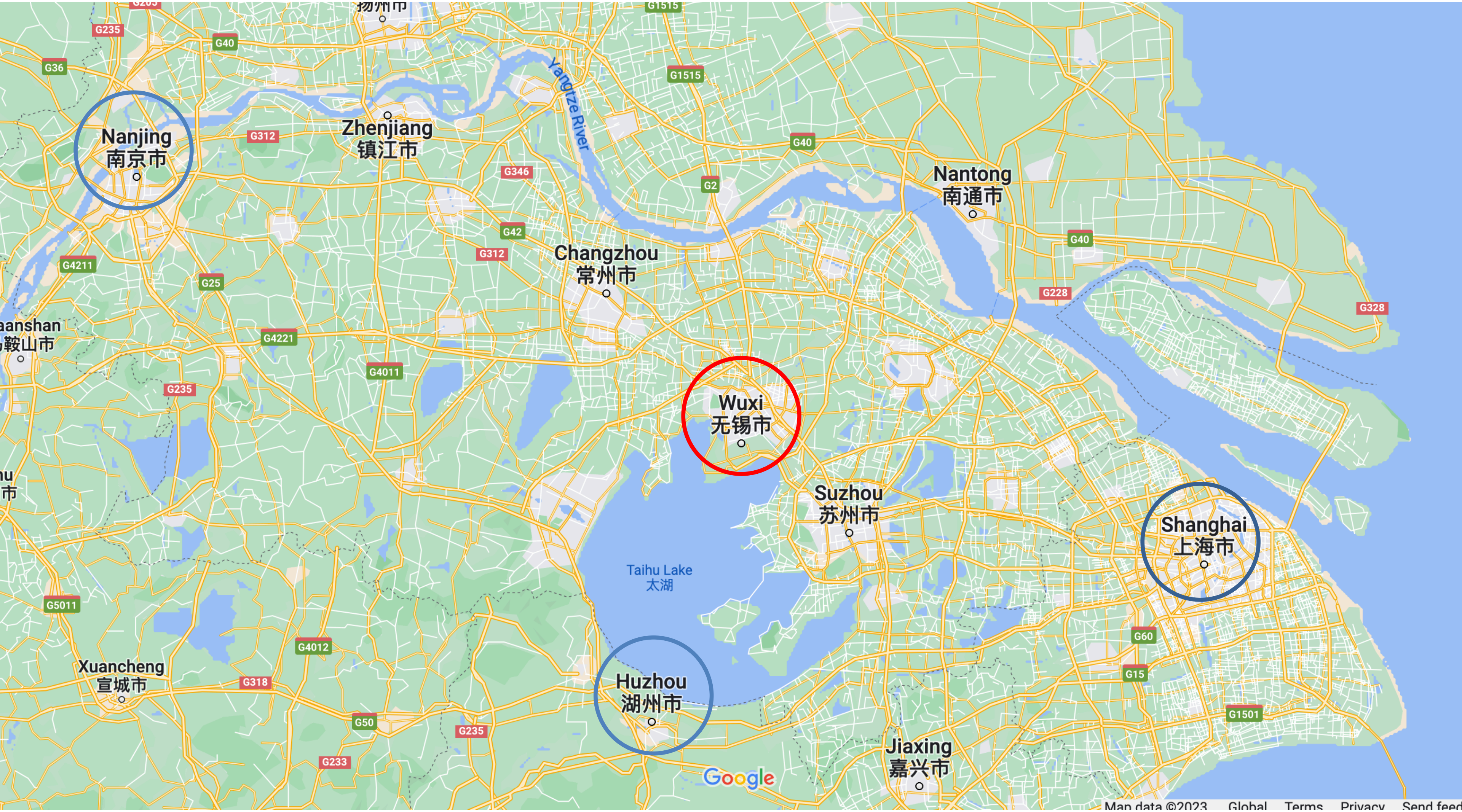
International Conference on Chirality and Wobbling in Atomic Nuclei （CWAN '23）

Pairing Phase Transition in Hot Nuclei

Lang Liu (刘 朗)

江南大学
JIANGNAN UNIVERSITY

2023-07-13 @ IMP, Huizhou


Nanjing
南京市
Zhenjiang
镇江市
Yangtze River
Nantong
南通市
Changzhou
常州市
Wuxi
无锡市
Suzhou
苏州市
Shanghai
上海市
Taihu Lake
太湖
Huzhou
湖州市
Jiaxing
嘉兴市
Xuancheng
宣城市
Google
Map data ©2023 Global Terms Privacy

Outline

- Introduction
- Theoretical framework
- Numerical details
- Results and discussion
- Summary

Introduction

✓ Pairing correlations are very crucial for nuclei;

The energy gap;

Odd-even effect of binding energy;

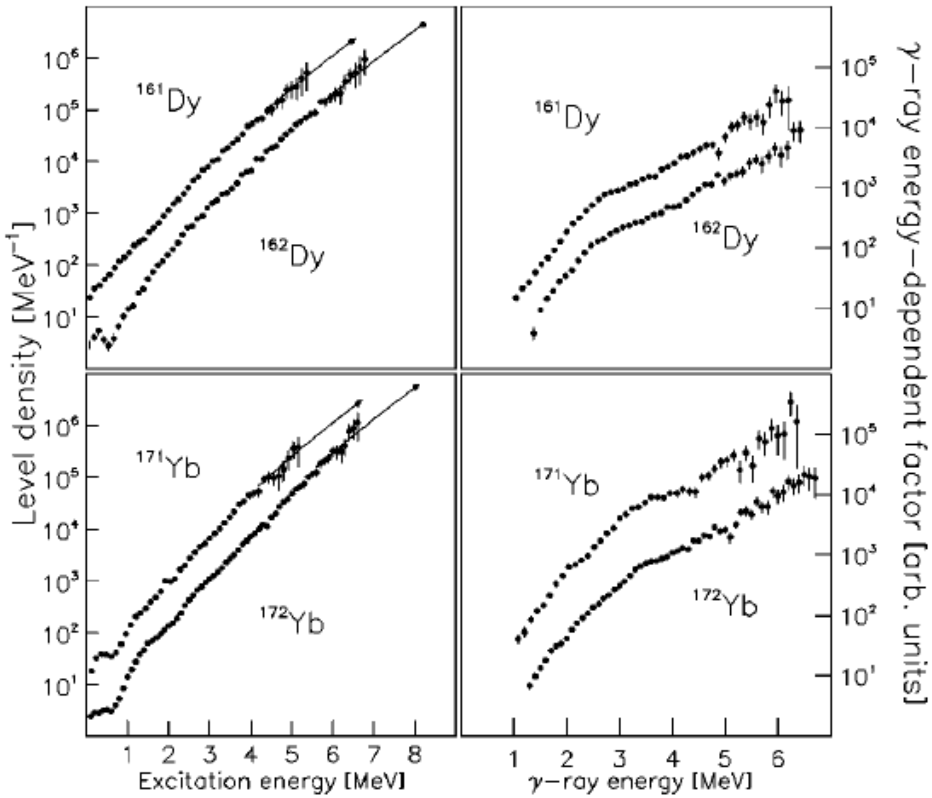
The moments of inertia;

The level density;

……

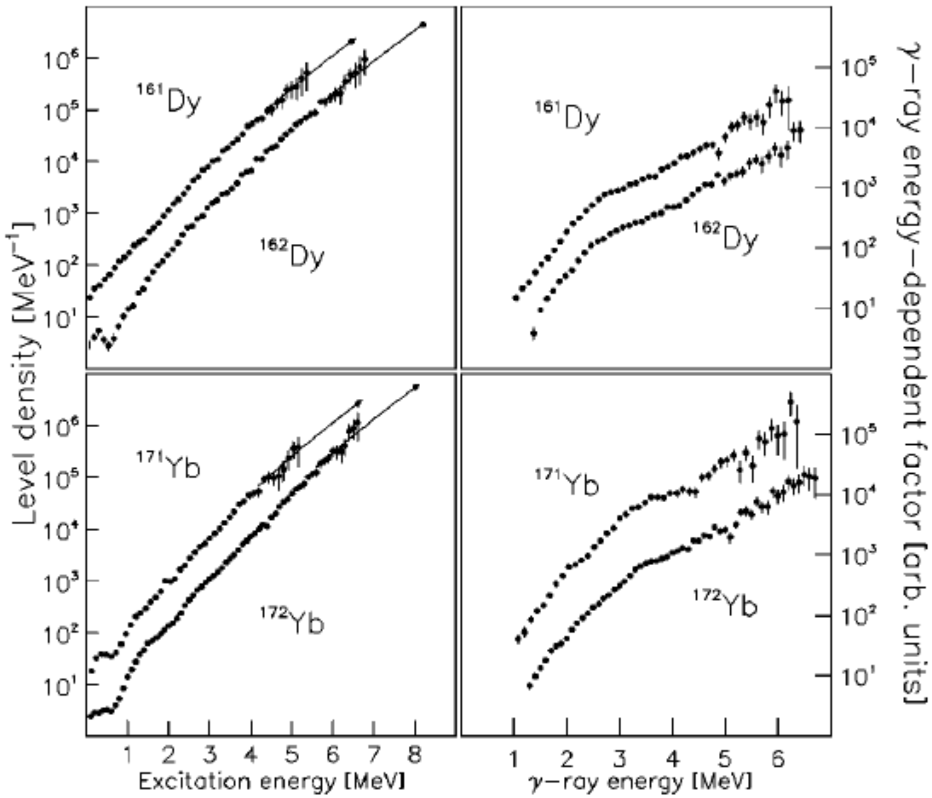
P. Ring and P. Schuck, "The Nuclear Many-Body Problem"
Springer-Verlag New York Inc. 1980

The accurate experiment of level density for $^{161,162}Dy$ and $^{171,172}Yb$



E. Melby, *et al*. *Phys. Rev. Lett.* **83** 3150 (1999)
A. Schiller, *et al*. *Phys. Rev. C* **63** 021306R (2001)

The accurate experiment of level density for ^{161,162}Dy and ^{171,172}Yb



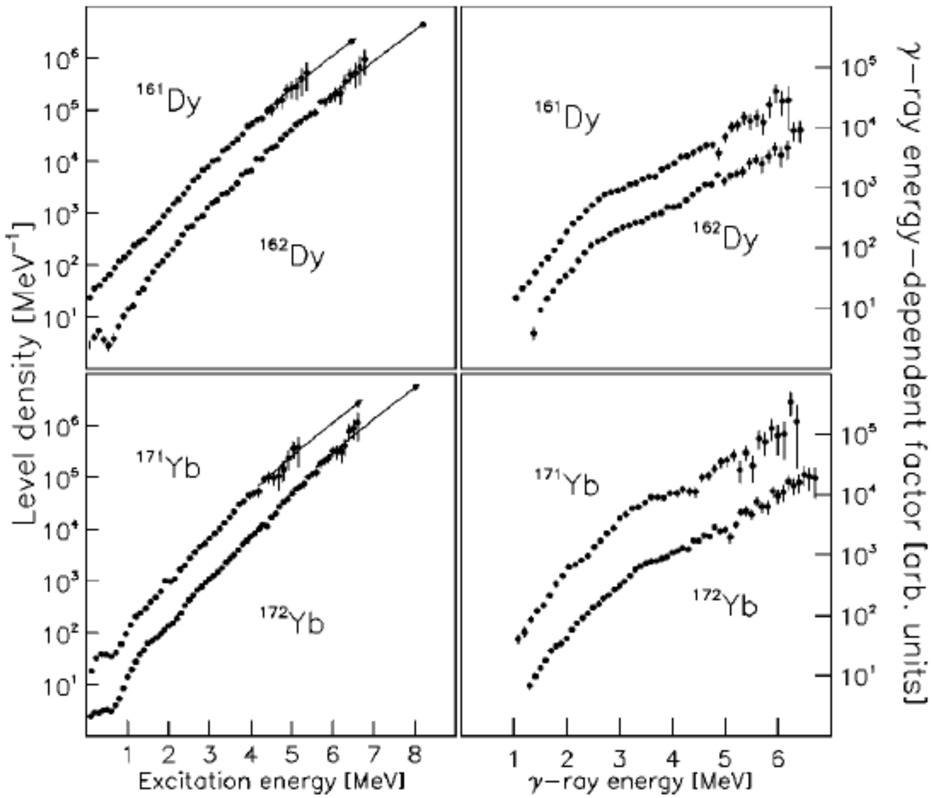
$$Z = \sum_{n=0}^{\infty} \rho(E_n) e^{-E_n/T},$$

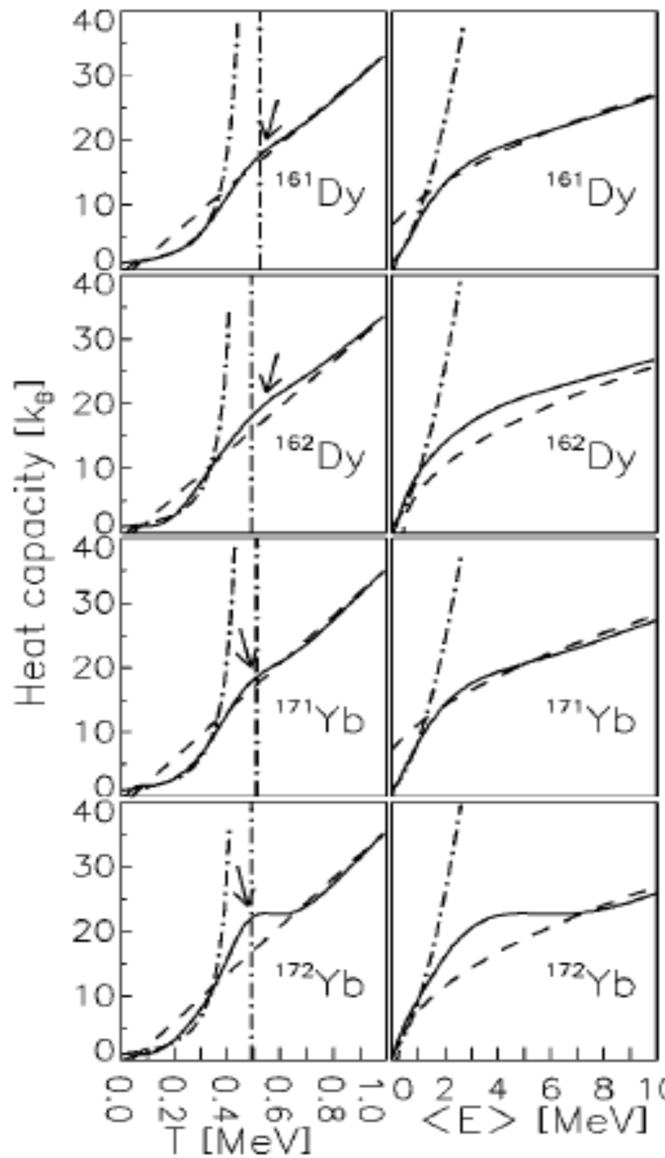
$$\langle E \rangle = \sum_{n=0}^{\infty} E_n \rho(E_n) e^{-E_n/T},$$

$$C_V = \frac{\partial \langle E \rangle}{\partial T}$$

E. Melby, *et al*. *Phys. Rev. Lett.* **83** 3150 (1999)
A. Schiller, *et al*. *Phys. Rev. C* **63** 021306R (2001)

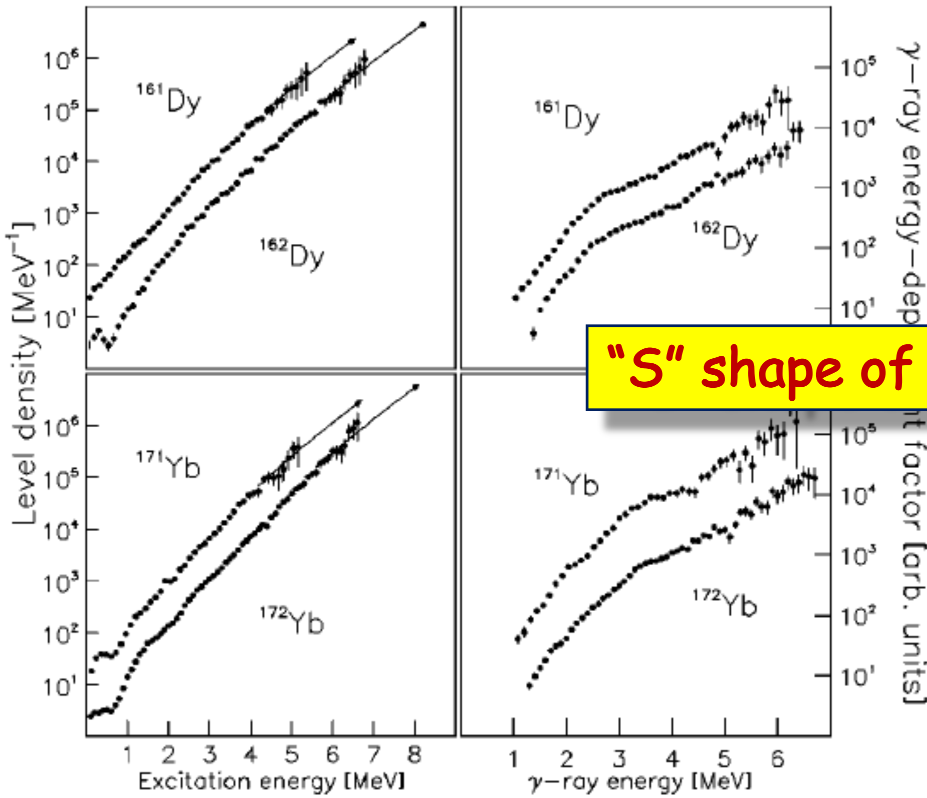
The accurate experiment of level density for ^{161,162}Dy and ^{171,172}Yb



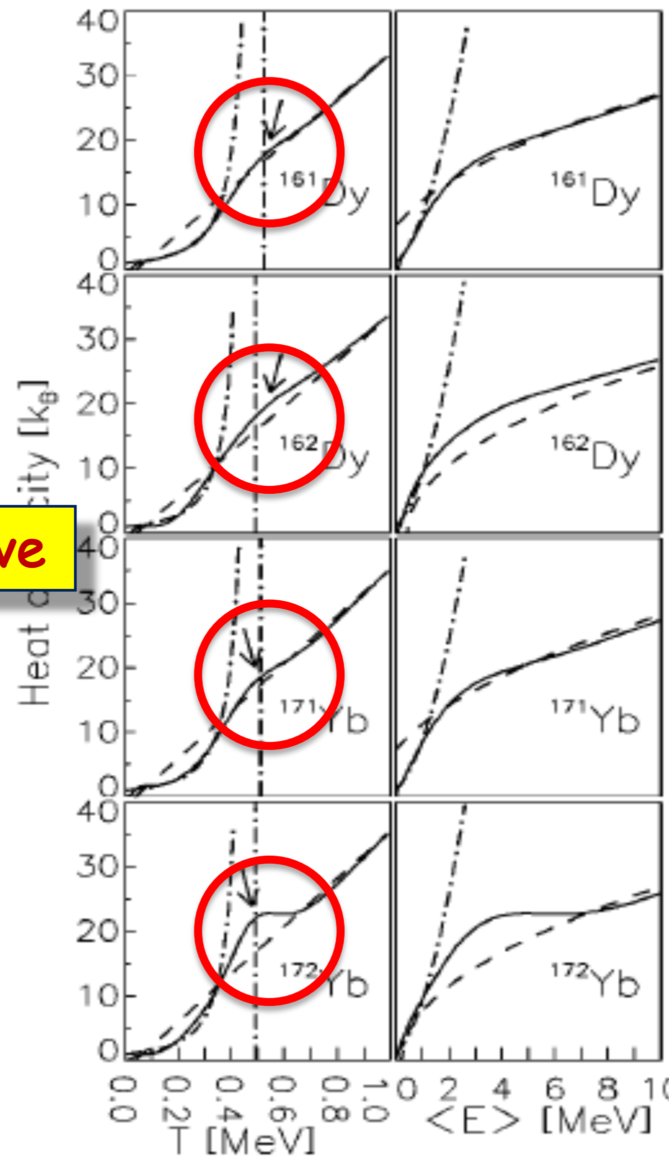


E. Melby, *et al*. *Phys. Rev. Lett.* **83** 3150 (1999)
A. Schiller, *et al*. *Phys. Rev. C* **63** 021306R (2001)

The accurate experiment of level density for ^{161,162}Dy and ^{171,172}Yb



"S" shape of Cv curve



E. Melby, *et al*. *Phys. Rev. Lett.* **83** 3150 (1999)
A. Schiller, *et al*. *Phys. Rev. C* **63** 021306R (2001)

Theoretical studies

✓ Based on BCS or Bogoliubov transformation:

- **Finite-temperature Hartree-Fock-Bogoliubov:**

  J. L. Egido, *et al.*, *Phys. Rev. Lett.* **85**, 26 (2000);

- **Relativistic Hartree-Fock-BCS:**

  B. K. Agrawal, *et al.*, *Phys. Rev. C* **62**, 044307 (2000);

- **Finite-temperature relativistic Hartree-Bogoliubov theory based on a point-coupling functional, with the Gogny or separable pairing force:**

  Y. F. Niu, *et al.*, *Phys. Rev. C* **88**, 034308 (2013);

  W. Zhang, *et al.*, Phys. Rev. C 97, 054302 (2018).

- **Continuum coupling are supplemented to the BCS equation:**

  N. Sandulescu, *et al.*, *Phys. Rev. C* **55**, 1250 (1997); Phys. Rev. C 61, 044317 (2000).

- **Relativistic Hartree-Fock-Bogoliubov:**

  J. J. Li, *et al.*, Phys. Rev.C **92**, 014302 (2015).

Theoretical studies

✓ Based on BCS or Bogoliubov transformation:

- **Finite-temperature Hartree-Fock-Bogoliubov:**

  J. L. Egido, *et al.*, *Phys. Rev. Lett.* **85**, 26 (2000);

- **Relativistic Hartree-Fock-BCS:**

  B. K. Agrawal, *et al.*, *Phys. Rev. C* **62**, 0443...

- **Finite-temperat... ...ed on a point-coupling functio... ...parable pairing force:**

  1) S shape of Cv;
  2) abrupt change of pairing gap

  Y. F. Niu, *et al.*, *Phys. Rev. C* **88**, 034308 (2013);

  W. Zhang, *et al.*, Phys. Rev. C 97, 054302 (2018).

- **Continuum coupling are supplemented to the BCS equation:**

  N. Sandulescu, *et al.*, *Phys. Rev. C* **55**, 1250 (1997); Phys. Rev. C 61, 044317 (2000).

- **Relativistic Hartree-Fock-Bogoliubov:**

  J. J. Li, *et al.*, Phys. Rev.C **92**, 014302 (2015).

Theoretical studies

✓ Based on projection method:

- **Particle-number projected statistics (PNPS):**

  C. Esebbag, *et al., Nucl. Phys. A* **552**, 205 (1993);

- **Finite-temperature variation before projection BCS (FT-VBP):**

  K. Esashika, *et al., Phys. Rev. C* **72**, 044303 (2005);

- **Finite-temperature variation after projection BCS (FT-VAP):**

  D. Gambacurta, *et al*., *Phys. Rev. C* **88**, 034324 (2013).

✓ Other works

- S. Rombouts, et al. *Phys. Rev. C* **58**, 3295 (1998); S. Liu, et al. *Phys. Rev. Lett.* **87**, 1 (2001);
- M. Guttormsen, et al. *Phys. Rev. C* **63**, 044301 (2001); *Phys. Rev. C* **64**, 034319 (2001).

Theoretical studies

✓ Based on projection method:

- Particle-number projected statistics (PNPS):

  C. Esebbag, *et al., Nucl. Phys. A* **552**, 205 (1993);

- Finite-temperature variation before projection BCS (FT-VBP):

  K. Esashika, *et al., Phys. Rev. C* **72**, 044303 (2005);

- Finite-temper ... jection BCS (FT-VAP):

  D. Gambacurta, ...

1) S shape of C_V;
2) gradual change of pairing gap

✓ Other works

- S. Rombouts, et al. *Phys. Rev. C* **58**, 3295 (1998); S. Liu, et al. *Phys. Rev. Lett.* **87**, 1 (2001);
- M. Guttormsen, et al. *Phys. Rev. C* **63**, 044301 (2001); *Phys. Rev. C* **64**, 034319 (2001).

division and difficulty

Phase transition of pairing ⇐ **interpretation of "S" shape of C_v** ⇒ **no phase transition**

others

K. Esashika, *et al*.

division and difficulty

Phase transition of pairing ⇦ **interpretation of "S" shape of C_V** ⇨ **no phase transition**

others

K. Esashika, *et al*.

⇩

what is the order of phase transition?

division and difficulty

Phase transition of pairing ⇐ interpretation of "S" shape of Cv ⇒ no phase transition

others — K. Esashika, *et al*.

⇓

what is the order of phase transition?

Ehrenfest's classification of phase transitions is based on the thermodynamic limits of large numbers of particles, and does not apply to small systems such as atomic nuclei.

P. Borrmann, *et al.*, Phys. Rev. Lett. **84**, 3511 (2000).

G. Jaeger, *et al.*, Exact. Sci. **53**, 51 (1998).

Introduction

A theorem on the distribution of roots of the grand parition function in small system.

T. D. Lee and C. N. Yang, Phys. Rev. **87**, 410(1952).

This theorem has been extended to the canonical ensemble through the analytic continuation of the inverse temperature in the complex plane.

S. Grossmann, *et al.*, Z. Phys. **207**, 138 (1967).

S. Grossmann, *et al.*, Z. Phys. **218**: 449-59 (1969).

A classification scheme for phase transition in finite systems, such as atomic systems, based on the distribution of zeros (DOZ) of the canonical partition function in complex temperature plane.

P. Borrmann, *et al.*, Phys. Rev. Lett. **84**, 3511 (2000).

O. Mülken, *et al.*, Phys. Rev. A **64**, 013611 (2001).

Motivation

Covariant density functional theory (CDFT)

P. Ring, Prog. Part. Nucl. Phys. **37**, 193 (1996)

J. Meng, *et al.*, AAPPS Bulletin **31** (2021).

Shell-like model approach (SLAP)

J. Y. Zeng, *et al.*, Nucl. Phys. A **405**, 1 (1983).

J. Meng, J. Y. Guo, L. Liu, *et al.*, Front. Phys. China 1, 38 (2006).

Outline

- ➢ Introduction
- ➢ Theoretical framework
- ➢ Numerical details
- ➢ Results and discussion
- ➢ Summary

SLAP Hamiltonian

Hamiltonian

$$H = H_{s.p.} + H_{pair}$$

where

$$\mathrm{H}_{s.p.} = \sum_{\nu>0} \boxed{\varepsilon_\nu} (a_\nu^+ a_\nu + a_{\bar{\nu}}^+ a_{\bar{\nu}}) \qquad \mathrm{H}_{pair} = -\boxed{G} \sum_{\mu,\nu>0}^{\mu\neq\nu} a_\mu^+ a_{\bar{\mu}}^+ a_{\bar{\nu}} a_\nu$$

single particle energy

pairing strength

1. Solve Dirac Eq. in CDFT to obtain single-particle levels;
2. Construct multi-particle configuration (MPC);
3. Diagonalize Hamiltonian in MPC.

J. Y. Zeng, and T. S. Cheng, *Nucl. Phys.* A **405**, 1 (1983).

J. Meng, J. Y. Guo, L. Liu, S. Q. Zhang, *Front. Phys. China* **1**, 38 (2006).

Multi-particle configuration (MPC)

1. Solve Dirac Eq. in CDFT to obtain single-particle levels;
2. Construct multi-particle configuration (MPC);
3. Diagonalize Hamiltonian in MPC.

➢ Fully paired state (s=0) : (s: *Seniority*)

$$|\phi_i^n\rangle = |\alpha_1\bar{\alpha}_1 \cdots \alpha_n\bar{\alpha}_n\rangle, \quad K = 0, \quad n\text{: number of pair}$$

➢ One pair broken state (s=2) :

$$|\phi_j^{n-1}\rangle = |\mu\bar{\upsilon}\alpha_1\bar{\alpha}_1 \cdots \alpha_{n-1}\bar{\alpha}_{n-1}\rangle, \quad K = \Omega_\mu \pm \Omega_\upsilon,$$

...

➢ For axial symmetrical case, K and parity are good quantum number, as well as the seniority, MPC for $\pi = +$ can be reduced as

$$\begin{array}{lllllll} & (s=0, K=0) & & & & & \\ \oplus & (s=2, K=0) & \oplus & (s=2, K=1) & \oplus & (s=2, K=2) & \oplus \quad \cdots \\ \oplus & (s=4, K=0) & \oplus & (s=4, K=1) & \oplus & (s=4, K=2) & \oplus \quad \cdots \\ \oplus & \quad\cdots & & & & & \end{array}$$

Wave functions and energies

1. Solve Dirac Eq. in CDFT to obtain single-particle levels;
2. Construct multi-particle configuration (MPC);
3. Diagonalize Hamiltonian in MPC.

⇓

energy spectra

$$E_m$$

wave function of the g.s. and excited states

$$|\Psi^{(m)}\rangle = \sum_i V_i^{(m)} |\phi_i^n\rangle + \sum_j V_j^{(m)} |\phi_j^{n-1}\rangle + \cdots$$

m=0 (g.s), 1, 2, … (excited states);
n: number of pair;
i, j: index of MPC

Thermodynamic quantities

energy spectra

$$E_m$$

wave function of the g.s. and excited states

$$|\Psi^{(m)}\rangle = \sum_i V_i^{(m)} |\phi_i^n\rangle + \sum_j V_j^{(m)} |\phi_j^{n-1}\rangle + \cdots$$

Partition Function $Z = \sum_{m=0}^{\infty} \rho(E_m)\, e^{-E_m/T}$

Average of physical quantities $\langle O \rangle = Z^{-1} \sum_{m=0}^{\infty} O_m\, \rho(E_m)\, e^{-E_m/T},$

Heat capacity $C_V = \dfrac{\partial \langle E \rangle}{\partial T}$

Outline

- Introduction
- Theoretical framework
- Numerical details
- Results and discussion
- Summary

Numerical details : ^{162}Dy

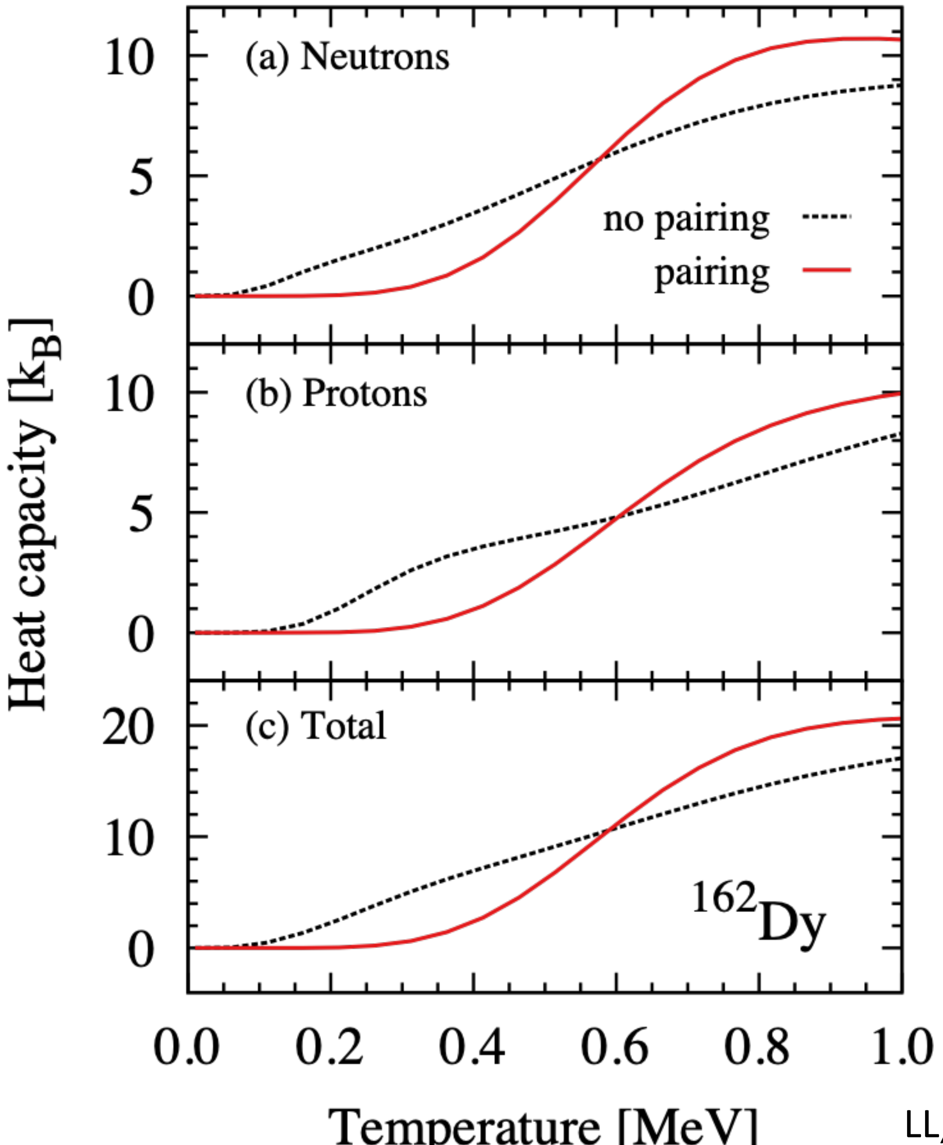
- RMF
  1) PK1 effective interaction;
  2) 14 oscillator major shells.

- SLAP
  1) 12 particles and 20 single-particle levels for either neutrons or protons;
  2) E_C = 30 MeV for either neutrons or protons;
  3) Dimension of MPCs: $5*10^5$ for neutrons, $3*10^5$ for protons;
  4) Pairing strength G is fitted according to experimental odd-even mass differences. ^{161,162,163}Dy for G_n, ^{161}Tb,^{162}Dy and ^{163}Ho for G_p. G_n=0.29 MeV, G_p=0.32 MeV.

Outline

- ➢ Introduction
- ➢ Theoretical framework
- ➢ Numerical details
- ➢ **Results and discussion**
- ➢ Summary

Heat capacity



$$\langle E \rangle = Z^{-1} \sum_{m=0}^{\infty} E_m \, \rho(E_m) \, e^{-E_m/T}$$

$$C_V = \frac{\partial \langle E \rangle}{\partial T}$$

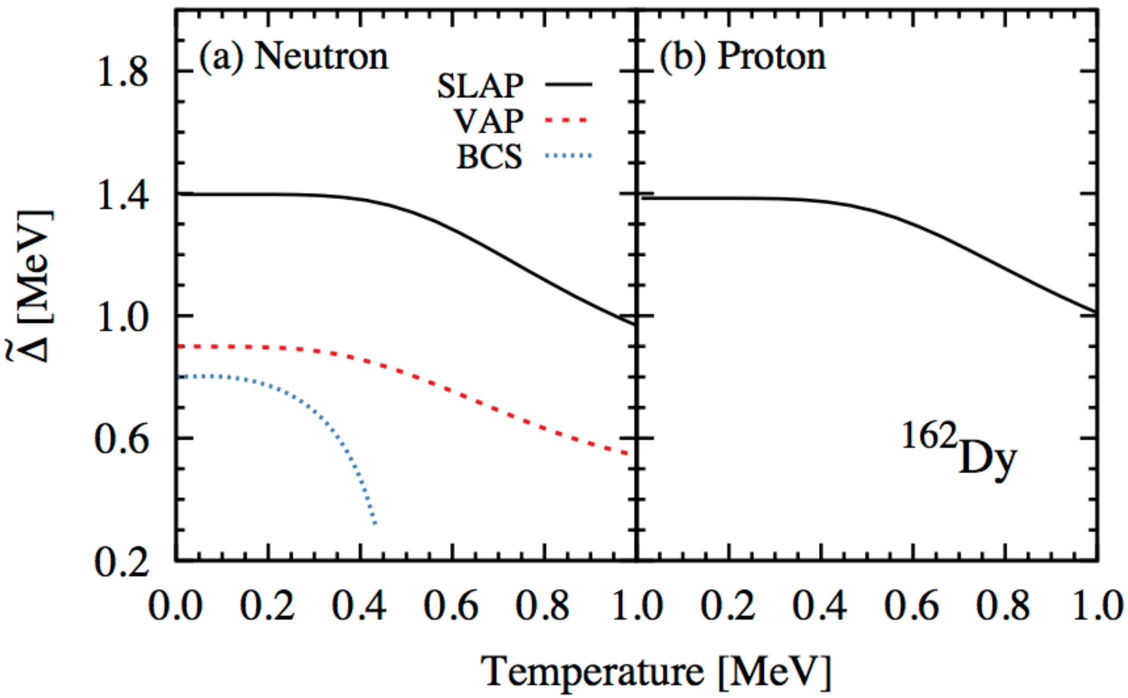
straight line w/o pairing

"S" shape with pairing

Pairing is important in hot nuclei

LL, Z. H. Zhang, P. W. Zhao, PRC **92**, 044304 (2015).

Pairing gap



$$\Delta^{(m)} = G\left[-\frac{1}{G}\langle\Psi^{(m)}|H_{\rm p}|\Psi^{(m)}\rangle\right]^{1/2}$$

L. F. Canto, et al.
Phys. Lett. B **161**, 21 (1985).

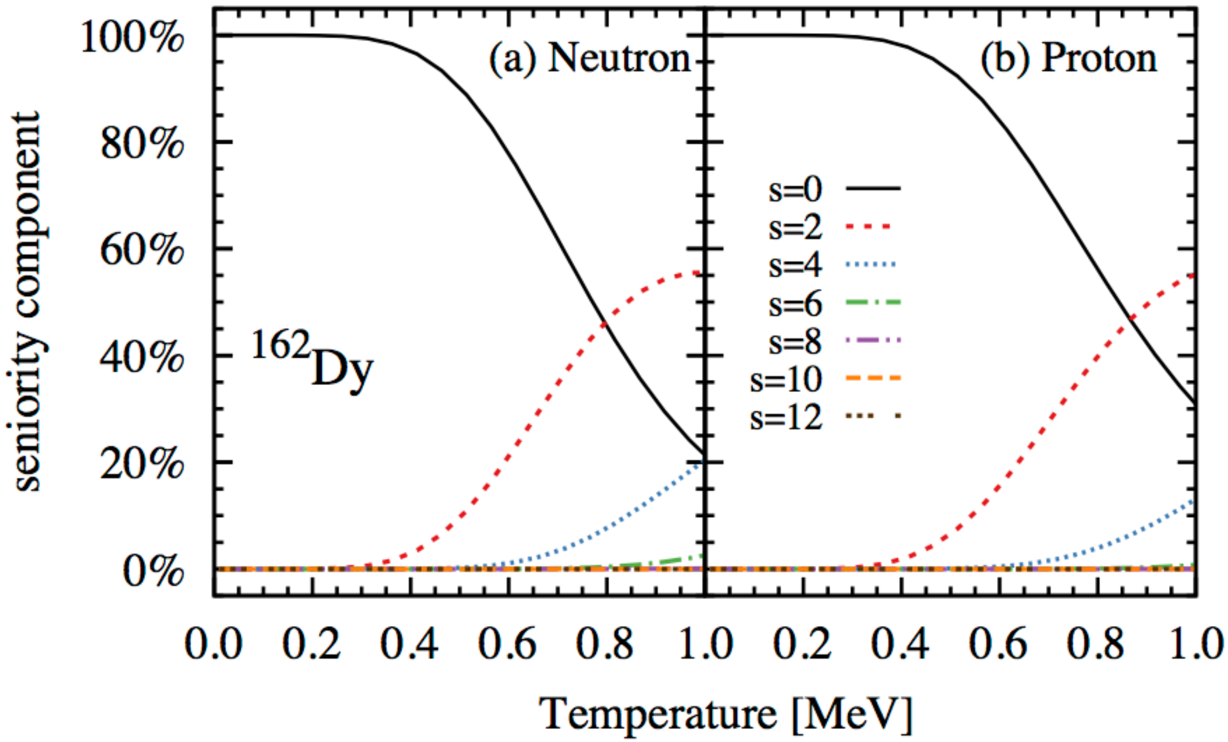
$$\tilde{\Delta} = Z^{-1}\sum_{m=0}^{\infty}\Delta^{(m)}\,\rho(E_m)\,e^{-E_m/T}$$

- ✓ Constant pairing gap at low T; ➡ ✓ difficult to excite;
- ✓ Gradually decrease at high T; ➡ ✓ many excited states appear;
- ✓ never collapse ➡ ✓ particle number conserving.

LL, Z. H. Zhang, P. W. Zhao, PRC **92**, 044304 (2015).

BCS & VAP: Phys. Rev. C **88**, 034324 (2013).

Seniority component



seniority component:

$$Z^{-1} \sum_{m \in \{s\}} \rho(E_m)\, e^{-E_m/T}$$

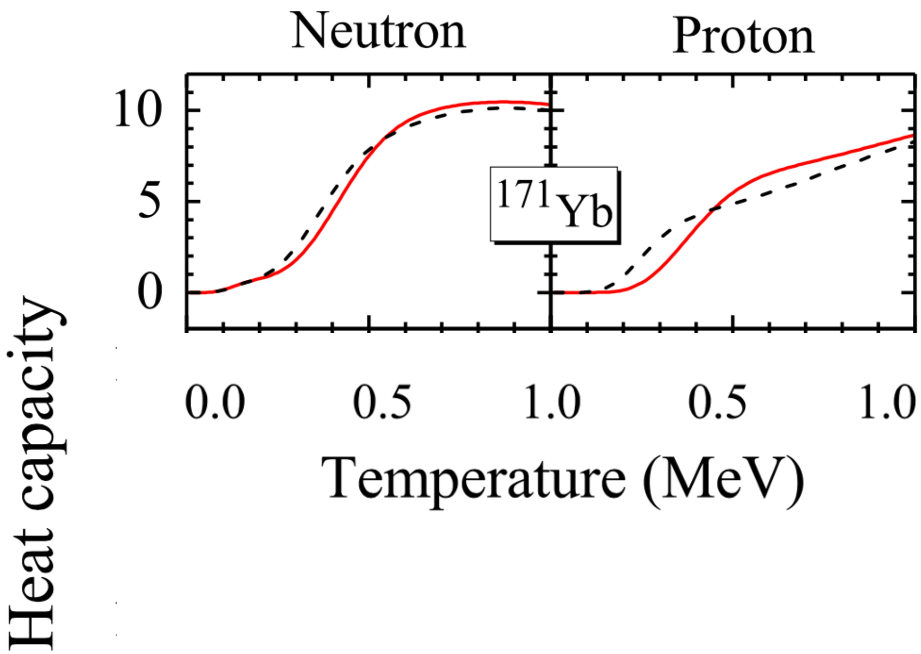
✓ s=0 states dominant at low T;

✓ s=2 states become important at high T;

✓ s=4 states contribute a little bit

LL, Z. H. Zhang, P. W. Zhao, PRC **92**, 044304 (2015).

Heat capacity for odd-A nuclei



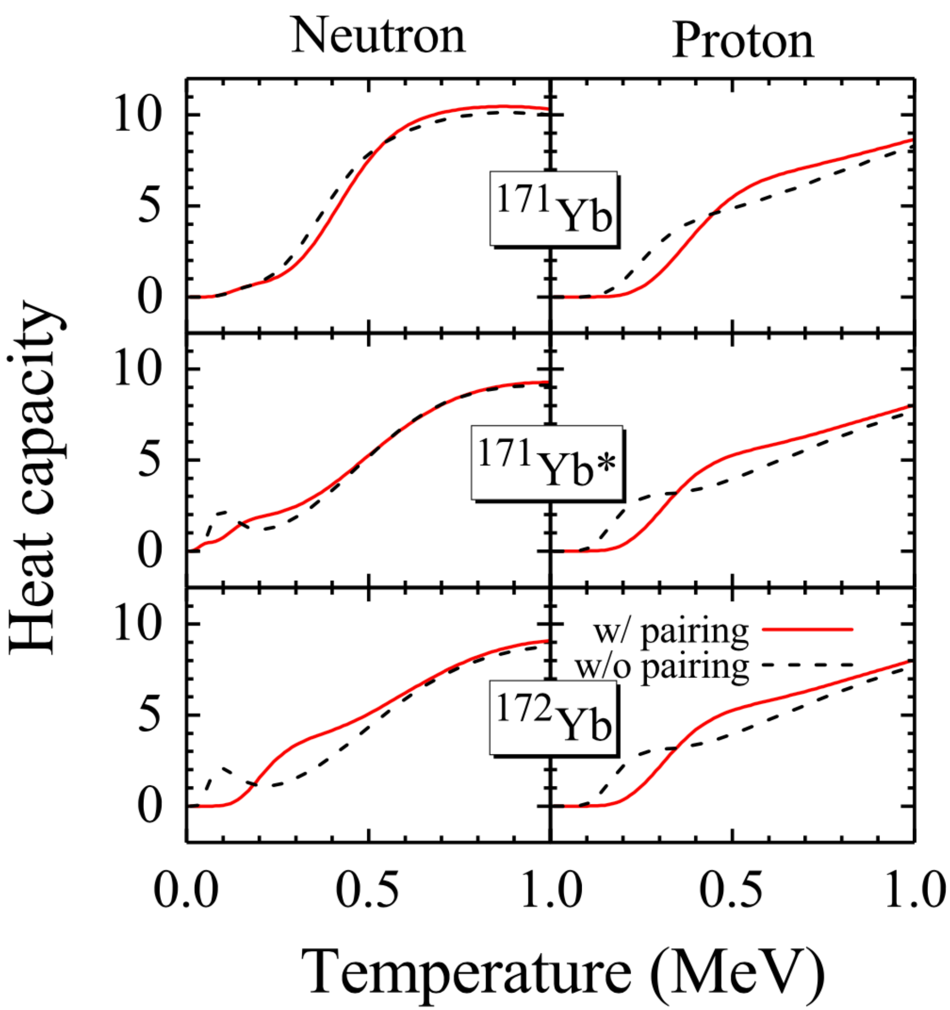
$$\langle E \rangle = Z^{-1} \sum_{m=0}^{\infty} E_m \, \rho(E_m) \, e^{-E_m/T}$$

$$C_V = \frac{\partial \langle E \rangle}{\partial T}$$

"S" shape with and w/o pairing

T. Yan, Y. L. Lin, LL, PRC **104**, 024303 (2021).

Heat capacity for odd nuclei



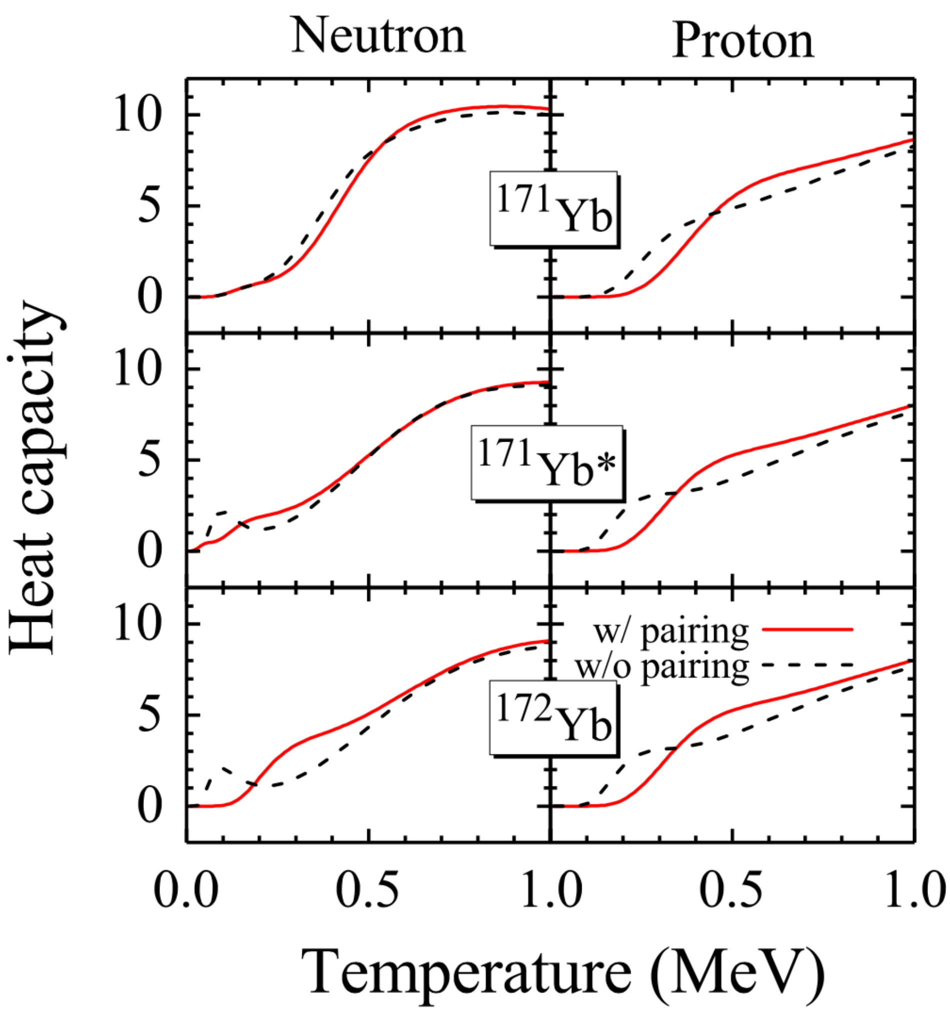
$$\langle E\rangle = Z^{-1}\sum_{m=0}^{\infty} E_m\,\rho(E_m)\,e^{-E_m/T}$$

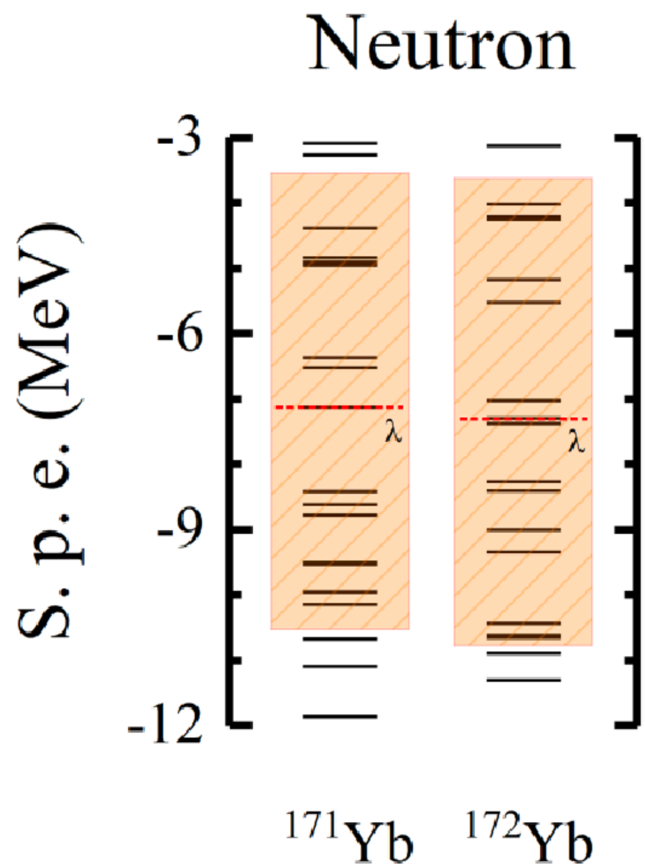
$$C_V = \frac{\partial\langle E\rangle}{\partial T}$$

"S" shape w/ and w/o pairing

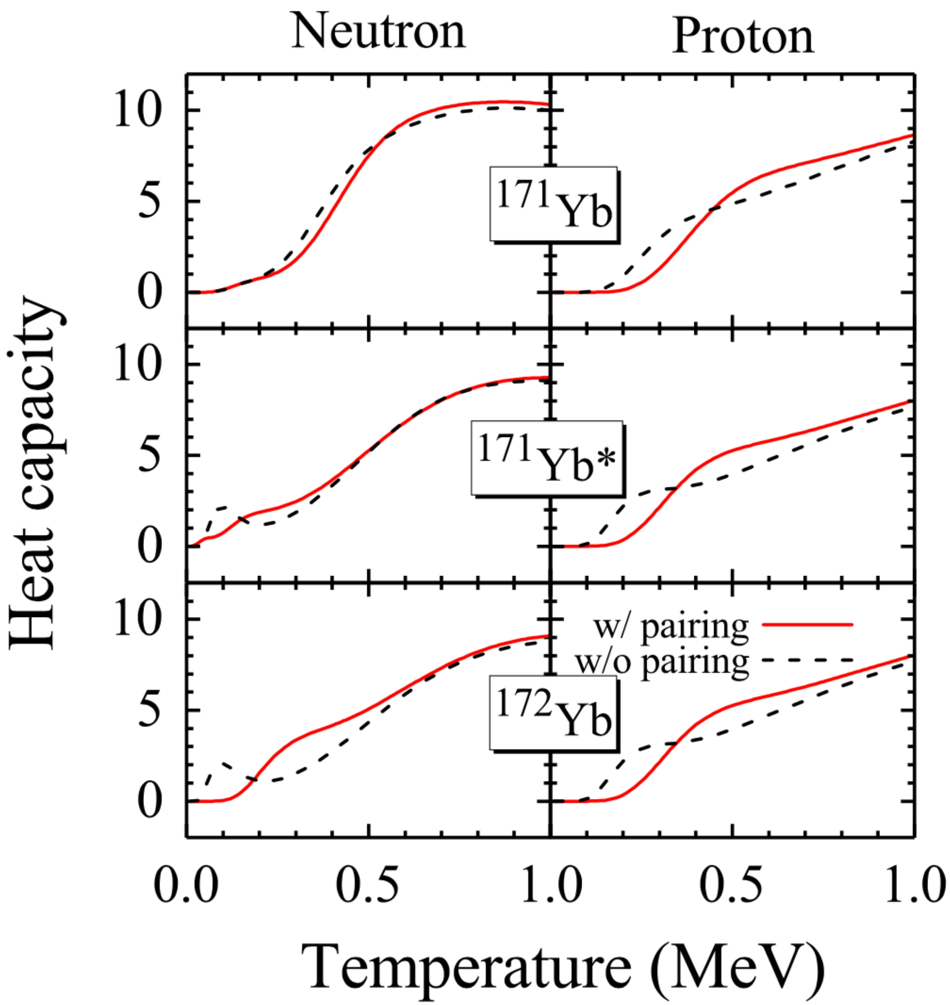
T. Yan, Y. L. Lin, LL, PRC **104**, 024303 (2021).

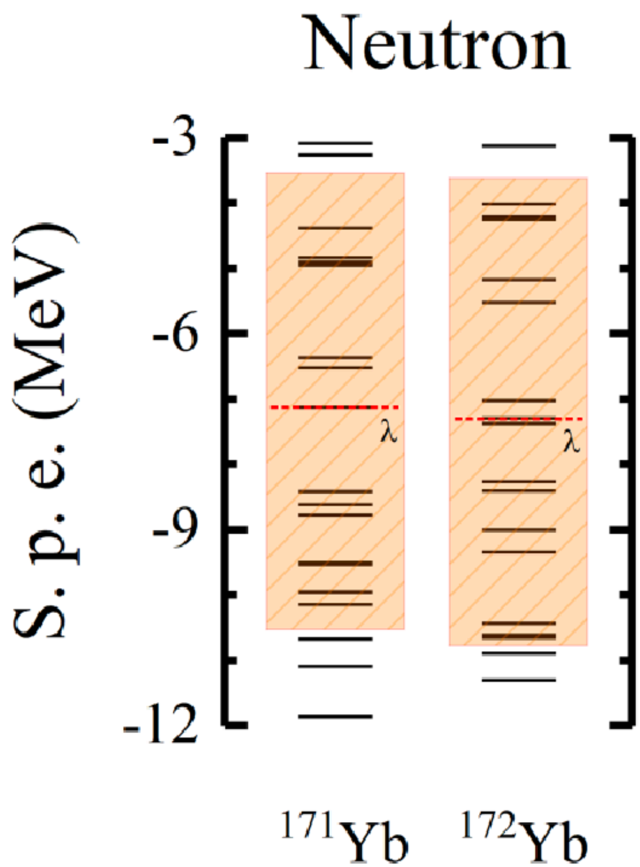
Single-particle level





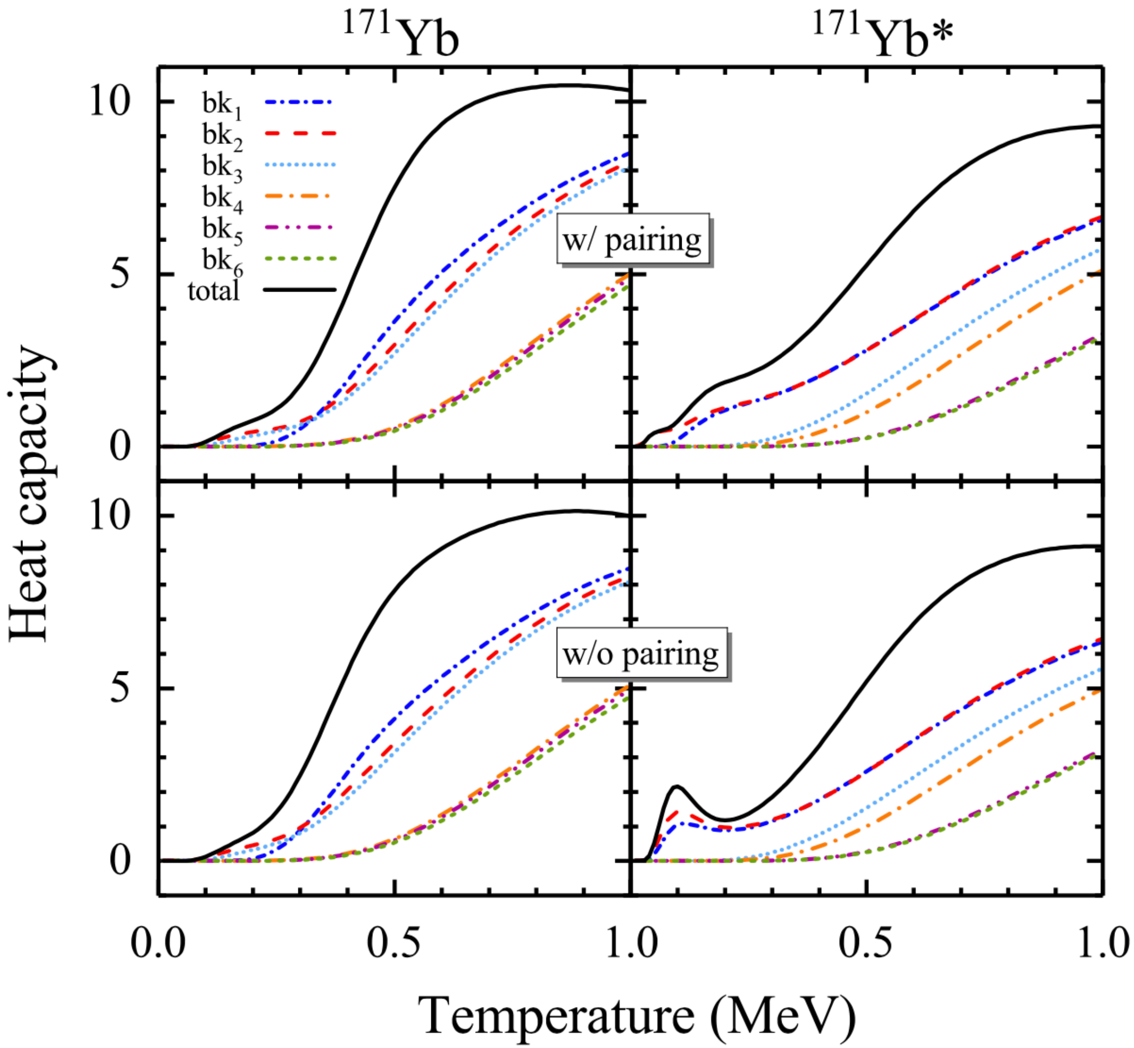
Single-particle level

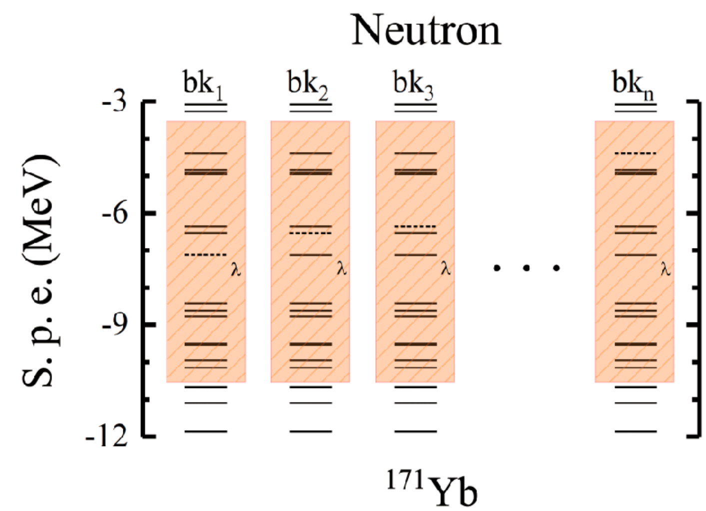




s.p.e structure can affect Cv curve

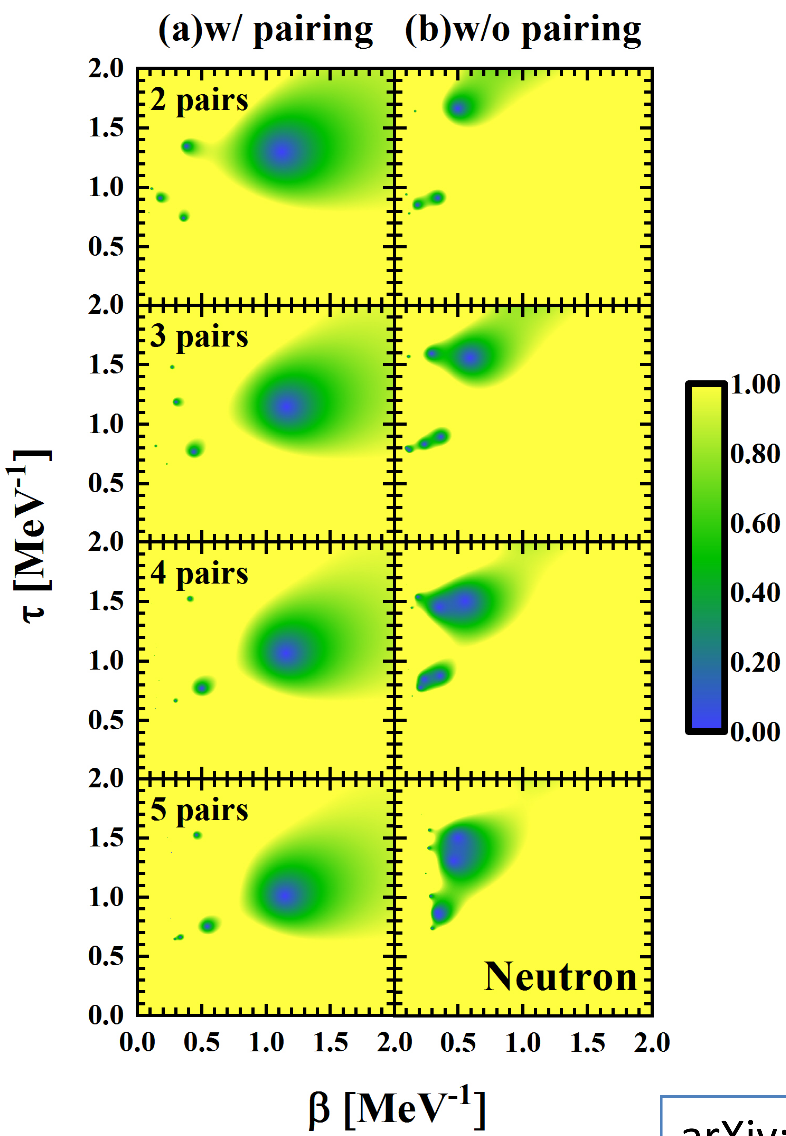
Blocking effect





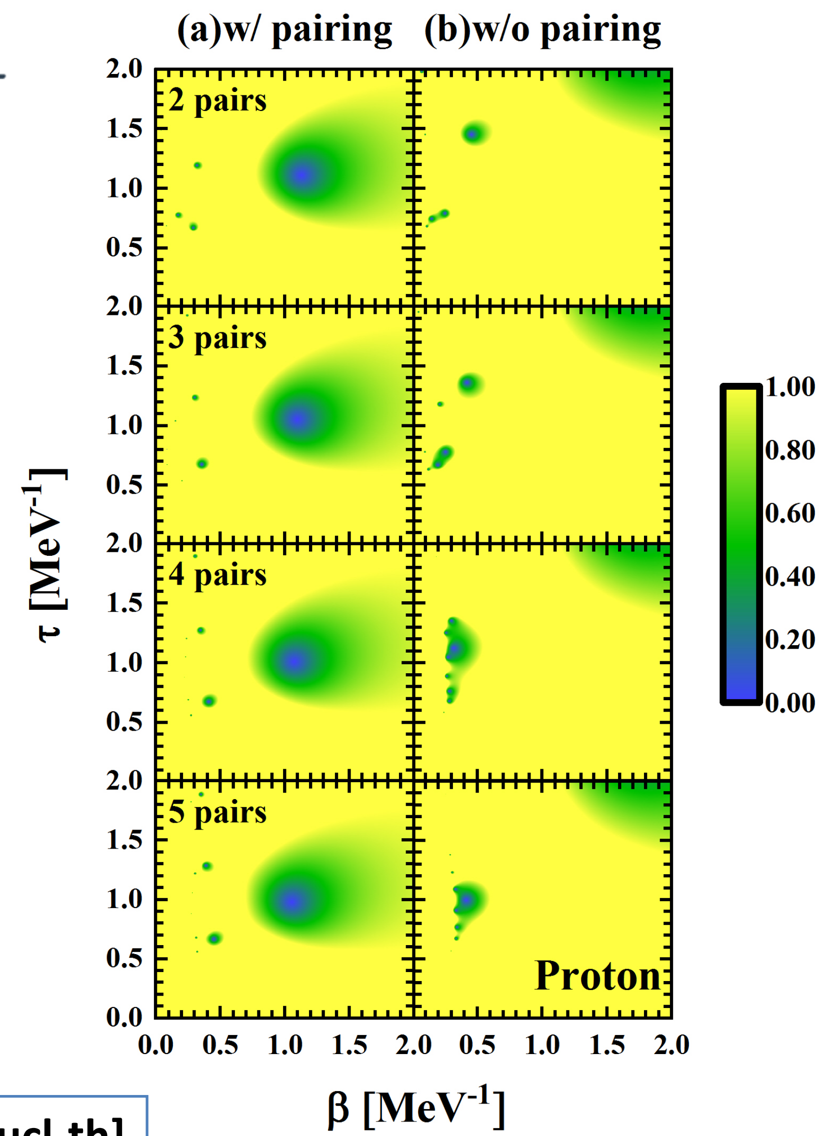
block s.p.e. from Fermi level one by one

The contour plots of the partition function



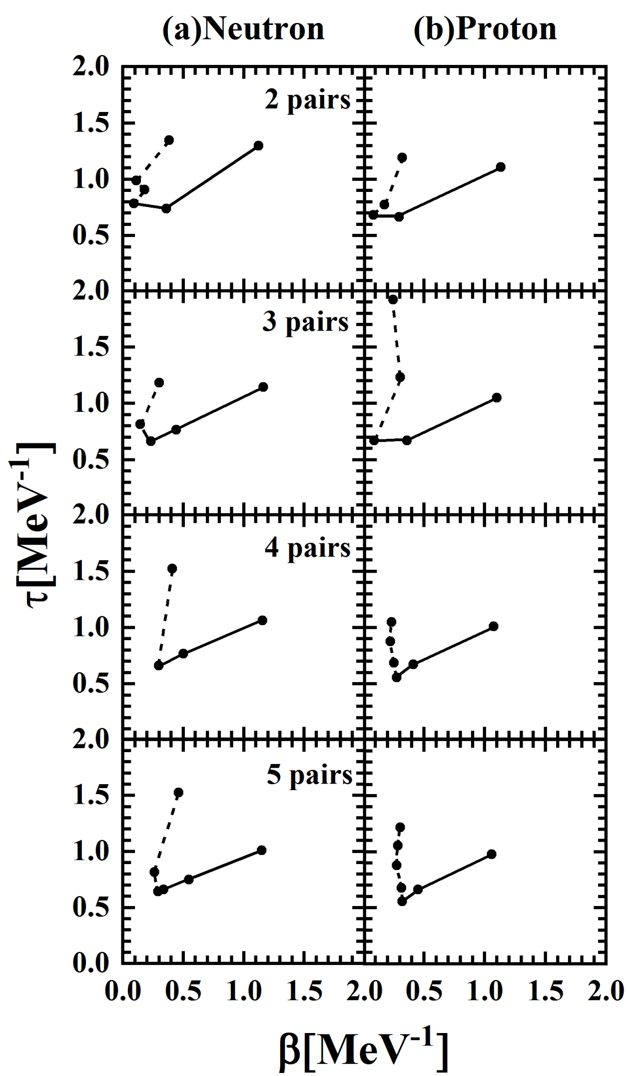
$$\mathcal{B} = \beta + i\tau$$

$$\beta = 1/T$$



arXiv:2303.09039 **[nucl-th]**

The DOZ of the partition function



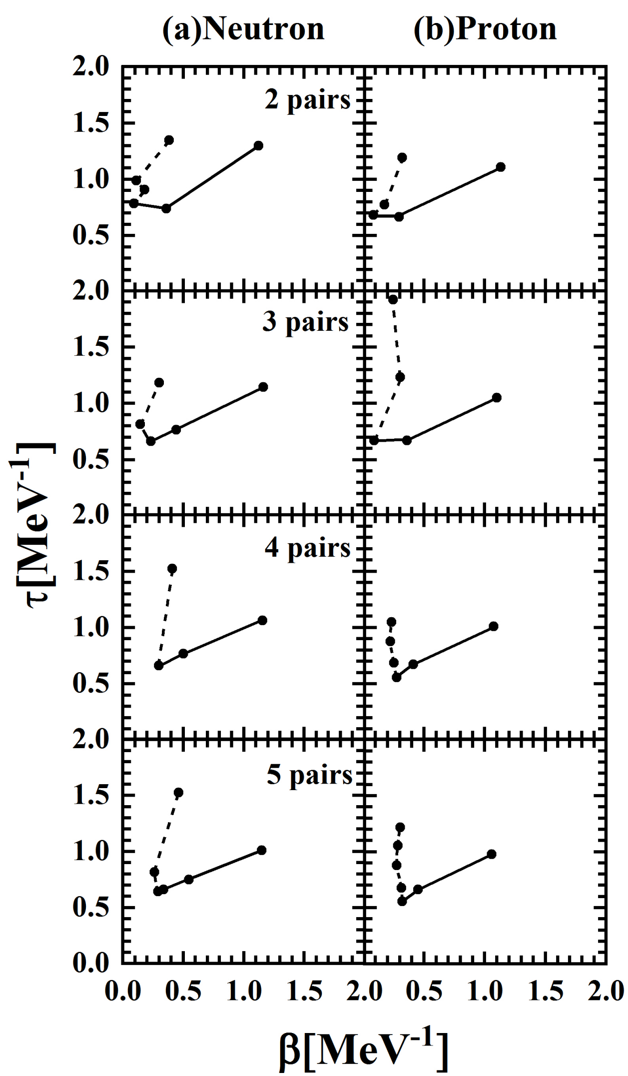
arXiv:2303.09039 [nucl-th]

√ **The dashed line** **quasiclassical phase**

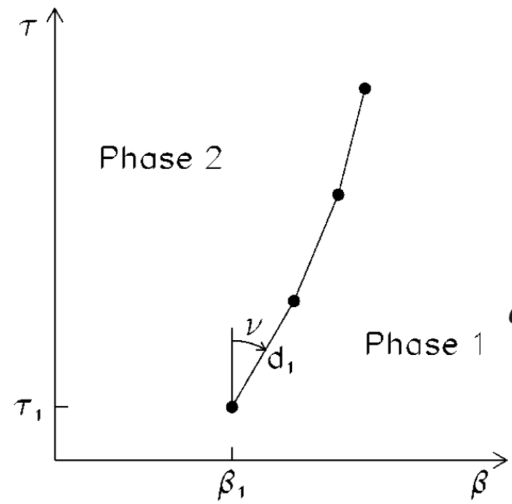
Phys. Rev. C **66**, 024322 (2002).

√ **The solid line** **represent the pairing phase transition.**

The DOZ of the partition function



arXiv:2303.09039 [nucl-th]



schematic diagram

$$\alpha = \frac{\ln \Phi(\tau_3) - \ln \Phi(\tau_2)}{\ln \tau_3 - \ln \tau_2}.$$

$$\Phi = \frac{1}{2}\left(\frac{1}{d_{j-1}} + \frac{1}{d_j}\right), \quad d_j = \sqrt{(\beta_{j+1} - \beta_j)^2 + (\tau_{j+1} - \tau_j)^2}.$$

$\alpha < 0$	first order
$0 < \alpha < 1$	second order
$\alpha > 1$	higher order

Phys. Rev. C **66**, 024322 (2002).

The DOZ of the partition function

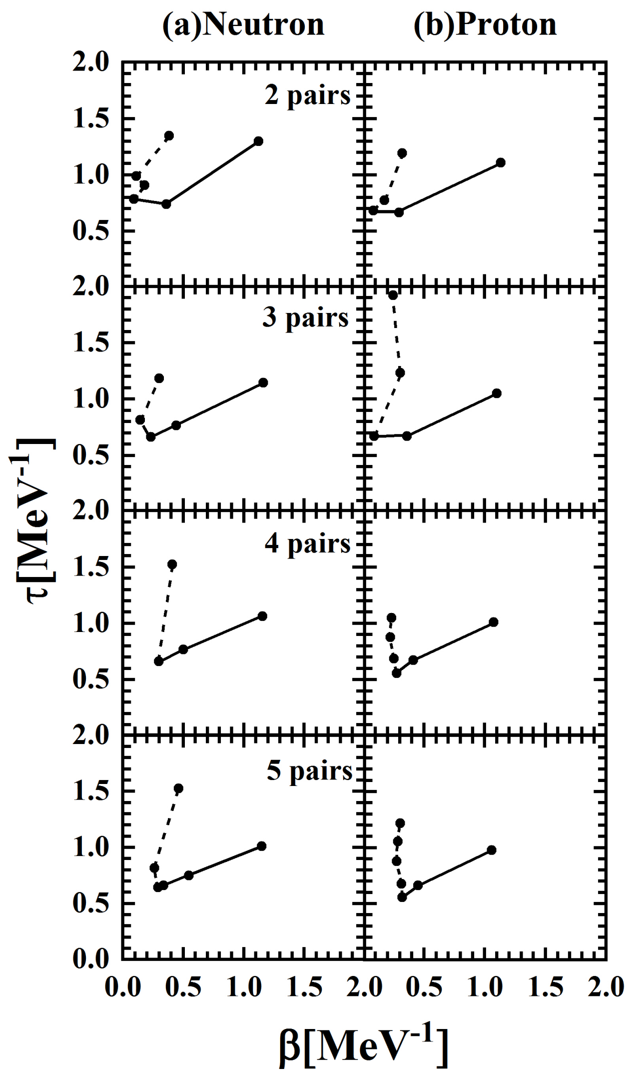


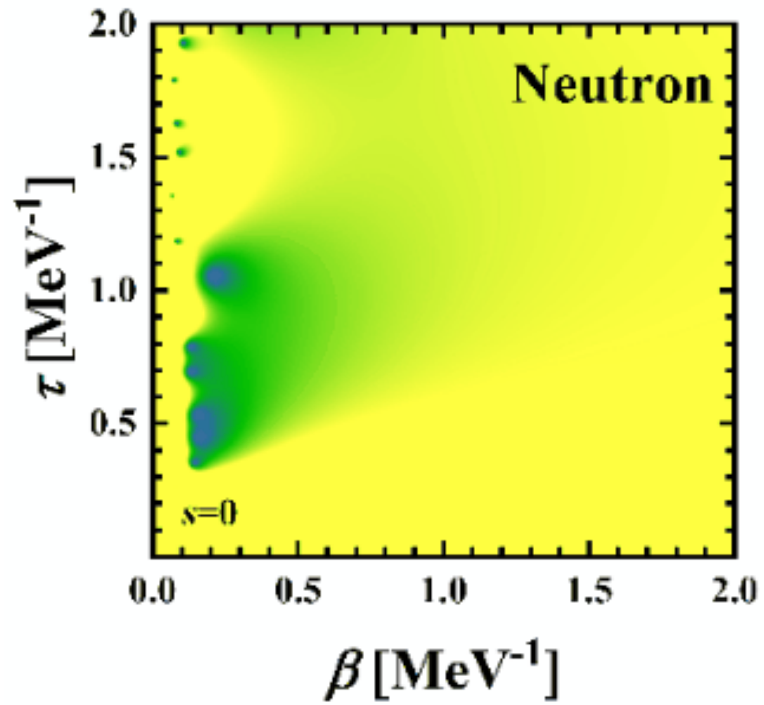
TABLE I. The value of α with 2, 3, 4, 5 pairs of neutrons and protons.

	2 pairs	3 pairs	4 pairs	5 pairs
neutron	α=-4.61	α=-4.31	α=-4.63	α=-4.74
proton	α=-5.5	α=-4.57	α=-4.55	α=-4.73

✓ **The solid line represent the pairing phase transition and the defined α indicates that this phase transition is a first order phase transition.**

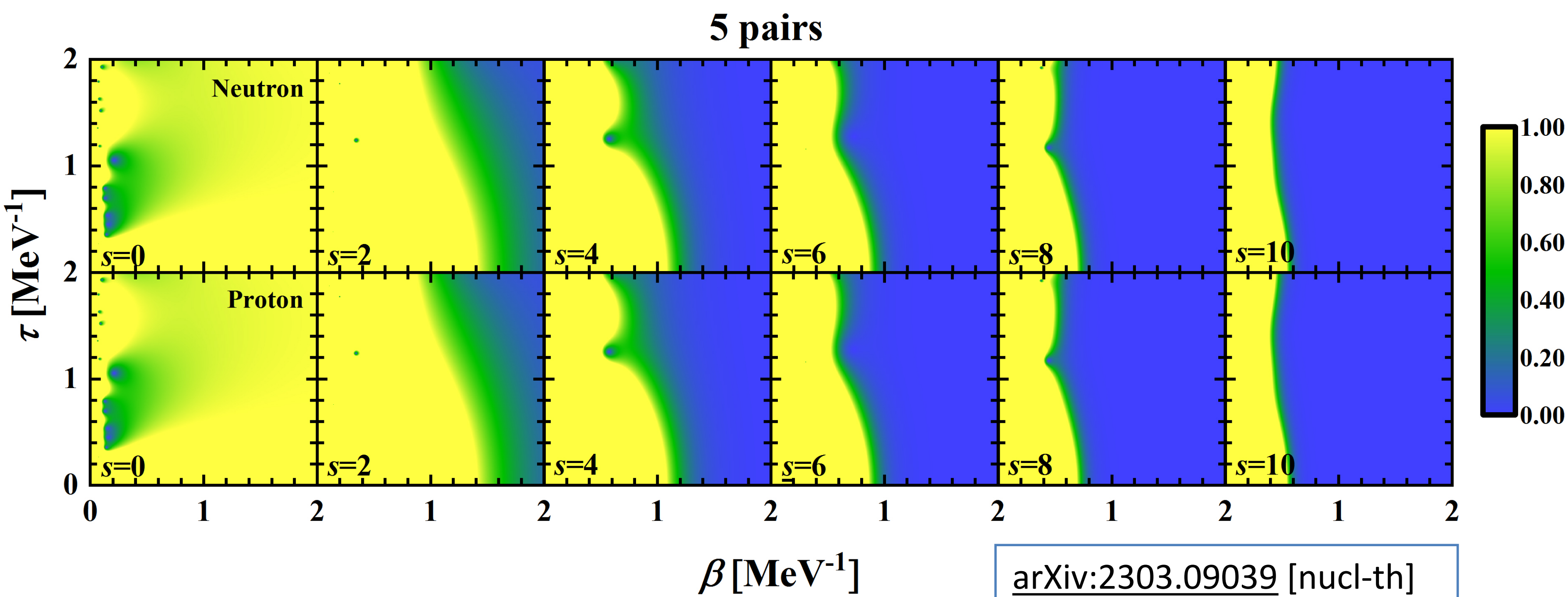
arXiv:2303.09039 [nucl-th]

Evolution of pairing phase transition



- ✓ s=0 (no pair broken) ✓ The nucleus is in **the superfluid phase;**
- ✓ s=2,4,6,8 ✓ **The normal and superfluid phases** coexist;
- ✓ s=10 (all pairs broken) ✓ The nucleus is entirely in **the normal phase.**

Evolution of pairing phase transition



arXiv:2303.09039 [nucl-th]

✓ *s*=0 (no pair broken) ✓ The nucleus is in the superfluid phase;

✓ *s*=2,4,6,8 ✓ The normal and superfluid phases coexist;

✓ *s*=10 (all pairs broken) ✓ The nucleus is entirely in the normal phase.

Outline

- Introduction
- Theoretical framework
- Numerical details
- Results and discussion
- Summary

Summary

- ☑ We address a strict particle number conserving calculation to investigate the properties of pairing correlations in hot nuclei with CDFT+SLAP framework.

- ☑ The clear "S" shape of C_V curves for neutrons and protons of ^{162}Dy are presented. seniority=2,4 states.

- ☑ The "S" shape of C_V for odd system is studied in terms of s.p.e and blocking effect.

- ☑ One calculates the negative values of α for this phase transition, indicating a first-order phase transition.

Thank you !

Collaborators:

Peking University : Peng-Wei Zhao

North China Electric Power University : Zhen-Hua Zhang

Jiangnan University : Yan Tao , Yan-Long Lin , Yu-Hang Gao

Institute of Physics and Nuclear Engineering: N. Sandulescu

Why complex temperature

correlation time, but some care is in order here. The time τ_i is not connected to a single system, but to an ensemble of infinitely many identical systems in a heat bath, with a Boltzmann distribution of initial states. Thus, the times

Phys. Rev. C **66**, 024322 (2002).

$$
\begin{aligned}
Z(\beta + i\tau) &= \mathrm{Tr}[\exp(-i\tau H)\exp(-\beta H)] \\
&= \langle \Psi_{\mathrm{can}} | \exp(-i\tau H) | \Psi_{\mathrm{can}} \rangle \\
&= \langle \Psi_{\mathrm{can}}(t=0) \mid \Psi_{\mathrm{can}}(t=\tau) \rangle
\end{aligned}
$$

A zero means the overlap of a time evoluted canonical state and the initial state vanishes.

The classification scheme for phase transition

1. Define the inverse complex temperature:

$$\mathcal{B} = \beta + i\tau$$

Where $\beta = 1/T$

2. Calculate the average inverse distance:

$$\Phi(\tilde{\tau}_j) = \frac{1}{d_j}$$

Where $\tilde{\tau}_j = (\tau_j + \tau_{j+1})/2,\ d_j = \sqrt{(\beta_{j+1} - \beta_j)^2 + (\tau_{j+1} - \tau_j)^2}$

3. Approximate the function:

$$\Phi(\tau_j) \propto \tau_j^{\alpha}$$

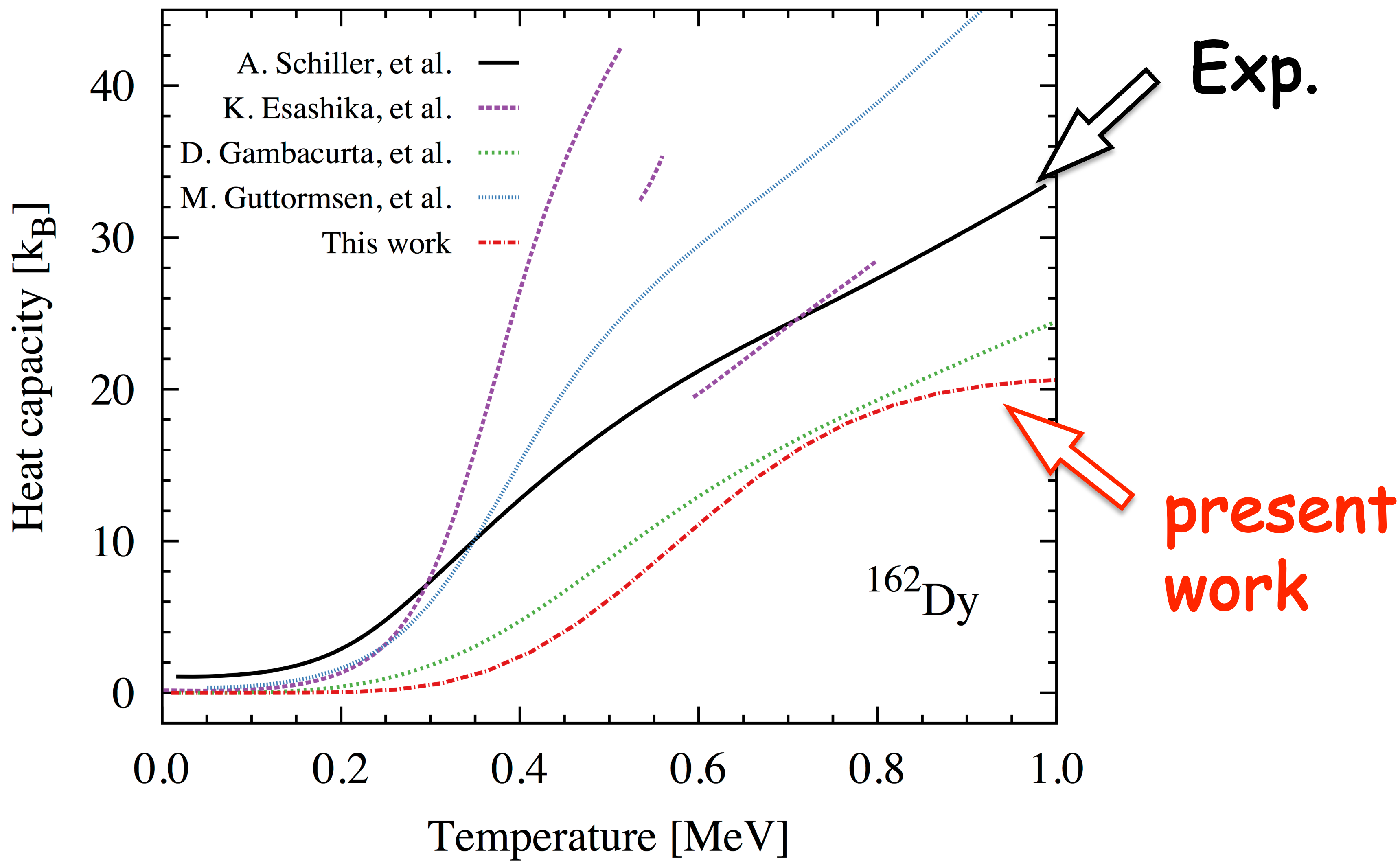
Then

$$\alpha = \frac{\ln \Phi(\tau_3) - \ln \Phi(\tau_2)}{\ln \tau_3 - \ln \tau_2}$$

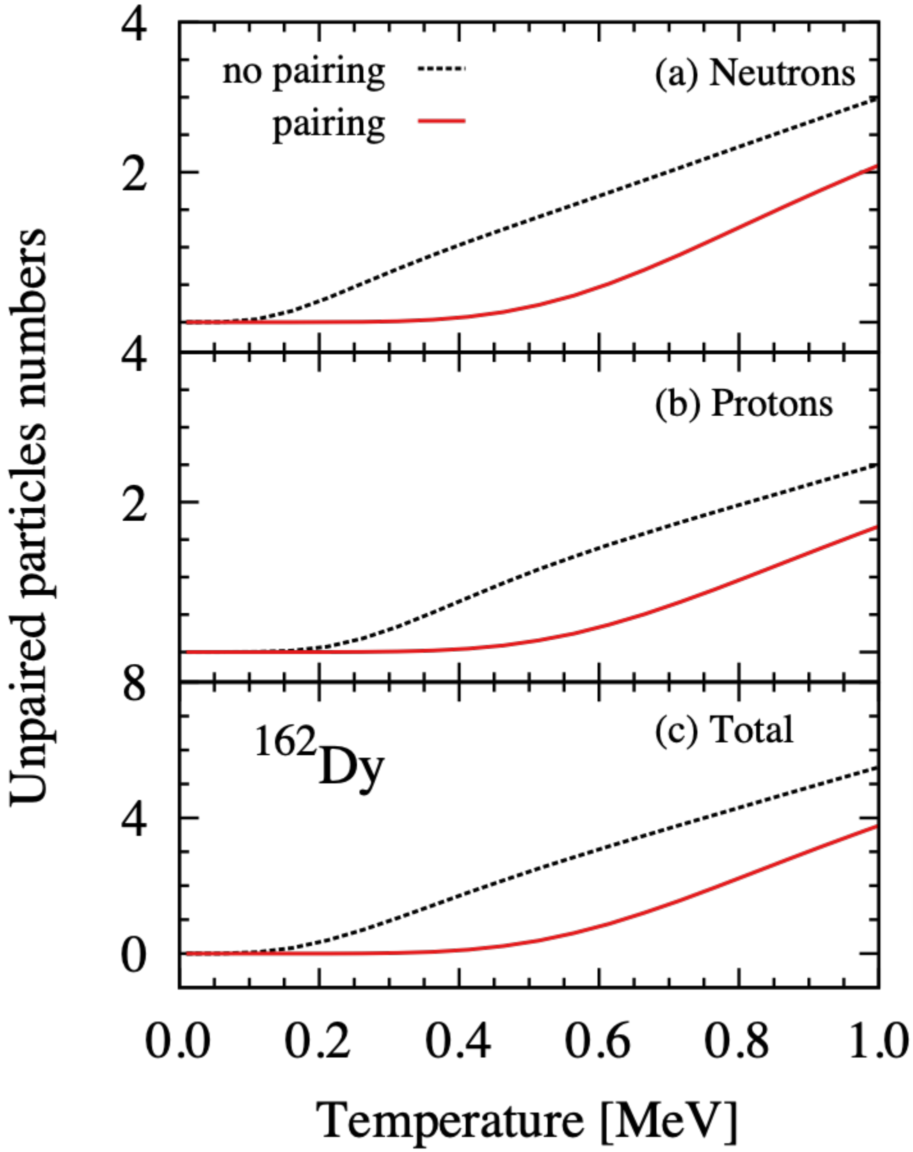
$$\begin{cases} \alpha < 0, & \textbf{first order} \\ 0 < \alpha < 1, & \textbf{second order} \\ 1 < \alpha, & \textbf{higher order} \end{cases}$$

A. Schiller, *et al.*, Phys. Rev. C 66, 024322(2002).

Comparison of Cv with Exp. and other calculations



Average unpaired numbers



Why "S" shape ?

Phase transition of pairing correlation ?

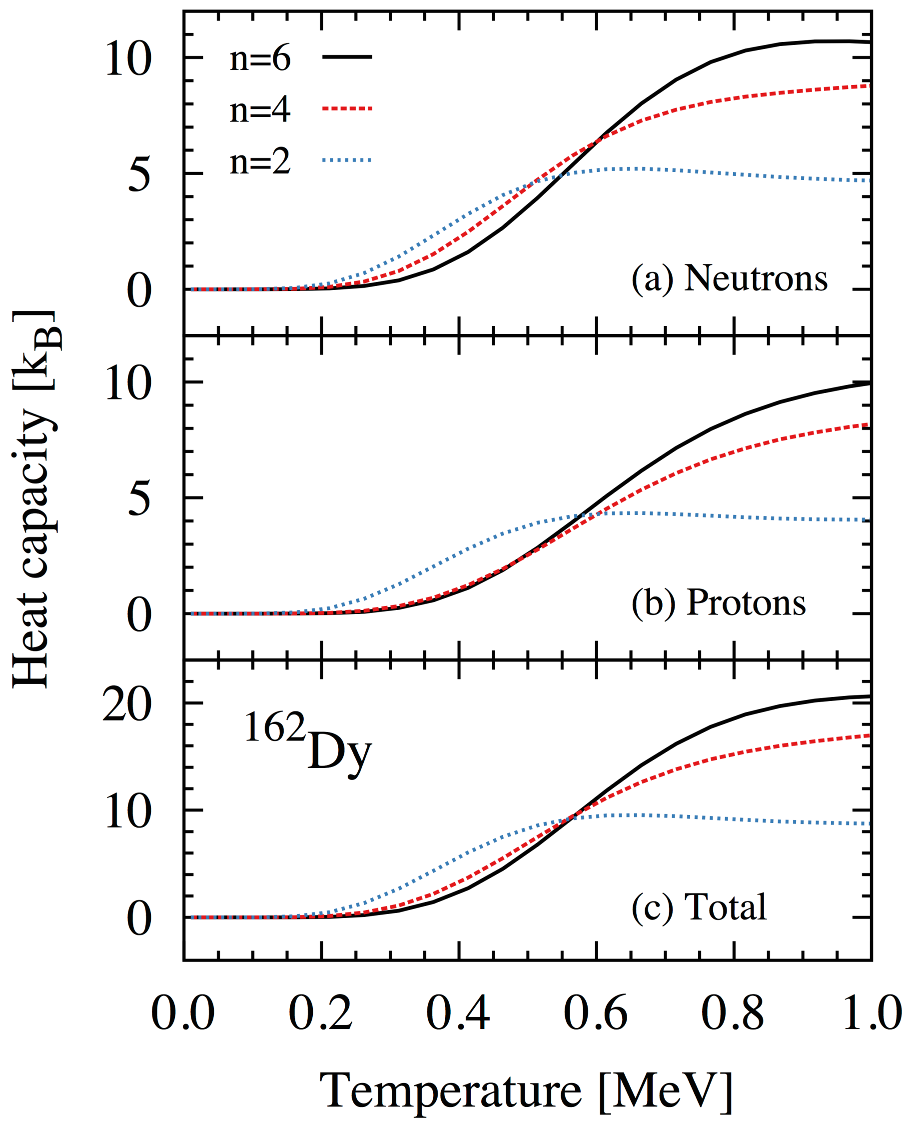
$$\langle s \rangle = Z^{-1} \sum_{m=0}^{\infty} s\, \rho(E_m)\, e^{-E_m/T}$$

s: seniority

- ✓ straight line w/o pairing;
- ✓ Low T (T<0.35 MeV) with pairing: fully paired;
- ✓ high T (T>0.35 MeV) with pairing: broken pairs,
- ✓ not all particles are broken.

no phase transition of pairing

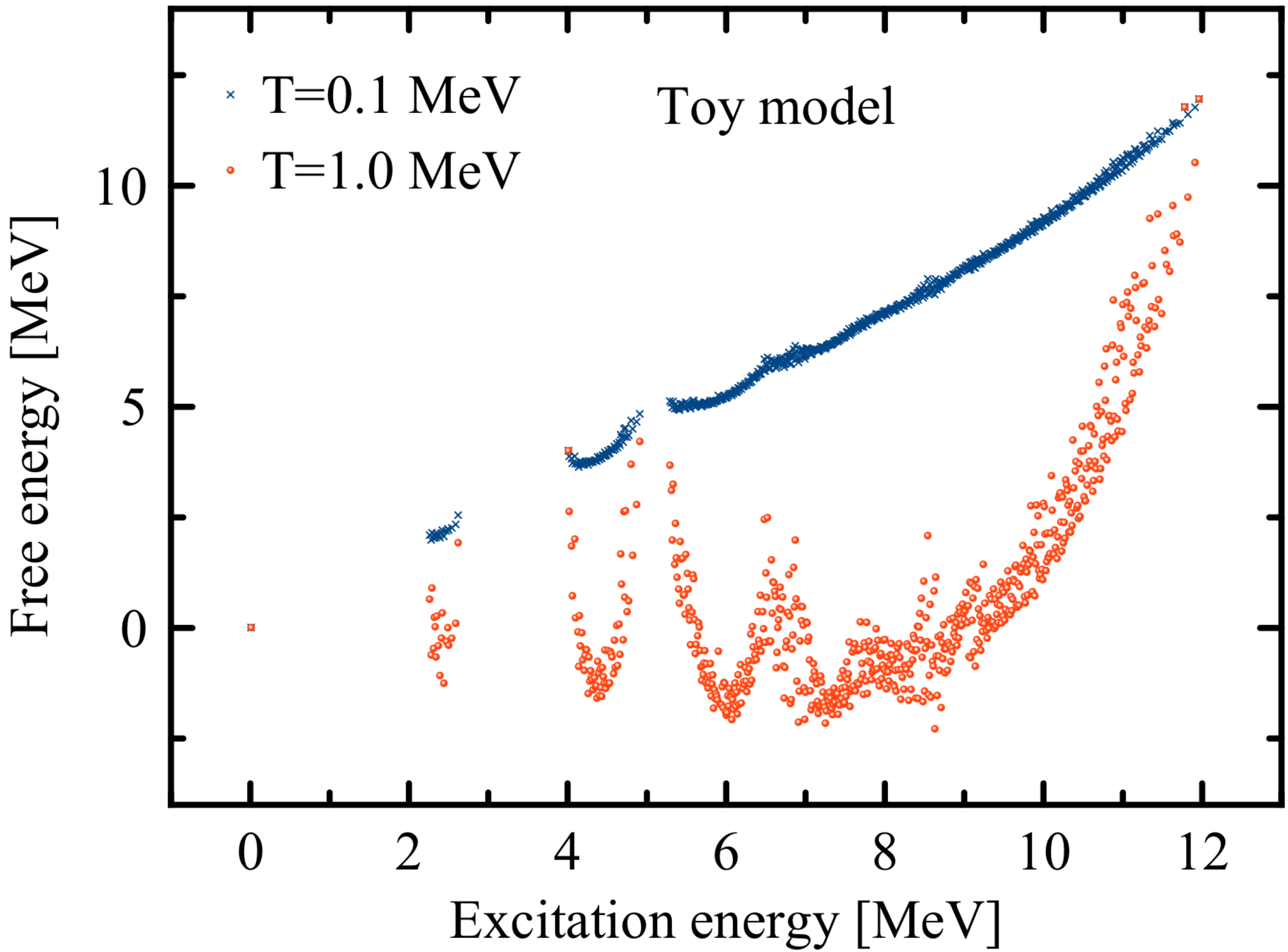
Number of particles dependence



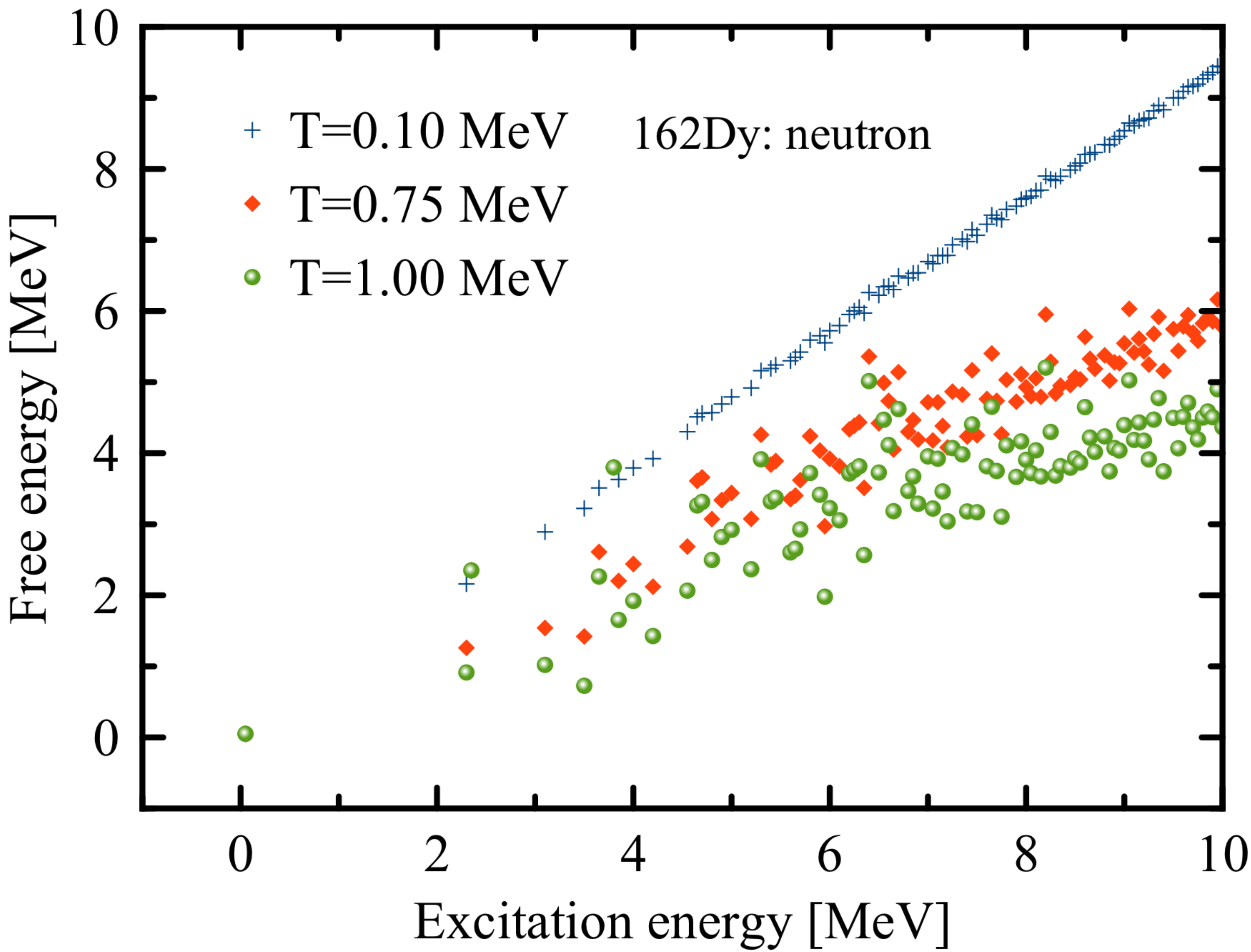
√ 12,8,4 particles (n=6,4,2) are included, respectively;

√ "S" shapes appear in all cases;

√ Values are different at high T;

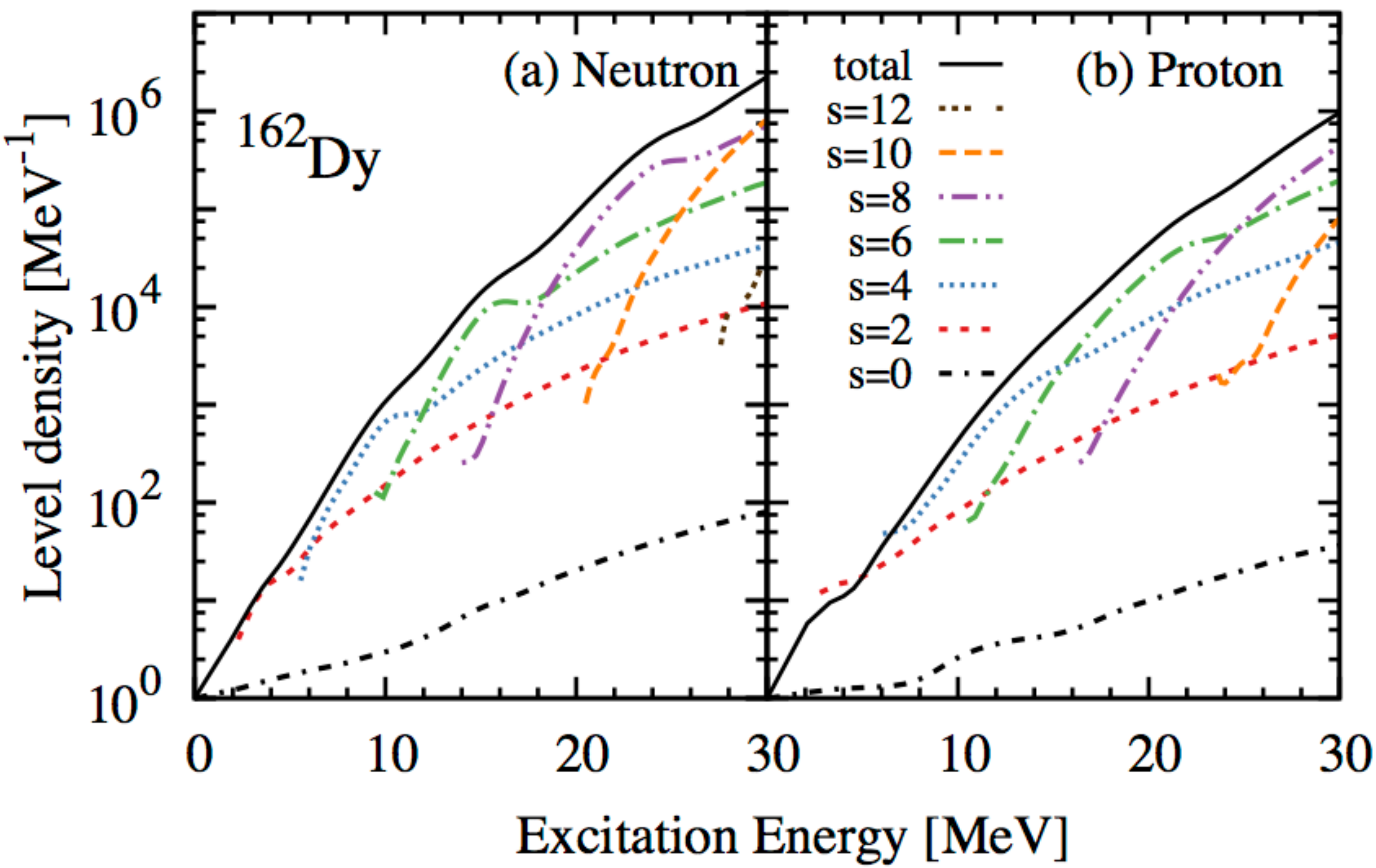


T=0.1 MeV
T=1.0 MeV
Toy model
Free energy [MeV]
Excitation energy [MeV]
0
5
10
0
2
4
6
8
10
12

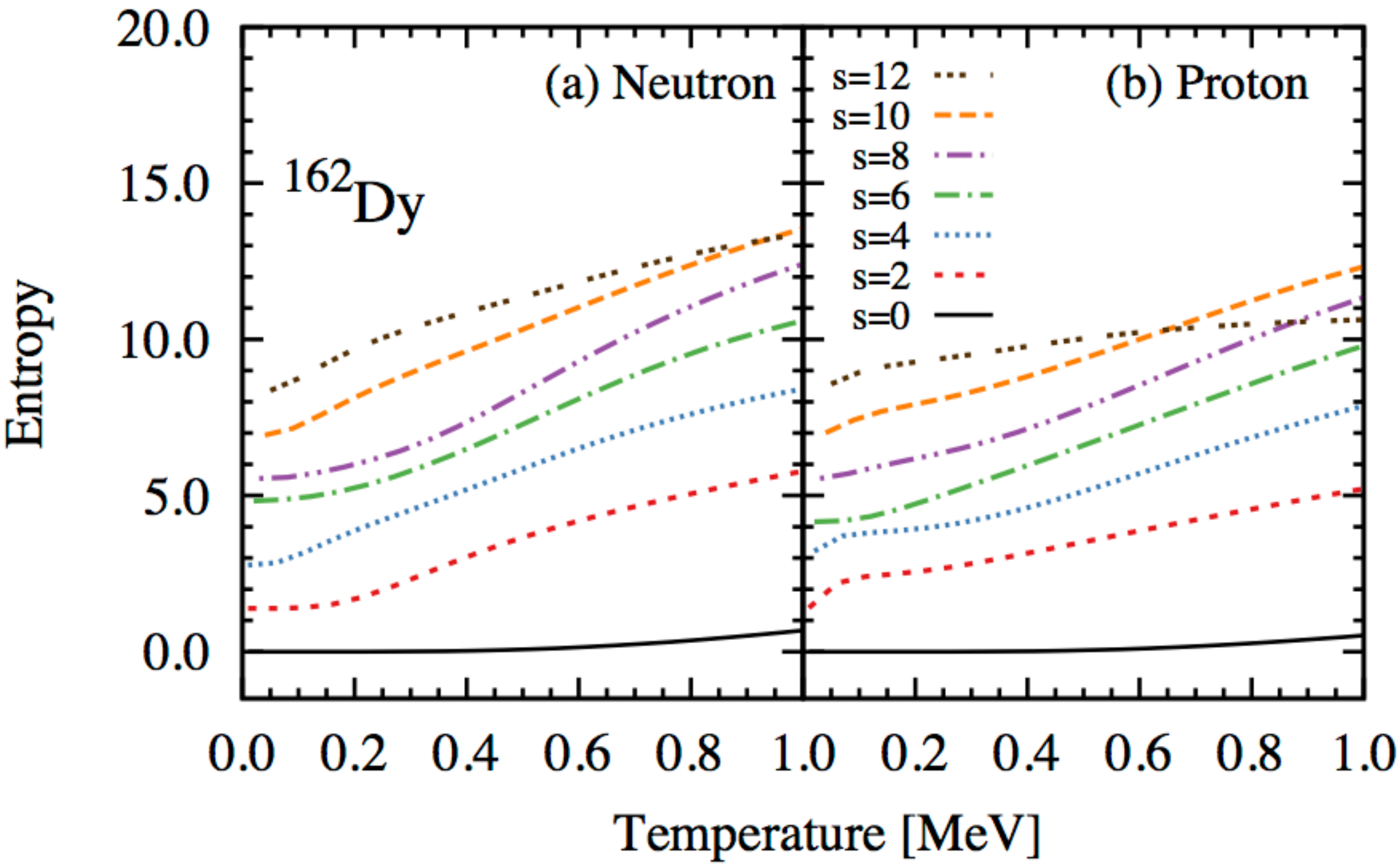


T=0.10 MeV
T=0.75 MeV
T=1.00 MeV
162Dy: neutron
Free energy [MeV]
Excitation energy [MeV]
0
2
4
6
8
10

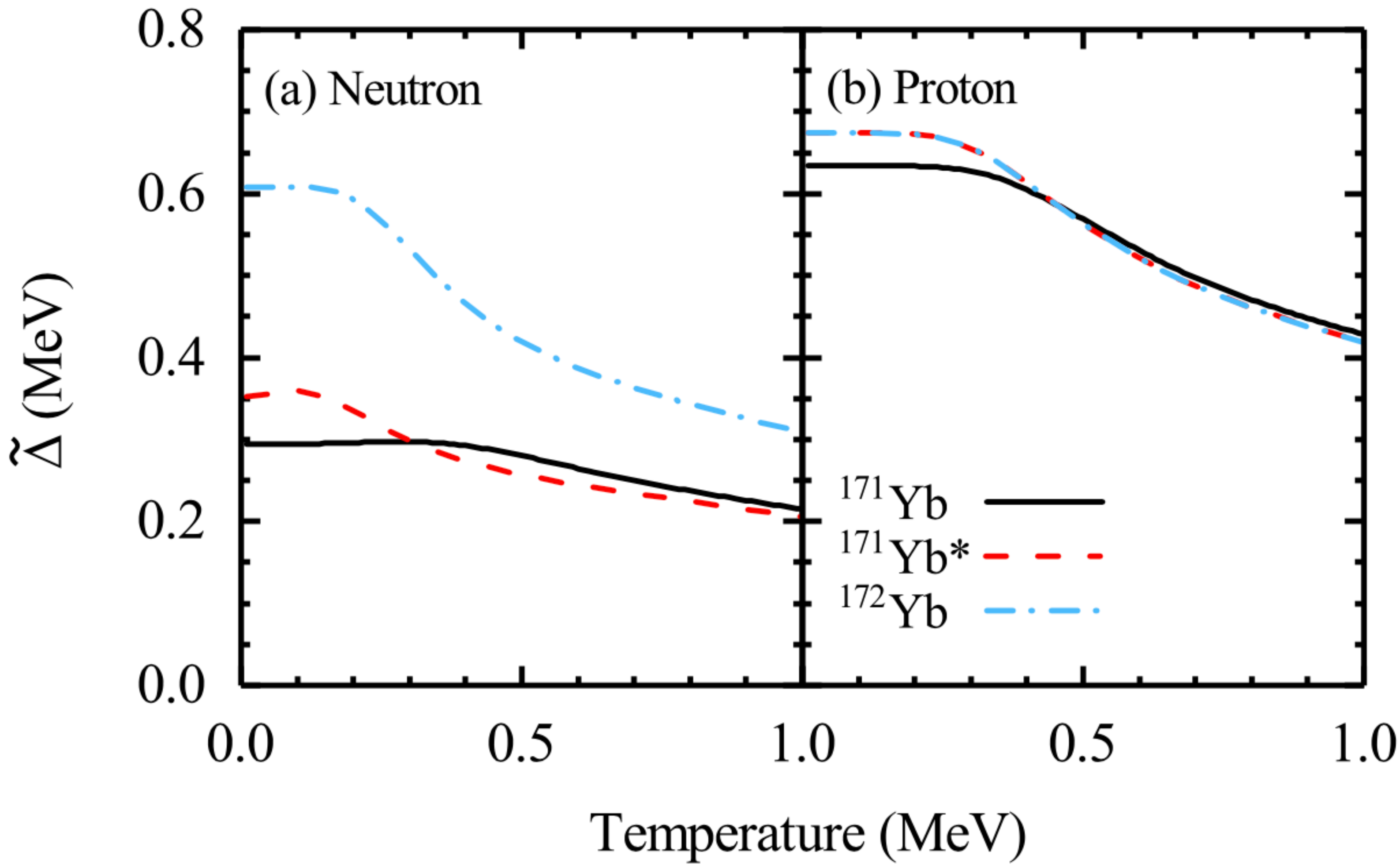
Level density



Entropy



(a) Neutron
(b) Proton
162Dy
s=12
s=10
s=8
s=6
s=4
s=2
s=0
Entropy
20.0
15.0
10.0
5.0
0.0
0.0 0.2 0.4 0.6 0.8 1.0 0.2 0.4 0.6 0.8 1.0
Temperature [MeV]



(a) Neutron
(b) Proton
$\tilde{\Delta}$ (MeV)
0.8
0.6
0.4
0.2
0.0
0.0
0.5
1.0
0.5
1.0
Temperature (MeV)
^{171}Yb
^{171}Yb*
^{172}Yb