578.4	237.9

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- The average occupancy of *pf*-shell does not reach beyond 5% of the valence nucleons for the nuclei considered. Such small average occupancies of *pf*-shell strikingly reduces the D_0 by $50 - 100\%$ emphasizing the importance of cross-shell excitations.
- T. Ghosh et al., Indispensability of cross-shell contributions in neutron resonance spacing, J. Phys. G. 51, 045105 (2024)

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Summary

- We obtained realistic nuclear level densities (NLDs) using the spectral distribution method within the framework of the many-body shell model Hamiltonian for the *pf* model space. By applying an appropriate parity equilibration scheme, these NLDs were then used to calculate D_0 and astrophysical reaction rates.
- Additionally, realistic shell-model NLDs of both parities were naturally obtained for a few *sd*-shell nuclei. These NLDs were employed to calculate D_0 and compared with experimental data.
- We also obtained temperature-dependent gamma strength functions using relativistic energy density functional theory and are currently studying various astrophysical reactions. The results are in a preliminary stage and are not shown here.

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