北京大學
PEKING UNIVERSITY

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Nuclear level density from DRHBc theory and combinatorial method

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r-process

- **The origin of elements is one of the most fundamental scientific problems**

  "How were the elements from iron to uranium made?"

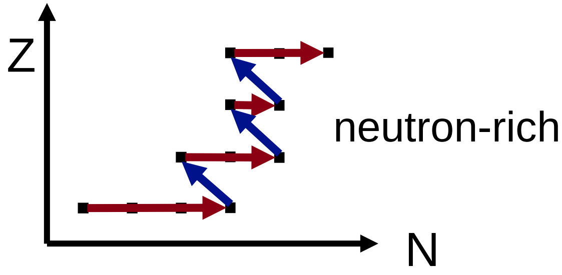
  National Research Council, Connecting Quarks with the Cosmos: Eleven Science Questions for the New Century (2003).

- **The rapid neutron capture process (*r*-process) produces about half of the elements heavier than iron in the universe**

  E. M. Burbidge, G. R. Burbidge, W. A. Fowler, and F. Hoyle, Rev. Mod. Phys. 29, 547 (1957).
  J. J. Cowan, C. Sneden, J. E. Lawler, et al., Rev. Mod. Phys. 93, 015002 (2021).

neutron capture (n,γ) β-decay

$$(Z,N) + Xn \rightarrow (Z,N+X) \rightarrow (Z+1,N+X-1) \rightarrow \cdots$$



- **The astrophysical environments are still ambiguous**

  core-collapse supernovae, neutron star mergers, …

- **Under all possible astrophysical conditions, neutron capture reactions play a crucial role**
  - Hot *r*-process: neutron capture reactions affect abundances during the freeze-out
  - Cold *r*-process: neutron capture reactions affect abundances during the full *r*-process

Neutron capture rate

- **Neutron capture rate is an important nuclear physics input**

  M. R. Mumpower, R. Surman, G. C. McLaughlin, and A. Aprahamian, Prog. Part. Nucl. Phys. 86, 86 (2016).

- **Measurement of neutron capture rates of neutron-rich nuclei is challenging**

  A. C. Larsen, A. Spyrou, S. N. Liddick, and M. Guttormsen, Prog. Part. Nucl. Phys. 107, 69 (2019).

- **The *r*-process studies rely on the theoretical predictions for the required neutron capture rates**

nuclear level density
γ-strength function
optical potential
→ Hauser-Feshbach model → (n,γ) cross section → (n,γ) reaction rate

↑ Maxwell-Boltzmann average, nuclear partition function

Reaction rate libraries for *r*-process

- JINA REACLIB https://groups.nscl.msu.edu/jina/reaclib/db/
- BRUSLIB http://www.astro.ulb.ac.be/bruslib/
- NON-SMOKER https://nucastro.org/nonsmoker.html

Nuclear level density (NLD)

- **The number of nuclear levels per unit energy interval** $\rho(E) = \Delta N/\Delta E$
- **Accurate prediction of NLD is challenging**
  - The exponential growth with increasing excitation energy
  - The complex nuclear structure and dynamics:
    shell structures, pairing correlations, collective motions, …

A. Bohr and B. R. Mottelson, Nuclear Structure, Vol. I (W. A. Benjamin, New York, 1969).

- **Microscopic methods**

Nuclear shell model based

- Shell-model monte carlo approach — Nakada+1997PRL; Alhassid+2007PRL
- Moment method — Sen'kov+2010PRC; Sen'kov+2016PRC
- Stochastic estimation method — Shimizu+2016PLB; Chen+2023PRC
- Extrapolated Lanczos matrix approach — Ormand+2020PRC
- Projected shell model — Wang+2023PRC

Self-consistent mean-field based

- Extended Thomas-Fermi + Skyrme forces + Statistical method — Kolomietz+2018PRC
- Skyrme Hartree-Fock + BCS + Statistical method — Demetriou+2001NPA
- Finite-temperature relativistic Hartree-Bogoliubov + Statistical method — Zhao+2020PRC
- Skyrme Hartree-Fock-Bogoliubov + Combinatorial method — Goriely+2008PRC
- Temperature-dependent Gogny Hartree-Fock-Bogoliubov + Combinatorial method — Hilaire+2012PRC
- Relativistic mean field theory + Combinatorial method — Geng+2023NST
- Relativistic Hartree-Bogoliubov + Combinatorial method — Jiang+2024PLB

Statistical vs Combinatorial

- **Statistical method (Darwin-Fowler method, Partition function method)**
  - An analogy with statistical mechanics
  - Performs an inverse Laplace transform of a partition function constructed from the single-particle levels
  - Quick
  - Introduces statistical approximations

- **Combinatorial method**
  - Exactly count the levels using **combinatorial mathematics**
  - Expand a generating function constructed from the single-particle levels
  - Provides the energy-, spin-, and parity-dependent NLD
  - Describes nonstatistical behaviors of NLD
  - Slow

S. Goko et al., Phys. Rev. Lett. 96, 192501 (2006).

Our work

- **We have developed:**

Combinatorial method based on relativistic Hartree-Bogoliubov (RHB) theory

- ✓ Pairing correlations are considered by Bogoliubov transformation
- ✓ Combinatorial method is used to calculate NLD
- ✓ Strutinsky method is adopted to remove the large fluctuations at low energy
- ✓ Inglis-Belyaev formula is used to calculate moments of inertia

XFJ, X. H. Wu, P. W. Zhao, and J. Meng, Phys. Lett. B 849, 138448 (2024).

Combinatorial method based on DRHBc theory

- ✓ DRHBc theory is adopted to provide nuclear properties
- ✓ Odd-odd and odd-*A* nuclei are included in the combinatorial method
- ✓ Towards a DRHBc database for neutron capture rates in *r*-process

Combinatorial method

- **The combinatorial method calculates NLD based on the nuclear properties predicted by nuclear density functional theory (DFT)**

✓ Incoherent particle-hole excitations
✓ Collective vibration excitations
✓ Collective rotation excitations

} Three kinds of excitations

DFT
↓
Single-particle levels
↓
Incoherent particle-hole state number

Generalized boson partition function
↓
Collective vibration state number

→ Total state number $C(U,K,P)$ → Total state density $\rho(U,K,P)$ → NLD $\rho_{\mathrm{NLD}}(U,J,P)$

Detailed formulism:

S. Hilaire, J. P. Delaroche, and M. Girod, Eur. Phys. J. A 12, 169 (2001).
S. Hilaire and S. Goriely, Nucl. Phys. A 779, 63 (2006).
S. Goriely, S. Hilaire, and A. J. Koning, Phys. Rev. C 78, 064307 (2008).

For deformed nuclei, Inglis-Belyaev moments of inertia are used to build rotational bands

Strutinsky method

The total state density

Total state number C is counted on a series of equally spaced excitation energies

$$U = n\varepsilon_0, \qquad n = 0,1,2,\ldots$$

Total state density ρ at each excitation energy U is given by

$$\rho(U,K,P) = C(U,K,P)/\varepsilon_0$$

It turns out that ρ strongly depends on ε_0, and one cannot obtain a smooth ρ as a function of U even at very small ε_0. A smoothing method is required!

The conventional smoothing method presents poor results at low excitation energy.

S. Hilaire, J. P. Delaroche, and M. Girod, Eur. Phys. J. A 12, 169 (2001).

Strutinsky method

$$\tilde{\rho}(U,K,P) = \frac{1}{\gamma_0}\int_{-\infty}^{+\infty} \rho(U',K,P) f\left(\frac{U'-U}{\gamma_0}\right) dU'$$

$$f(x) = P(x)w(x)$$

$$w(x) = \frac{1}{\sqrt{\pi}} e^{-x^2}$$

$$P(x) = L_{M_0}^{1/2}(x^2) = \sum_n^{M_0} a_{2n} x^{2n}$$

- ✓ Remains unchanged if smoothed again
- ✓ Fulfills the conservation of the state number

P. Ring and P. Schuck., *The nuclear many-body problem*, Springer-Verlag, Berlin Heidelberg (1980).

Numerical details

- **The RHB equation**
  - Relativistic density functional: PC-PK1 — P. W. Zhao et al., Phys. Rev. C 82, 054319 (2010).
  - Pairing strength: G = 728 MeV fm^3 — Y. Tian, Z. Y. Ma, and P. Ring, Phys. Lett. B 676, 44 (2009).
  - Major shells of harmonic oscillator basis: 14
- **Combinatorial method**
  - Cut-off of the excitation energy: 20 MeV
  - Cut-off of the angular momentum: 49 $\hbar$
  - Energy unit: $\varepsilon_0 = 0.05, 0.01, 0.005$ MeV
- **Strutinsky method**
  - Smoothing range: $\gamma_0 = 0.2$ MeV
  - The order of the generalized Laguerre polynomial: $M_0 = 1$

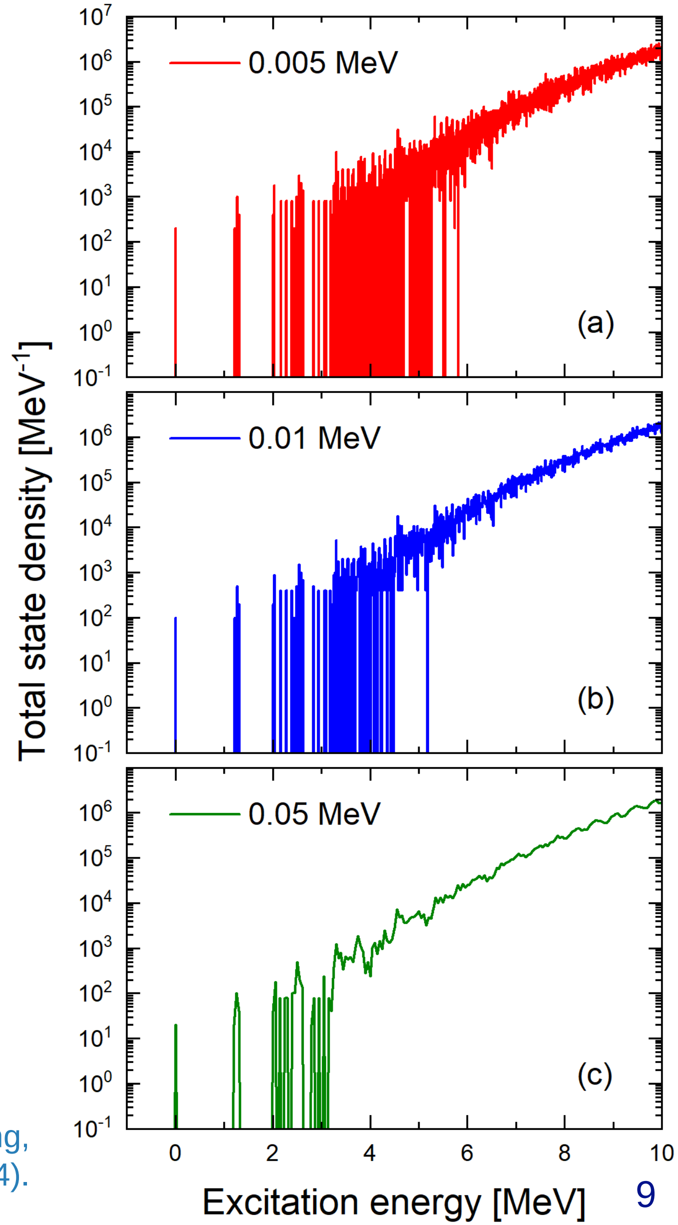
The nucleus ^{112}Cd is taken as an example to show the results.

Results

Total state density

$$\rho(U,M,P) = \frac{C(U,M,P)}{\varepsilon_0}$$

- The total state density ρ strongly depend on the energy unit ε_0.
- A very small energy unit ε_0 does not lead to a smooth ρ.
- A smoothing method is required to obtain smooth ρ against the excitation energy.

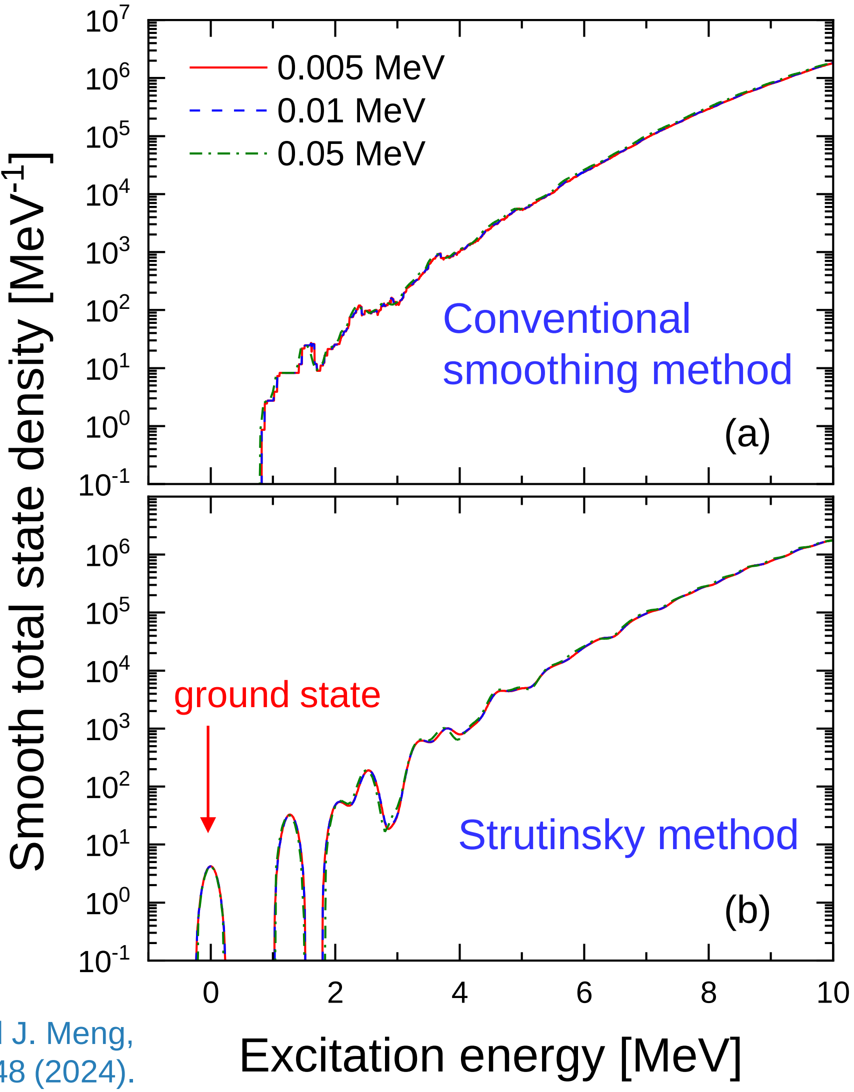


XFJ, X. H. Wu, P. W. Zhao, and J. Meng, Phys. Lett. B 849, 138448 (2024).

Results

■ Smooth total state density

- ☐ The total state densities are significantly smoothed by both methods.
- ☐ The Strutinsky method can better present the details at low excitation energy and in particular the ground state.
- ☐ The Strutinsky method can be regarded as an improvement over the conventional smoothing method and would be adopted in the present work.



XFJ, X. H. Wu, P. W. Zhao, and J. Meng, Phys. Lett. B 849, 138448 (2024).

Results

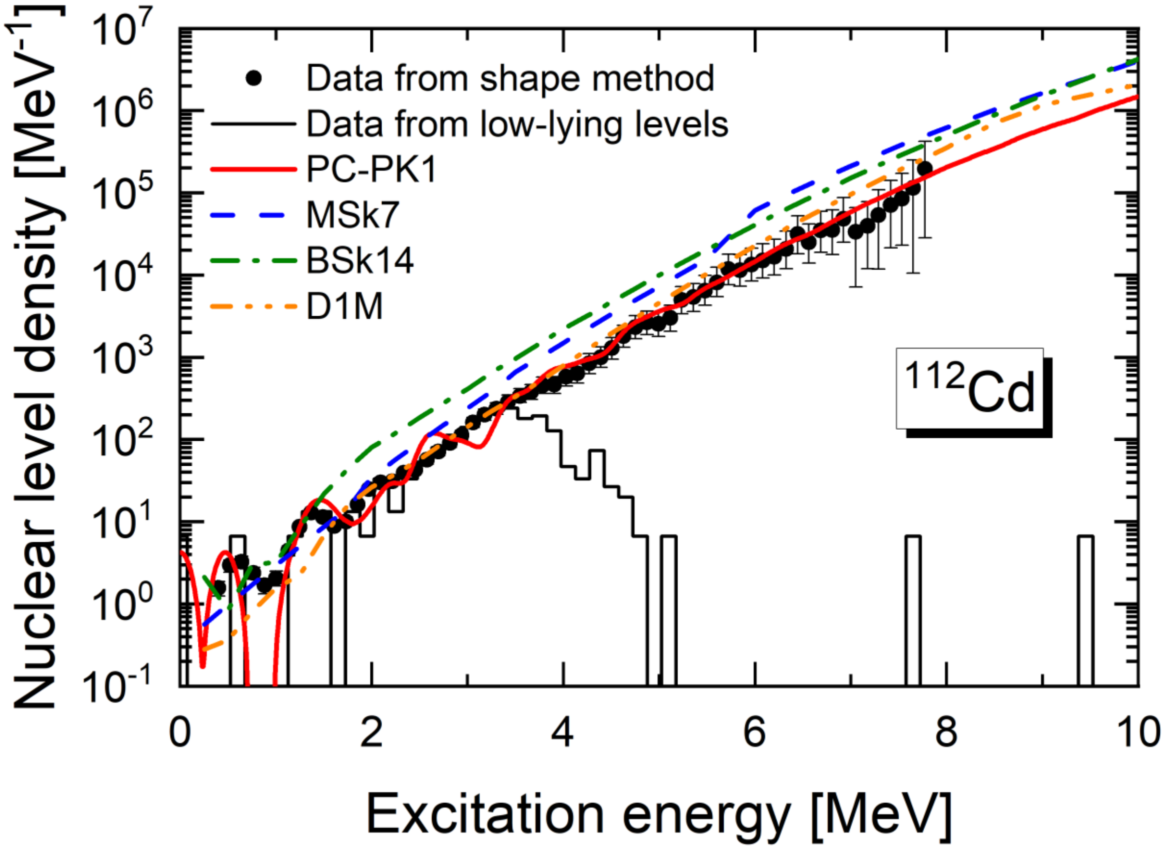
■ **Comparison with results based on non-relativistic DFT**

MSk7: Skyrme HF + BCS + Stat.

BSk14: Skyrme HFB + Comb.

D1M: Gogny Temp. HFB + Comb.

(Taken from TALYS code package)



XFJ, X. H. Wu, P. W. Zhao, and J. Meng, Phys. Lett. B 849, 138448 (2024).

□ The NLD based on PC-PK1 reproduces the ^{112}Cd experimental data quite well.

NLD from DRHBc

- **The deformed relativistic Hartree-Bogoliubov theory in continuum (DRHBc) has been successful in describing nuclear ground-state and excited properties**

see P. Guo's talk

- **The nuclear properties required for the combinatorial method have been provided by the DRHBc Collaboration**

- **Odd-odd and odd-*A* nuclei are included in the combinatorial method**

  - Different from even-even nuclei, the ground-state spin $K_{g.s.}$ and parity $P_{g.s.}$ should be considered by transform the total state density into the sum of the following two terms

$$\rho(U, K, P) = \rho(U, K - K_{g.s.}, P \times P_{g.s.}) + \rho(U, K + K_{g.s.}, P \times P_{g.s.})$$

Numerical details

- **DRHBc calculation**
  - The following nuclear properties are taken from DRHBc calculation:

    nuclear single-particle levels, masses, deformations, moments of inertia

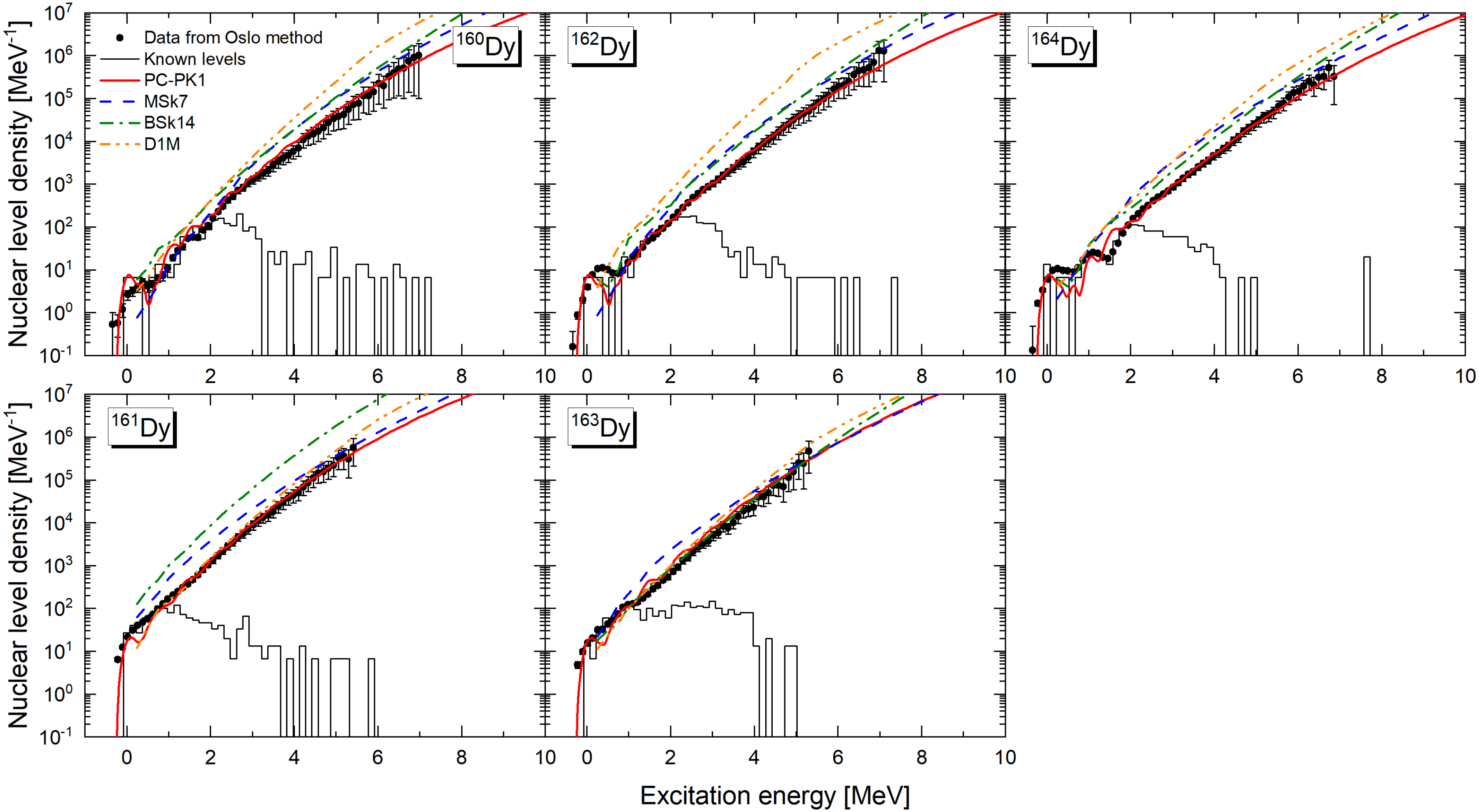
Zhang, et al. (DRHBc Mass Table Collaboration), At. Data Nucl. Data Tables 144, 101488 (2022).
P. Guo. et al. (DRHBc Mass Table Collaboration), At. Data Nucl. Data Tables 158, 101661 (2024).

- **Combinatorial method**
  - Cut-off of the excitation energy: 20 MeV
  - Cut-off of the angular momentum: 49 $\hbar$
  - Energy unit: $\varepsilon_0 = 0.01$ MeV

- **Strutinsky method**
  - Smoothing range: γ_0= 0.2 MeV
  - The order of the generalized Laguerre polynomial: $M_0 = 1$

Results

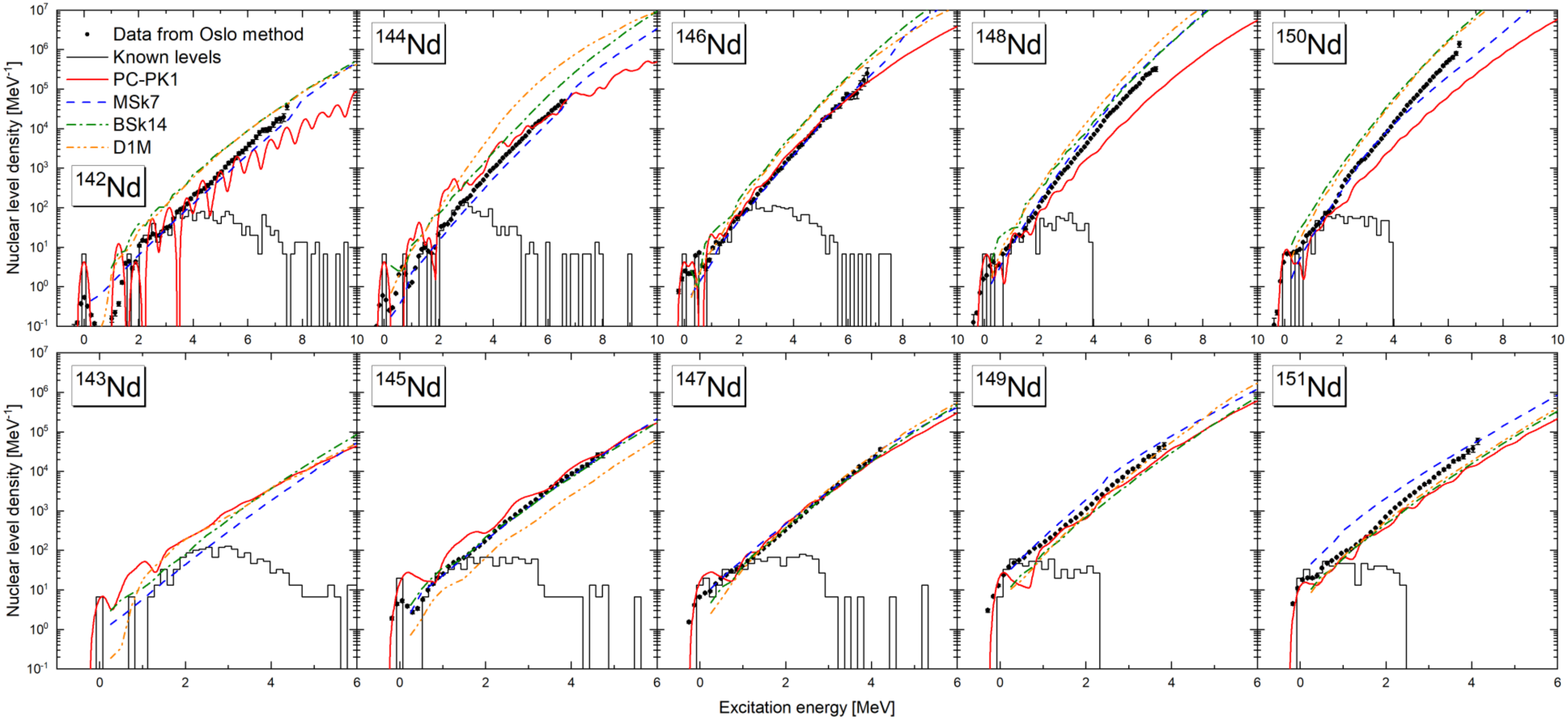
■ $^{160-164}$Dy



- For $^{160-164}$Dy, the NLDs from DRHBc with PC-PK1 reproduce the experimental data quite well.

Results

■ $^{142\text{-}151}$Nd



- For ^{148}Nd and ^{150}Nd, the NLDs from DRHBc with PC-PK1 deviates obviously from the experimental data
- Checks have made on the nuclear properties but the reason is still unclear

Results

- **A possible reason: the model dependence of the extraction procedure of NLD experimental data**
  - In the standard Oslo method the slope of the NLD is not experimentally constrained.
  - The measured NLD data are traditionally renormalized to the low-lying levels and the total NLD at the neutron separation energy deduced from the s-wave neutron spacing value D_0 for a given phenomenological NLD model (e.g. Cst-T, BSFG)

This model-dependent procedure leads to uncertainties in NLD slope

  - A consistent renormalisation procedure has been proposed.

S. Goriely, A.-C. Larsen, and D. Mücher, Phys. Rev. C 106, 044315 (2022).

Summary

- The Combinatorial method based on RHB theory is developed

✓ The Strutinsky method effectively removes the large fluctuations at low excitation energy and smoothes the total state density

✓ The NLD based on the relativistic density functional PC-PK1 well reproduces the ^{112}Cd experimental data

- The Combinatorial method based on DRHBc theory is developed

✓ For $^{160-164}$Dy, the NLDs from DRHBc reproduce the experimental data quite well

✓ For ^{148}Nd and ^{150}Nd, the NLDs from DRHBc deviates obviously from the experimental data and the reason is still unclear

- More checks on the nuclear peoperties
- A possible reason: the model dependence of the extraction procedure of NLD experimental data → the consistent renormalisation procedure

Outlook

- **Systematic calculations applied to the whole chart of nuclide**
  - even-Z
  - odd-Z

dir.out

- **DRHBc database for neutron capture rates in *r*-process**

nuclear level density
γ-strength function
optical potential

→ Hauser-Feshbach model → (n,γ) cross section → (n,γ) reaction rate

(Maxwell-Boltzmann average, nuclear partition function)

nuclear level density: Combinatorial method based on DRHBc

γ-strength function: Finite amplitude method based on DRHBc

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The End

Thanks for your attention!

Appendix

Relativistic DFT

Energy density functional

$$E = \int d^3r[\sum_{i=1}^{A} \psi_i^\dagger(\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta M)\psi_i$$
$$+ \frac{1}{2}\alpha_S\rho_s^2 + \frac{1}{3}\beta_S\rho_s^3 + \frac{1}{4}\gamma_S\rho_s^4 + \frac{1}{2}\delta_S\rho_s\Delta\rho_s + \frac{1}{2}\alpha_V j_\mu j^\mu + \frac{1}{2}\gamma_V(j_\mu j^\mu)^2 + \frac{1}{2}\delta_V j_\mu\Delta j^\mu$$
$$+ \frac{1}{2}\alpha_{TV} j_{3\mu} j_3^\mu + \frac{1}{2}\delta_{TV} j_{3\mu}\Delta j_3^\mu + eA_\mu j_c^\mu + \frac{1}{2}A_\mu\Delta A^\mu] + \frac{1}{2}\mathrm{Tr}[\Delta\cdot\kappa]$$

The relativistic Hartree-Bogoliubov (RHB) equation

$$\begin{pmatrix} \hat{h}_\mathrm{D} - \lambda_\tau & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h}_\mathrm{D}^* + \lambda_\tau \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}$$

where $\hat{h}_\mathrm{D}$ is the single-nucleon Dirac Hamiltonian, λ_τ is the Fermi energy ($\tau = n/p$ for neutrons and protons), $\hat{\Delta}$ is the pairing potential, U_k and V_k are the quasi-particle wavefunctions, and E_k is the corresponding quasi-particle energy. The single-nucleon Dirac Hamiltonian $\hat{h}_\mathrm{D}$ reads

$$\hat{h}_\mathrm{D} = \boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta(m + S) + V$$

The RHB equation is solved self-consistently to obtain nuclear single-particle levels, masses, radii, and deformations.

J. Meng, ed., Relativistic Density Functional for Nuclear Structure (WorldScientific, 2015).

Moments of inertia

- **Collective rotation effects**
  - For a spherical nucleus, the NLD is given by

$$\rho_{\mathrm{sph}}(U,J,P) = \tilde{\rho}(U,M=J,P) - \tilde{\rho}(U,M=J+1,P)$$

  - For deformed nuclei, collective rotation effects are included by building up rotational bands on the folded states

$$\rho_{\mathrm{def}}(U,J,P) = \frac{1}{2}\left[\sum_{K=-J,K\neq 0}^{J} \tilde{\rho}(U-E_{\mathrm{rot}}^{J,K},K,P)\right] + \tilde{\rho}(U-E_{\mathrm{rot}}^{J,0},0,P)\left[\delta_{(J=\mathrm{even})}\delta_{(P=+)} + \delta_{(J=\mathrm{odd})}\delta_{(P=-)}\right]$$

rotation energy

$$E_{\mathrm{rot}}^{J,K} = \frac{\hbar^2}{2\mathcal{J}_\perp}\left[J(J+1)-K^2\right]$$

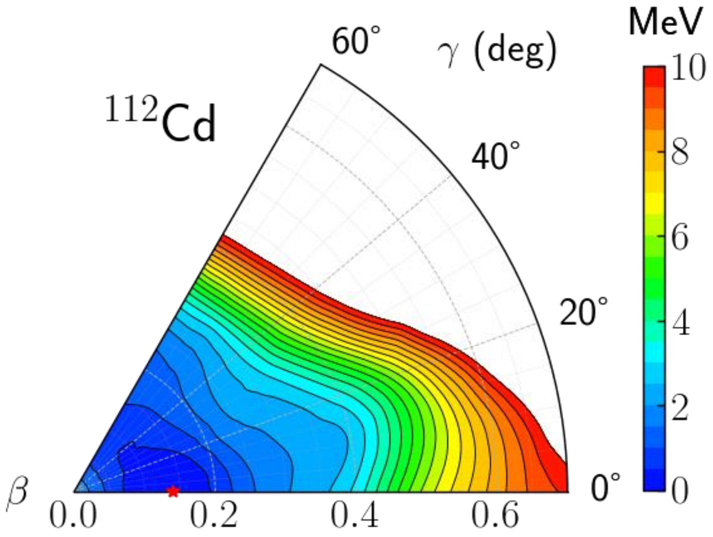
Moments of inertia Inglis-Belyaev formula

$$\mathcal{J}_\kappa = \sum_{i,j} \frac{(u_i v_j - v_i u_j)^2}{E_i + E_j} |\langle i|\hat{J}_\kappa|j\rangle|^2$$

D. R. Inglis, Phys. Rev., 103, 1786 (1956).
S. T. Beliaev, Nucl. Phys., 24, 322 (1961).
P. Ring and P. Schuck., *The nuclear many-body problem*, Springer-Verlag, Berlin Heidelberg (1980).

Appendix

- **The details of the RHB calculation**
  - Relativistic density functional PC-PK1
  - Finite-range separable pairing force, G = 728 MeV fm^3
  - RHB equation is solved by expanding the quasi-particle wavefunctions in terms of a 3-dimensional harmonic oscillator basis in Cartesian coordinates which contains 14 major shells



^{112}Cd ground-state deformation

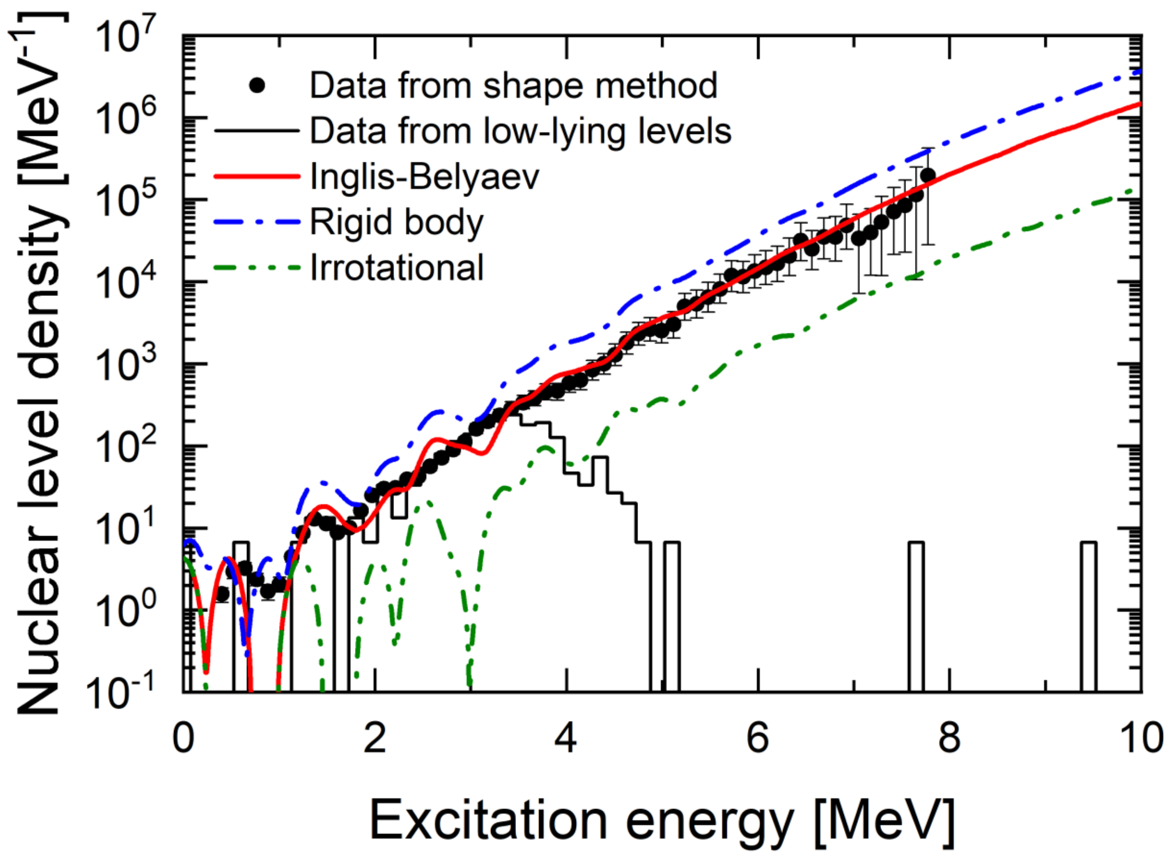
β_2 = 0.145

Figure from: http://nuclearmap.jcnp.org

Y. L. Yang, Y. K. Wang, P. W. Zhao, and Z. P. Li, Phys. Rev. C 104, 054312 (2021)

Results

■ Moments of inertia

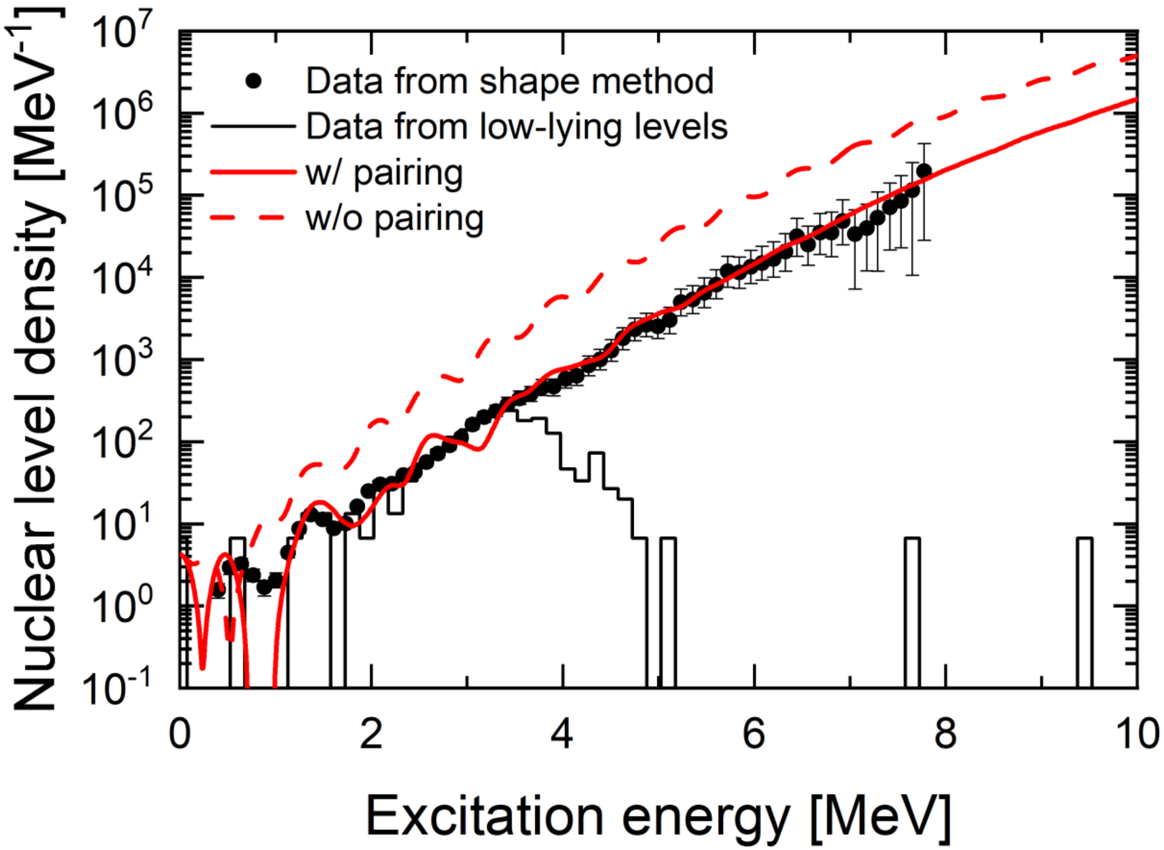


XFJ, X. H. Wu, P. W. Zhao, and J. Meng, Phys. Lett. B 849, 138448 (2024).

- The Inglis-Belyaev formula provides a proper moment of inertia and it reproduces the experimental data quite well.

Results

■ **Pairing correlations**



- ☐ The calculation with pairing correlations well reproduces the experimental data.
- ☐ The calculation without pairing correlations provides nuclear level densities of about one order of magnitude higher.

Combinatorial method

Particle/hole states

DRHBc theory provides single-particle levels characterized by

- ε_i energy
- m_i angular momentum projection onto the symmetry axis
- p_i parity
- Δ_i pairing energy

n/p particle states

$$\begin{cases} \varepsilon_i^p = \varepsilon_{Z+i}^\pi - \varepsilon_\mathrm{F}^\pi \\ m_i^p = m_{Z+i}^\pi \\ p_i^p = p_{Z+i}^\pi \\ \Delta_i^p = \Delta_{Z+i}^\pi \end{cases}$$

n/p hole states

$$\begin{cases} \varepsilon_i^h = \varepsilon_\mathrm{F}^\pi - \varepsilon_{Z-i+1}^\pi \\ m_i^h = -m_{Z-i+1}^\pi \\ p_i^h = p_{Z-i+1}^\pi \\ \Delta_i^h = \Delta_{Z-i+1}^\pi \end{cases}$$