Microscopic approaches to nuclear level densities

(核準位密度に対する微視的アプローチ)

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@ RIKEN (Sep. 25, 2008)

Contents :

I. Introduction

Nuclear level densities (↔ **partition fn.**)

— **one of the key inputs**

in calculations of nuclear-astrophysics

for $A(a,b)B$ **reaction** $\sigma_{(a,b)} \propto \sum_{J_f\pi_f} \int dE_f\, T^{(a)}_{J_i\pi_i}(E_i)\, T^{(b)}_{J_f\pi_f}(E_f)\, \rho_{J_f\pi_f}(E_f)$

↔ **Hauser-Feshbach formula**

$T^{(a/b)}_{J\pi}(E)$ **: transmission coefficient from compound state**

$\rho_{J\pi}(E)$ **: level density**

e.g. s**- &** r**-processes** $\cdots$ (n,γ) ***vs.*** β**-decay**

$\sigma_{(n,\gamma)} \quad \leftarrow \quad (a=n,\ b=\gamma)$

$E_i = E_f + E_\gamma - S_n \quad (\rightarrow E_f \lesssim S_n)$

rp**-process** $\cdots$ (p,γ) ***vs.*** β**-decay**

Experimental methods to measure nuclear level densities

1. **Direct counting of levels — lowest-lying states or light nuclei** ($E_x \lesssim 2-3\,\mathrm{MeV}$)

2. **Level spacing among neutron resonances** ($\rho = \bar{D}^{-1}$)
   — small energy range around $E_x = S_n \sim 8\,\mathrm{MeV}$**, restricted to** s**-wave**

3. **Ericson fluctuation —** $E_x \sim 20\,\mathrm{MeV}$

4. **Charged particle reactions (← reaction model)**

5. **'Oslo method'** $\cdots$ γ**-ray matrix** $P(E_x, E_\gamma) = C(E_x)\,F(E_\gamma)\,\rho(E_x - E_\gamma)$
   (← Brink-Axel hypothesis)

   Refs.: T. S. Tveter *et al.*, Phys. Rev. Lett. 77, 2404 ('96)
   E. Melby *et al.*, Phys. Rev. Lett. 83, 3150 ('99)
   A. Schiller *et al.*, Phys. Rev. C 61, 044324 ('00)
   M. Guttormsen *et al.*, Phys. Rev. C 62, 024306 ('00)

   — $E_x \sim 3-7\,\mathrm{MeV}$

II. Phenomenology (→ Why microscopic ?)

Conventional approach to nuclear level densities

★ **Backshifted Bethe's formula** (← Fermi-gas model)

$$\rho(E_x) = \frac{\sqrt{\pi}}{12} a^{-1/4} (E_x - \Delta)^{-5/4} \exp\left[2\sqrt{a(E_x - \Delta)}\right] \qquad \text{(for state density)}$$

$\cdots$ **fits well to experimental data (except at very low E_x),**
if the parameter a (& Δ) is adjusted

(Δ : backshift ↔ pairing & shell effects)

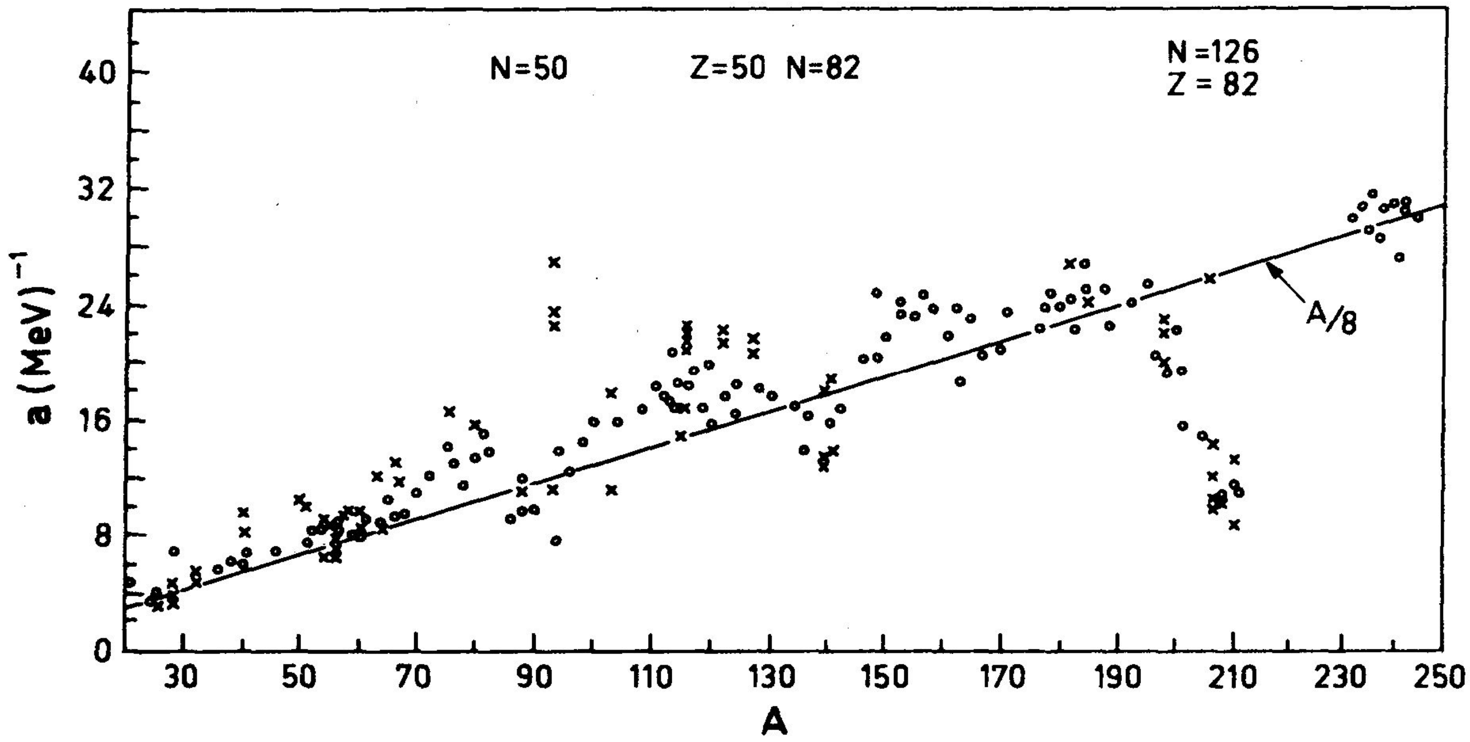
$$\rho_{J,\pi}(E_x) = \rho(E_x)\,\frac{2J+1}{4\sqrt{2\pi}\sigma^3} \exp\left[-J(J+1)/2\sigma^2\right] ; \qquad \sigma = \mathcal{I}\sqrt{(E_x - \Delta)/a}$$

$$\left(\rho(E_x) = \sum_{J,\pi} (2J+1)\, \rho_{J,\pi}(E_x)\right)$$

However, **1)** $a = A/6 \sim A/10\,\mathrm{MeV}^{-1}$,
in contrast to the Fermi-gas prediction $a \approx A/15$

2) a **: nucleus-dependent (not only A-dependent)**
— shell effects, *etc.*

fitted values of a:



Ref.: Bohr & Mottelson, vol. 1

Note: 10% **change in** a $\rightarrow$ **change in** $\rho(E_x)$ **by greater than factor** 10**!**

(for $A \sim 150,\ E_x \sim 8\,\mathrm{MeV}$**)**

For better E_x-dep. — **correction for low E_x part**

★ **Constant-T formula** ($\leftrightarrow$ T-dep. of pairing)

$$\rho(E_x) \propto \exp[(E_x - E_1)/T_1] \quad \text{for } E_x < E_M$$

$\rightarrow$ **matching to BBF at $E_x = E_M$**

To get less A-dep. parameters — **nucl.-dep. corrections**

★ $a \rightarrow E_x$**-dep.** : $a(E_x) = \tilde{a}\left(1 + \delta W \dfrac{1 - \exp[-\gamma(E_x - \Delta)]}{E_x - \Delta}\right)$

δW : **shell correction energy,** $\gamma = \gamma_1 A^{-1/3}$

★ **Collective enhancement factor** $K_{\rm vib}(E_x)$, $K_{\rm rot}(E_x)$

$$\textit{e.g.}\quad K_{\rm rot}(E_x) = \max\left(\left[0.01389 A^{5/3}\left(1 + \frac{\beta_2}{3}\right)\sqrt{\frac{E_x - \Delta}{a}} - 1\right] \frac{1}{1 + \exp(\frac{E_x - E_c}{d_c})} + 1, 1\right)$$

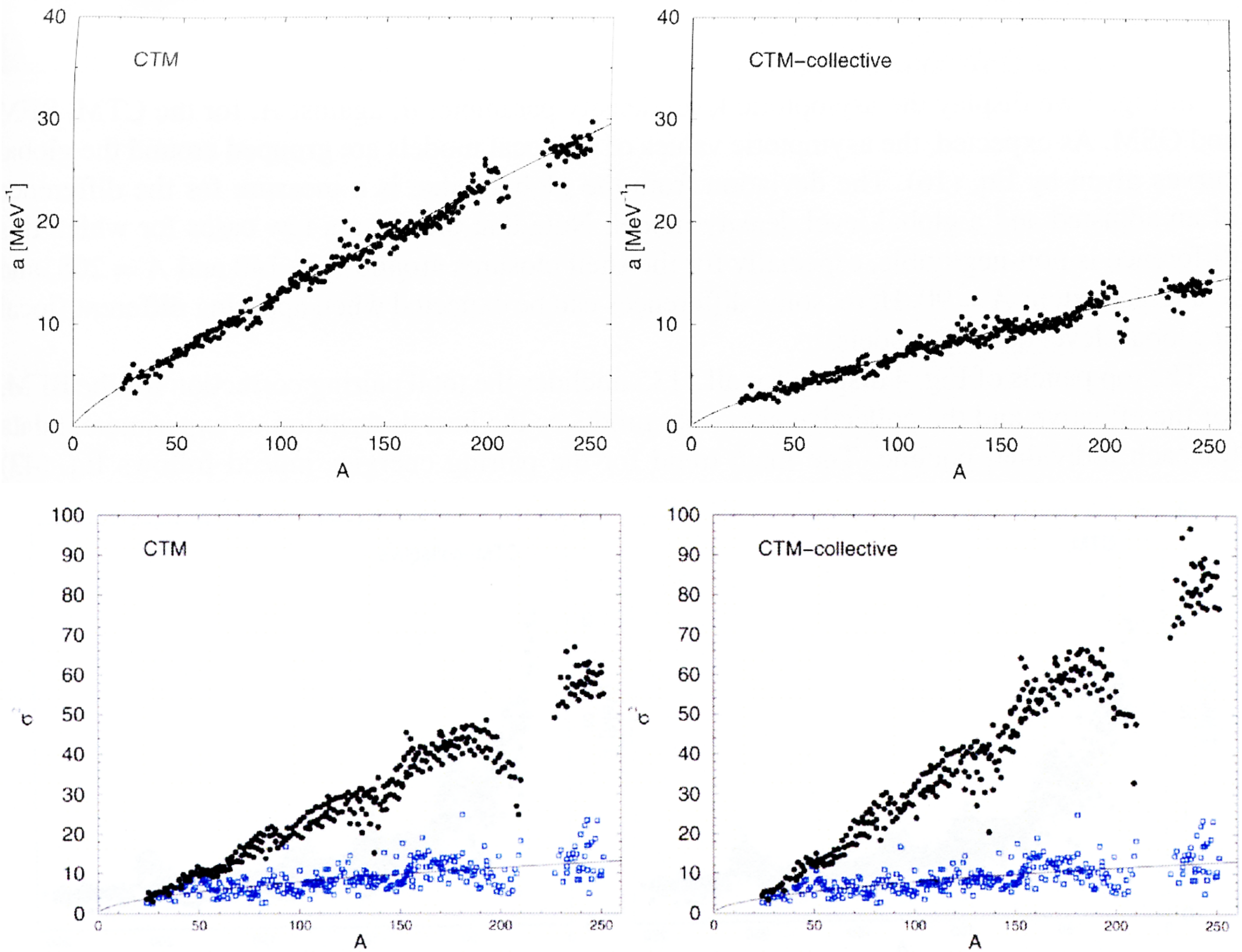
$\rightarrow$ **can be harmonious with $a \approx A/15\,\mathrm{MeV}^{-1}$ (Fermi-gas value)**

- **many corrections & parameters introduced**

  — **origin ? estimate ? (physics ?)**

- **significant nucleus-dependence still remains**

  e.g. **for $\tilde{a}$(: "asymptotic value" of a) & σ**



Ref.: A. J. Koning *et al.*, Nucl. Phys. A810, 13 ('08)

$\Longrightarrow$ **It has been difficult to predict nuclear level densities to good accuracy**

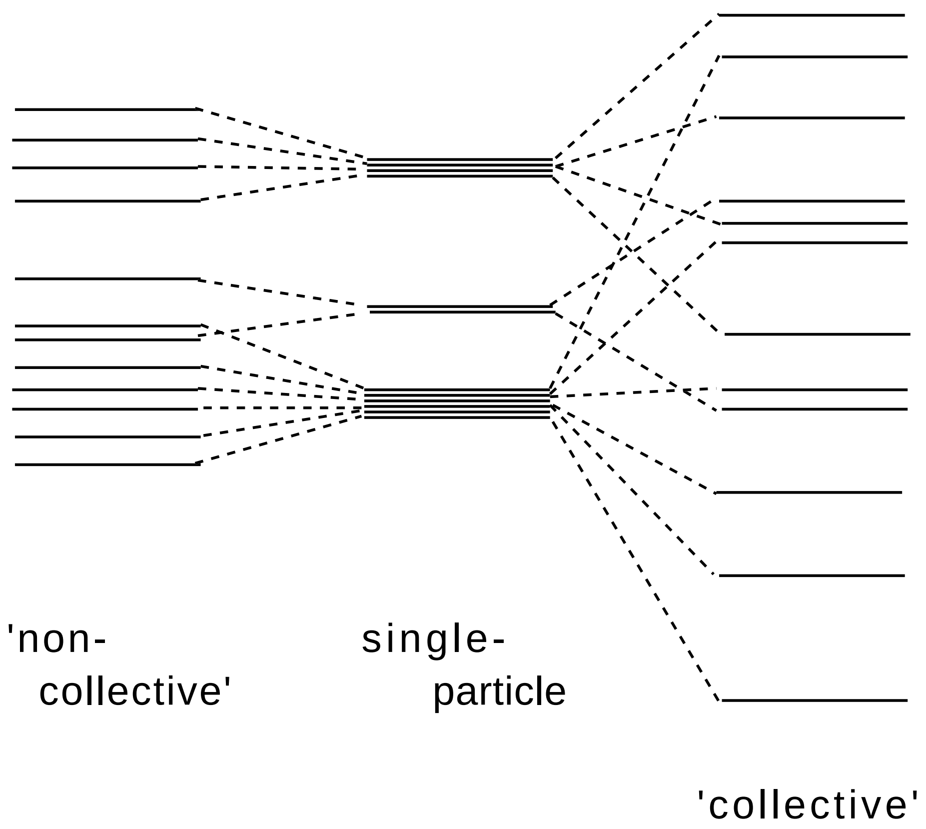
III. Microscopic approaches

What is needed ?

(1) shell effects (2) 'collective' 2-body correlations

e.g. $V = -\frac{\kappa}{2}\,\hat{\rho}^2$ **(**$\hat{\rho}$ **: 1-body op.)**

typically, κ **: large** $\leftrightarrow$ **collective**



Why microscopic ?

- deeper understanding
- fewer parameters (in Hamiltonian) $\}$ → $\{$ good accuracy
- direct cal. of $\rho(E_x)$ (not via BBF) $\}$ → $\{$ proper nucleus-dependence

What is "microscopic" ? ··· starting from NN (shell model) int.

A) microscopic s.p. model → $\{$ evaluation of (BBF) parameters; combinatorial counting

— not really microscopic ***e.g.*** needs phen. $K_{\rm vib}(E_x)$, $K_{\rm rot}(E_x)$

B) NN int. → dist. of levels in terms of moments (J. B. French *et al.*)

— works well in certain cases

- ∘ g.s. energy ? → exponential convergence (M. Horoi *et al.*)
- ∘ influence of phase transition ? deformed nuclei ?

C) full shell model — exact treatment of int. ···desirable !

→ (1) shell effects & (2) 2-body correlations
are fully taken into account within the model space

— large model space required
⟶ shell model Monte Carlo (SMMC) (H.N. & Y. Alhassid)

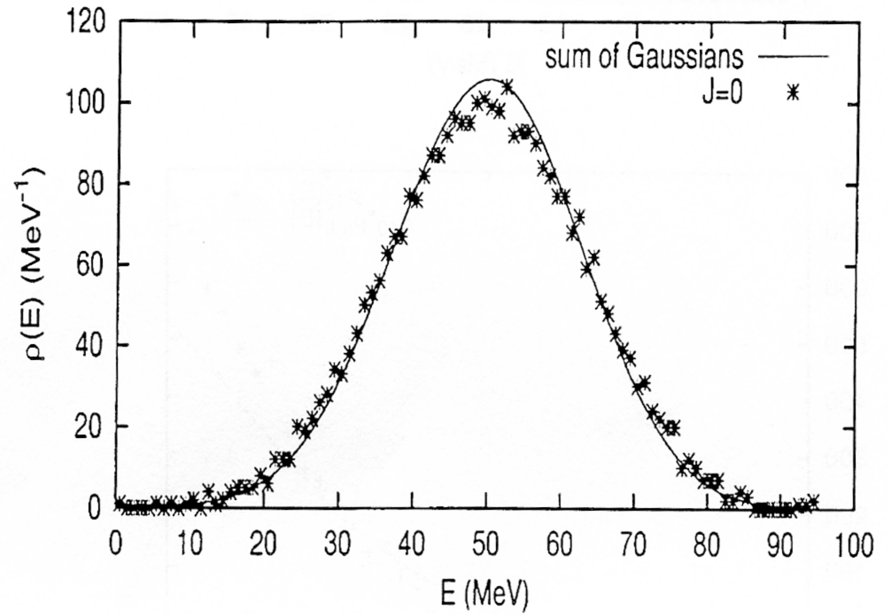
Moment method (spectral averaging method) $\leftarrow$ **shell model picture**

for each shell model config. $[m]$

$$M_\nu([m]) = \frac{1}{d_{[m]}} \mathrm{Tr}_{[m]}(H^\nu) \longrightarrow \rho_{[m]}(E) \longrightarrow \rho(E) = \sum_{[m]} d_{[m]}\, \rho_{[m]}(E)$$

(J,π specified $\rightarrow \rho_{J,\pi}(E)$)

$\rho(E) \longrightarrow \rho(E_x)$; $\quad E_x = E - E_0 \quad$ (E_0 : g.s. energy $\leftarrow$ separate estimate)



^{28}Si (?), $J = 0$ levels
within sd-shell config.

Ref. : M. Horoi *et al.*,
P.R.C 67, 054309 ('03)

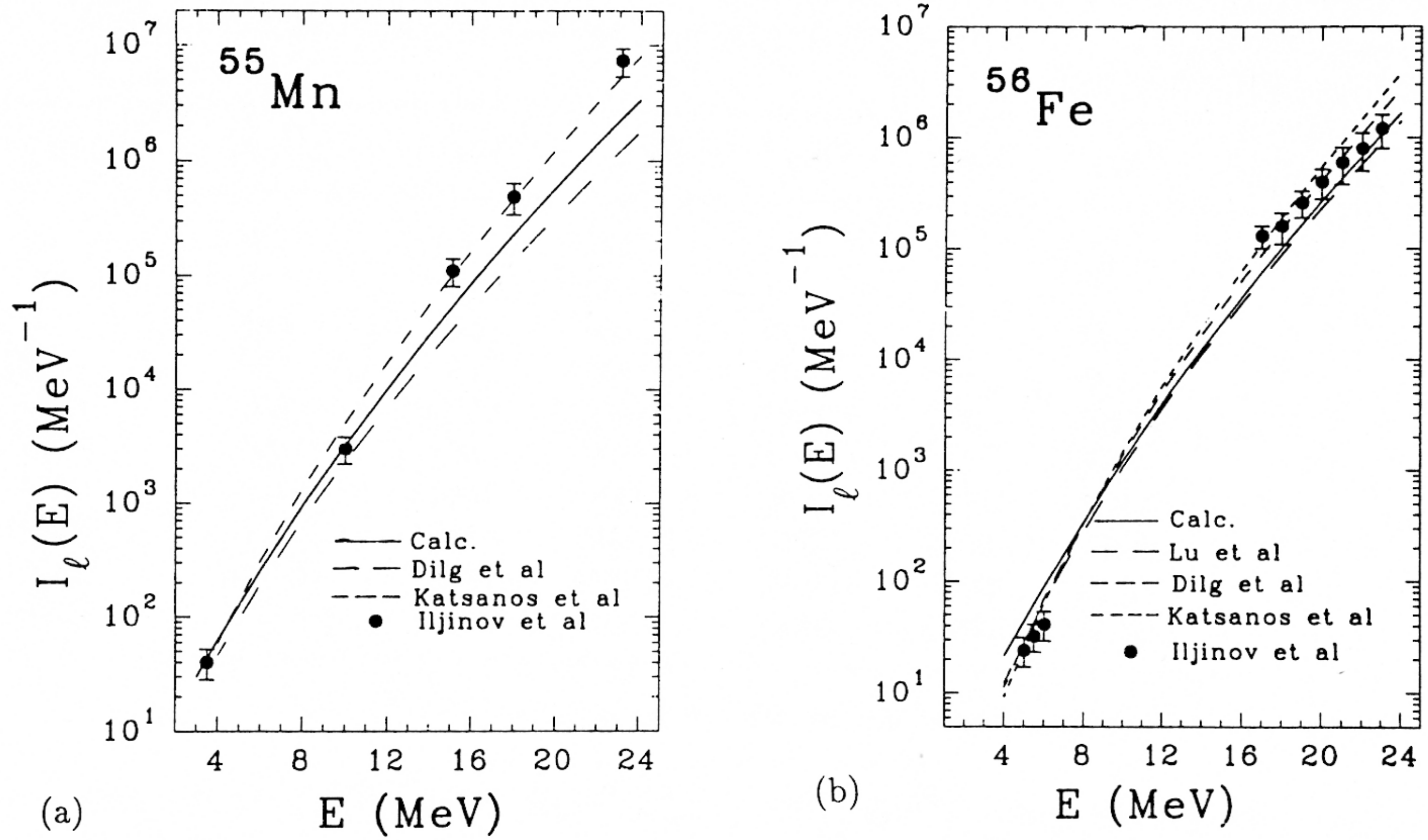
- **meaningful comparison in linear scale !**

cf. comparison of a (& Δ)

- model space $\rightarrow$ physical only at low-energy ($E_x \lesssim 20\,\mathrm{MeV}$)

Level density by moment method

pf**-shell nuclei** $\leftarrow sd + pf + 0g_{9/2}$**-shell, SDI,** $\nu \leq 4$



Ref.: V. K. B. Kota & D. Majumdar, N.P. A604, 129 ('96)

$\cdots$ seems good for nearly spherical nuclei

for well-deformed nuclei? — **no justification (needs test)**

IV. Brief survey of SMMC

'**Nuclear temperature**' $\leftrightarrow$ **(average) excitation energy**

$\rightarrow$ **finite-T formalism** $\left\{ \begin{array}{l} \textbf{Fermi gas} \rightarrow \textbf{BBF} \\ \textbf{MF} \\ \textbf{SMMC} \end{array} \right.$ $\begin{array}{l} \cdots \textbf{grand-can. ens.} \\ \cdots \textbf{can. ens.} \end{array}$

$\rightarrow$ **statistical properties** — **thermodynamics in finite systems**

state density **partition fn.**

$$\rho(E) = \mathrm{Tr}\,\delta(E - H) \quad \longleftrightarrow \quad Z(\beta) = \mathrm{Tr}(e^{-\beta H}) = \int dE\, \rho(E) e^{-\beta E}$$

Laplace transform. (Tr : **can. trace**)

saddle-point approx. ($\leftrightarrow$ **smoothening for** E**, nuclear temp.**)

$$\rightarrow \rho(E) \approx \frac{e^S}{\sqrt{2\pi\beta^{-2}C}}\,; \quad S = \beta E + \ln Z(\beta), \;\; \beta^{-2}C = -\frac{dE}{d\beta}$$

(S : **entropy**, C : **heat capacity**)

cf. grand-can. $\cdots$ $\rho_{\rm gc}(E) \approx \dfrac{e^{S_{\rm gc}}}{\sqrt{(2\pi)^3(\varDelta N_p)^2(\varDelta N_n)^2\beta^{-2}C_{\rm gc}}}$ $\rightarrow$ **nucl.-dep. ?**

SMMC $\rightarrow$ **evaluate** $\langle\mathcal{O}\rangle_\beta = \mathrm{Tr}(\mathcal{O}e^{-\beta H})/Z(\beta)$ **(*e.g.*** $E(\beta) = \langle H\rangle_\beta$**)**

H **: shell model Hamiltonian (1- + 2-body)**

$e^{-\beta H}$ $\rightarrow$ **auxiliary-fields** **(**$\sigma_\alpha(\tau)$**)** **path integral rep.**

- **2-body int.** $\rightarrow$ **Pandya transform.**
- $e^{-\beta H}$ **: Suzuki-Trotter decomp.**
  $\rightarrow$ **Hubbard-Stratonovich transform.**

MC sampling $\sigma_k = \{\sigma_\alpha(\tau)\}_k \rightarrow \langle\mathcal{O}\rangle_\beta \approx \frac{1}{N_k}\sum_k \langle\mathcal{O}\rangle_{\sigma_k}$ **(with stat. error)**

- **advantage : easier to handle large model space**
  ($\because$ $\sigma_\alpha(\tau) \leftrightarrow$ **"mean-field"**)
- **finite-**T **method** $\rightarrow$ **suitable for statistical properties**
  (but not for distinguishing discrete levels)
- **conservation laws** $\rightarrow$ **projections** **(**(Z, N)**,** π**,** J**,** ***etc.*****)**
- $E_0 = \lim_{\beta\rightarrow\infty}\langle H\rangle_\beta$ $\cdots$ **evaluated also by SMMC**
- **disadvantage : sign problem**
  — propagator $\mathrm{Tr}(e^{-\beta h(\sigma_k)})$ **: not necessarily positive-definite**

dominant part of nuclear int. — sign good !

V. SMMC level densities

★ **Nuclei around Fe-Ni region**

- **setup**

  model space : **full** $pf + 0g_{9/2}$

  Hamiltonian : **s.p. energy** $\leftarrow$ **W-S pot.**

  int. $\begin{cases} T = 1 \textbf{ monopole pairing} \\ \quad \textbf{strength} \leftarrow \textbf{even-odd mass difference} \\ T = 0 \textbf{ surface-peaked multipole } (\lambda = 2, 3, 4) \\ \quad \textbf{strength} \leftarrow \textbf{self-consistency + renorm.} \\ \quad \textbf{renorm. factor} \leftarrow \textbf{realistic int.} \end{cases}$

  no adjustable parameters !

- **applications**

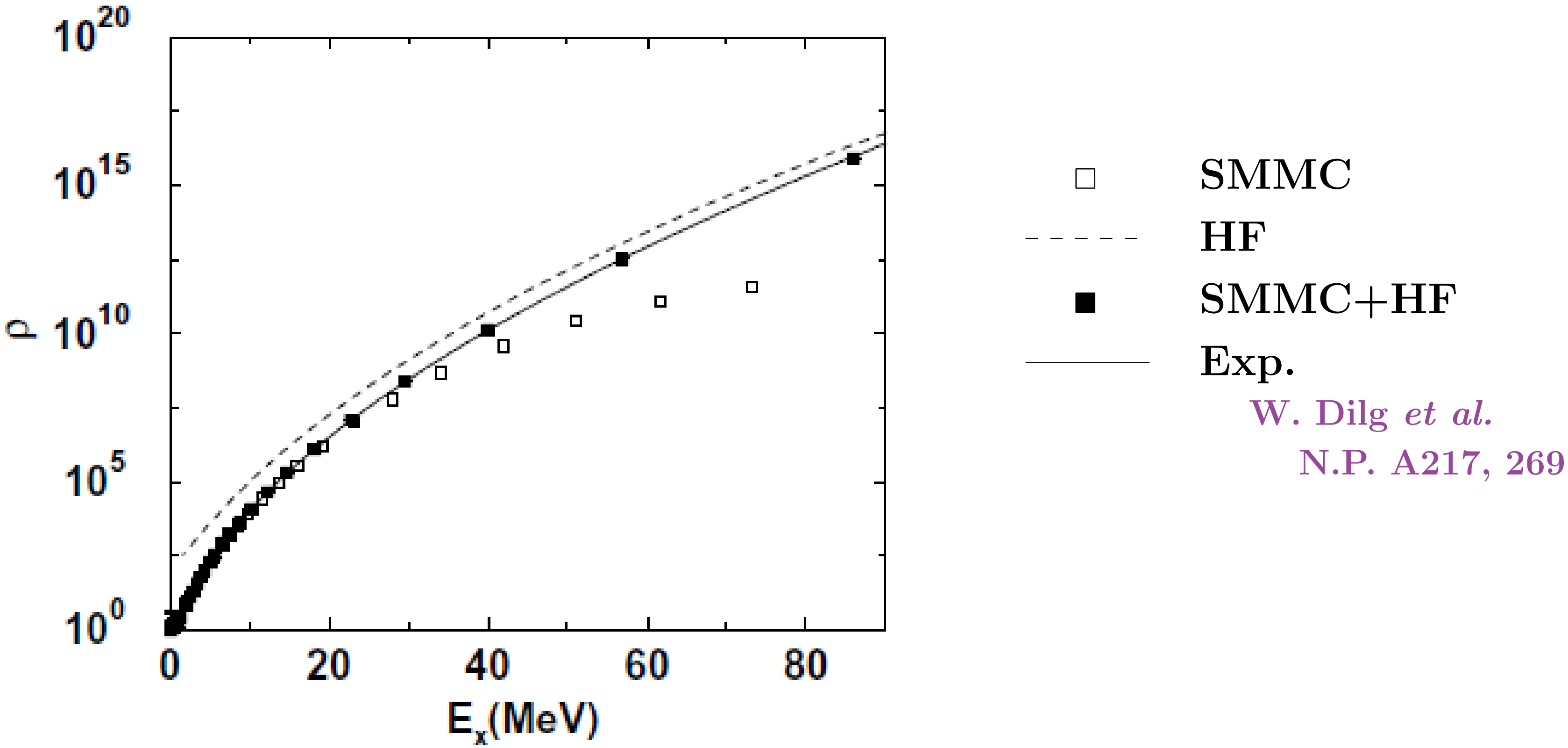
  $\rho(E_x) \quad \rightarrow \begin{cases} \textbf{comparison to BBF} \\ \textbf{extention to higher } E_x \textbf{ (via connection with HF)} \end{cases}$

  $\rho_\pi(E_x)$ **(**$\leftarrow$ π**-proj.)**

  $\rho_J(E_x)$, $\rho_{J\pi}(E_x)$ **(**$\leftarrow$ J**-proj.)** $\rightarrow$ **comparison to spin cut-off model**

State density $\rho(E_x)$ of ^{56}Fe : Ref. : Y. Alhassid *et al.*, P.R.C 68, 044322 ('03)

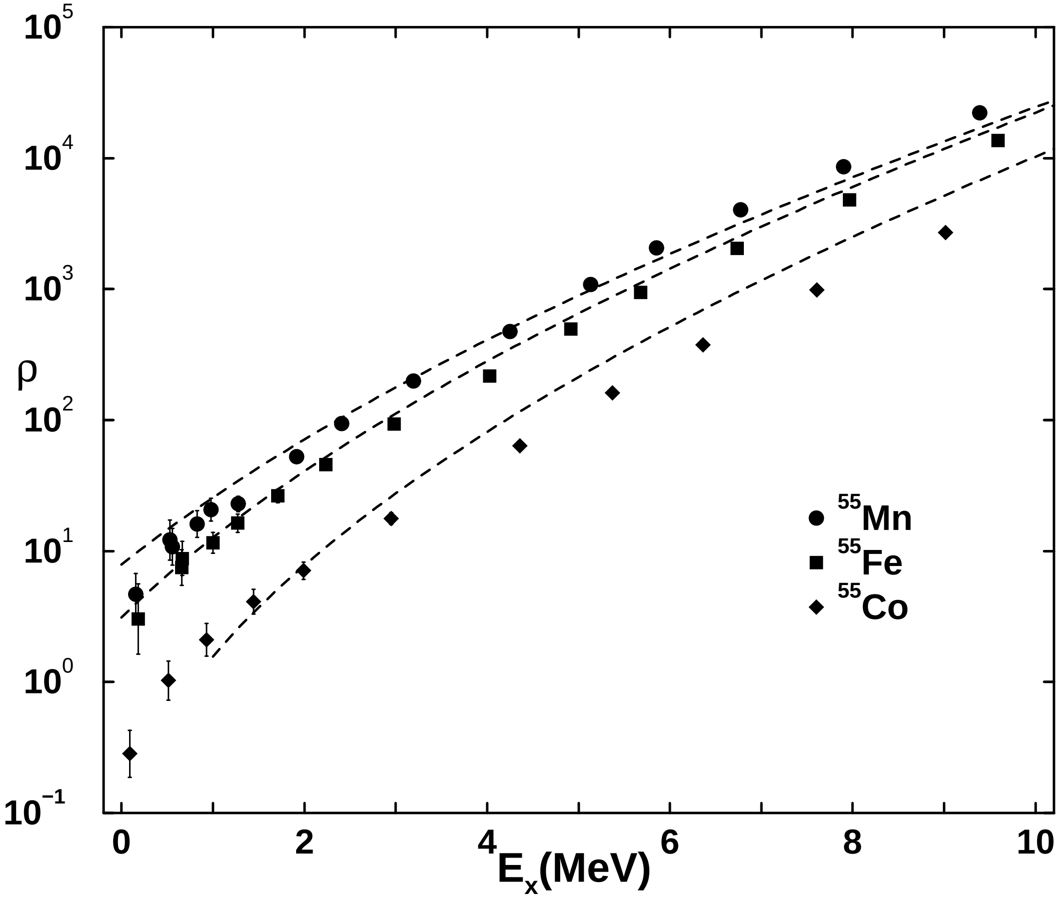
SMMC for $pf + g_{9/2}$
finite-T HF $\Big\} \rightarrow$ **connection of $F(\beta) \rightarrow \rho(E)$**



$\Big\{$ $E_x \lesssim 10\,\mathrm{MeV}$ — **strong correlations inside $pf + g_{9/2}$ shell**
$E_x \gtrsim 25\,\mathrm{MeV}$ — **weak correlation, s.p. d.o.f. is essential**

State density $\rho(E_x)$ of $A = 55$ isobars :

Ref. : Y. Alhassid, S. Liu, H.N., P.R.L. 83, 4265 ('99)



Many empirical formulae predict equal $\rho(E_x)$ among odd-A isobars

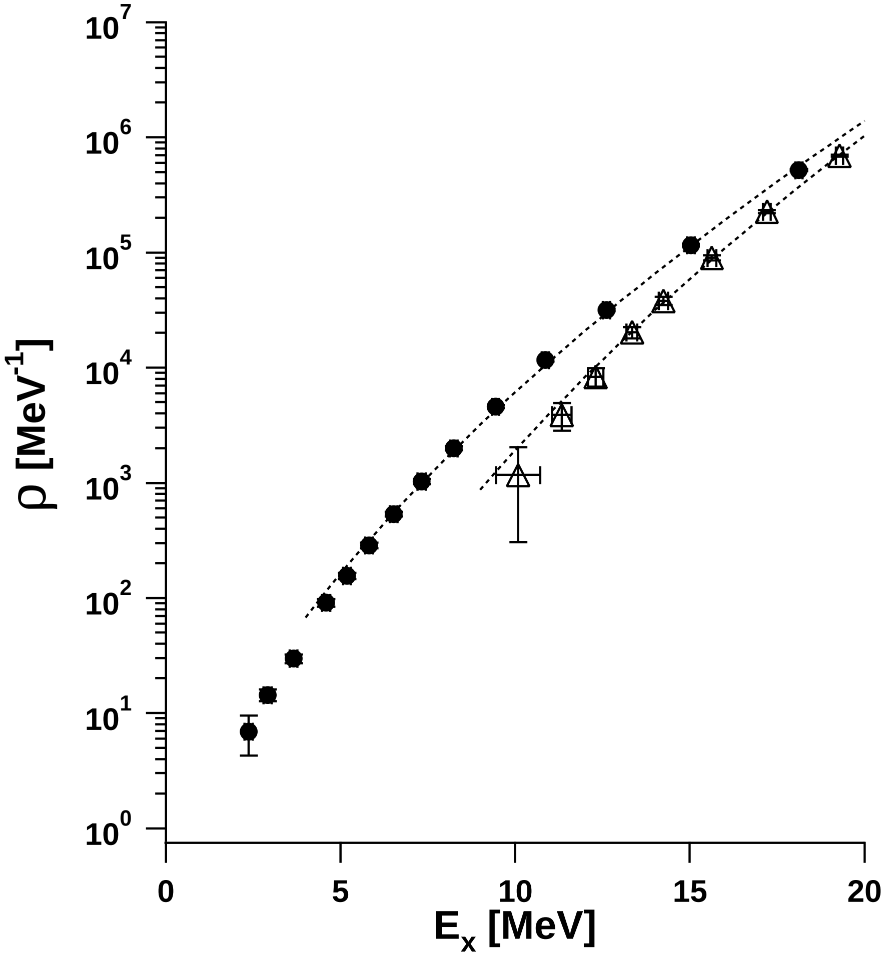
— not true !

(← exp. & micro. cal.)

Exp. : W. Dilg *et al.*, Nucl. Phys. A217, 269 ('73)

π-dep. state density $\rho_\pi(E_x)$ of ^{56}Fe:

Ref.: H.N. & Y. Alhassid, P.R.L. 79, 2939 ('97); P.L.B 436, 231



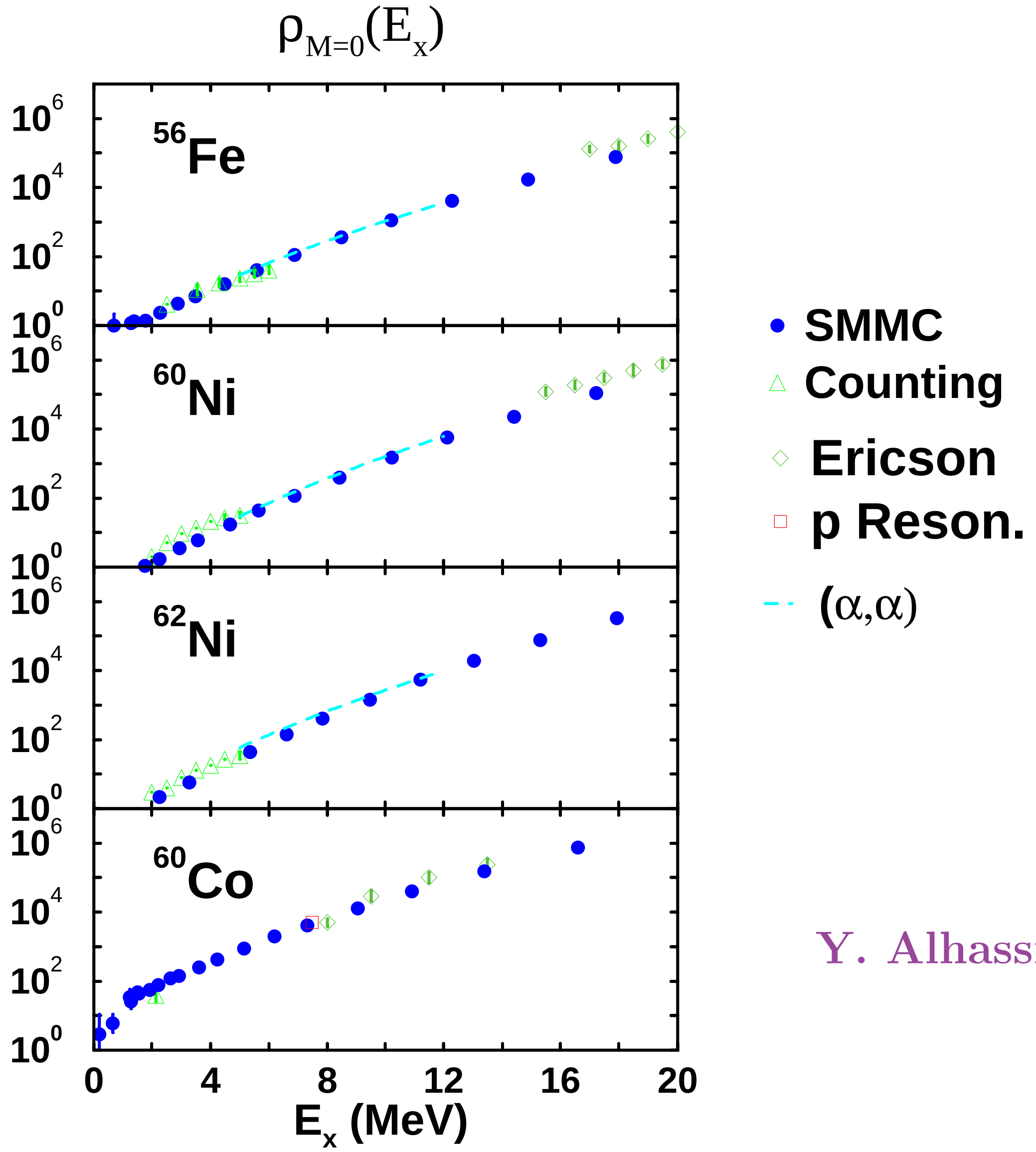
$\Rightarrow$ strong parity-dependence?

recent exp. $\rightarrow$
exc. out of *sd*-shell play a role

Ref.: Y. Kamylov *et al.*
Phys. Rev. Lett. 99, 202502

Level density $\sum_{J\pi} \rho_{J\pi}(E_x) = \rho_{M=0}(E_x)$ **of** ^{56}**Fe,** ^{60,62}**Ni,** ^{60}**Co:** **(←** J_z**-proj.)**

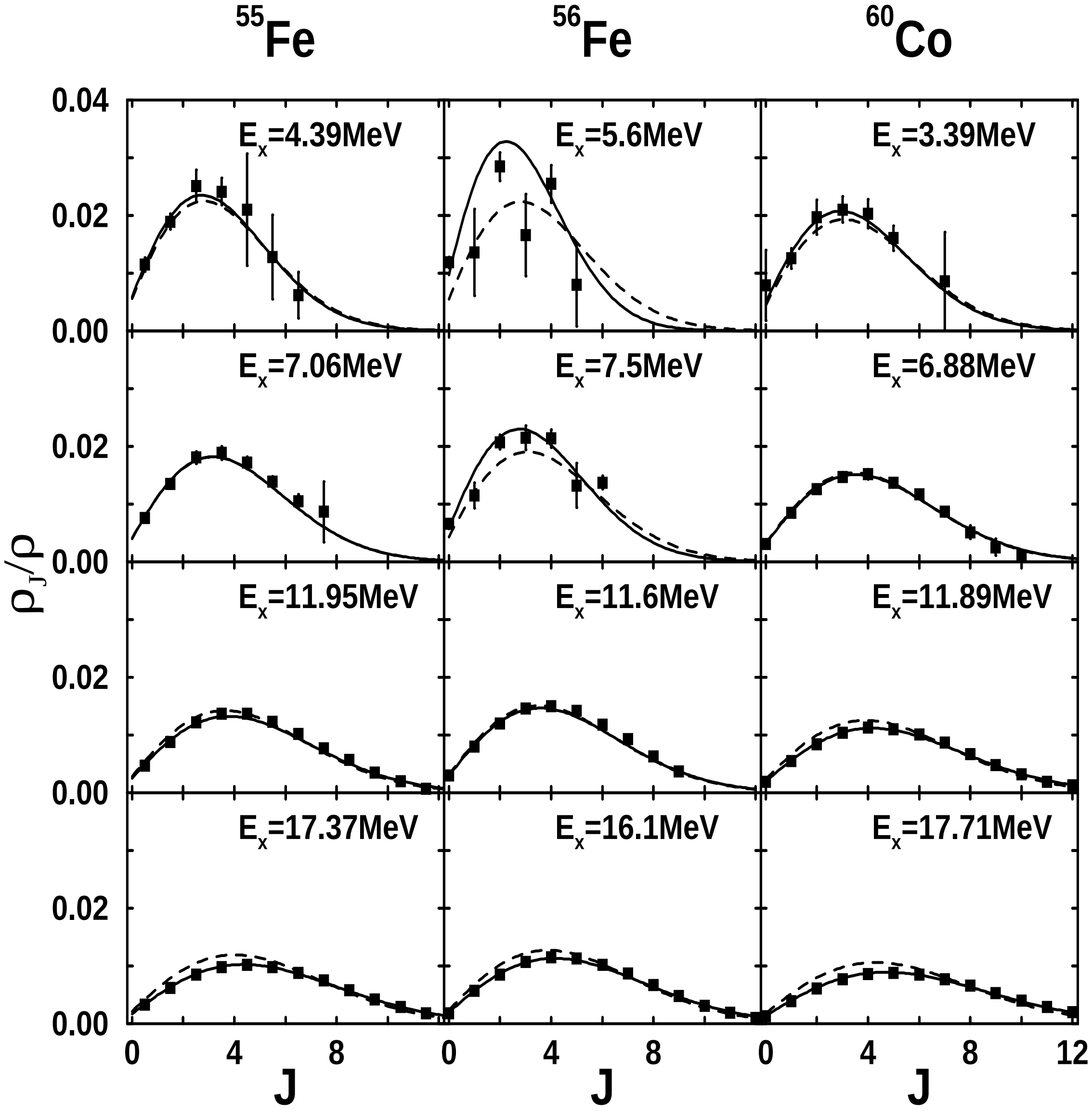
→ straightforward comparison with exp.



Y. Alhassid, S. Liu & H.N., unpublished

J-dep. level density $\rho_{J\pi}(E_x)$ of ^{56}Fe :

Ref. : Y. Alhassid, S. Liu, H.N., P.R.L. 99, 162504 ('07)



■ SMMC results

spin-cutoff model with σ

- —— fitted to SMMC
- - - - from rigid-body $\mathcal{I}$

significant deviation from spin-cutoff model

- at low E_x &
- in even-even nuclei

$\leftrightarrow$ influence of pairing

★ Well-deformed rare-earth nuclei

Ref: Y. Alhassid, L. Fang & H.N., P.R.L. 101, 082501 ('08)

- setup

model space: $\begin{cases} p : (Z = 50 - 82 \textbf{ shell}) + 1f_{7/2} \\ n : 0h_{11/2} + (N = 82 - 126 \textbf{ shell}) + 1g_{9/2} \end{cases}$

$\leftarrow$ expand def. WS solutions by sph. WS orbitals

$(0.1 < \langle \hat{n}_{\alpha j} \rangle / (2j + 1) < 0.9)$

Hamiltonian: s.p. energy $\leftarrow$ W-S pot. + HF-type correction

int. $\begin{cases} pp \text{ \& } nn \textbf{ monopole pairing} \\ \quad \text{strength} \leftarrow \text{even-odd mass difference} \\ \qquad\qquad + \text{fit to } \mathcal{I}_g \\ (p+n) \textbf{ surface-peaked multipole } (\lambda = 2, 3, 4) \\ \quad \text{strength} \leftarrow \text{self-consistency + renorm.} \\ \quad \text{renorm. factor for } \lambda = 2 \leftarrow \text{fit} \end{cases}$

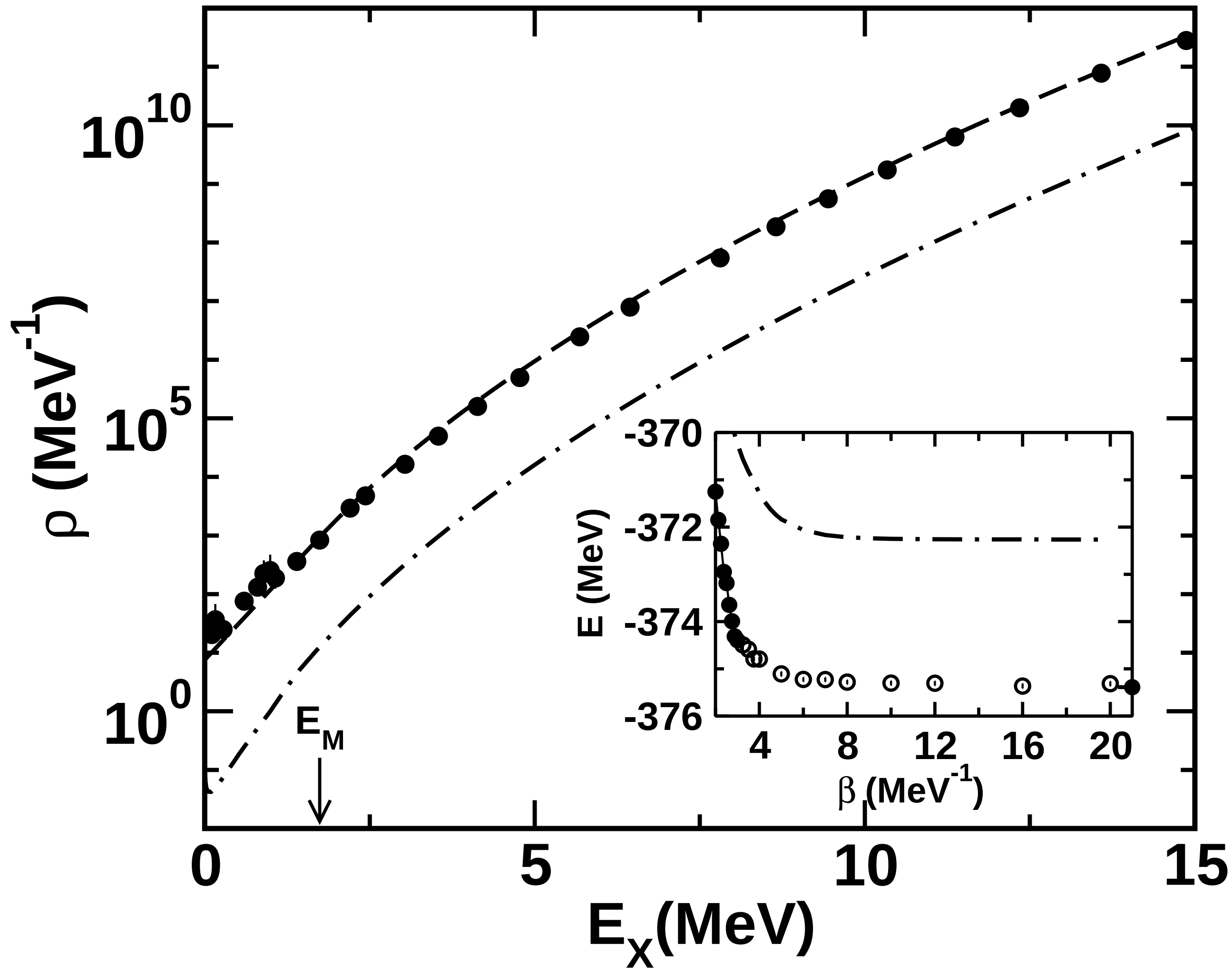
adjust. parameters $\cdots$ insensitive to nuclide (?)

- applications

$\rho(E_x)$ $\longrightarrow$ comparison to exp.

(represented by (BBF + constant-T)-model)

SMMC state density in ^{162}Dy *vs.* exp. & HFB



- excellent agreement with exp.
- almost equal "slope" at high E_x, but factor 10^2 enhancement from finite-T HFB $\leftrightarrow$ collective rotation

VI. Summary & future prospect

Summary — Microscopic approaches are promising in reproducing and predicting nuclear level densities to good precision.

Future prospect (problems to be solved)

- **Further tests in well-deformed nuclei !**
  — odd-A & odd-odd nuclei, *etc.*

- **Better understanding ?**
  - effects of 'phase transitions'
  - role of collectivity (quantitative estimate)
  - others ?

- **Systematic calculations !**
  ←
  - connection of different model spaces !
  - powerful & massive CPUs (+ man-power) ?
  - simplification based on physics understanding ?

  ··· "RIPL-4 hopefully contain SMMC level densities"
  (by Capote-Noy @ SNP2008)

Appendix : SMMC calculation in ^{162}Dy

★ **Biggest SMMC calculations to date !**

★ **Nucleus-dependence of setup ?** (↔ predictability)

- **Methods should be generic !**
- **Actual values ?**
  - ◦ **model space ··· might be nucleus-dep., but only moderately**
    → can be the same for a certain region of nuclei
  - ◦ **renorm. parameters ··· nucleus-dep. seems small**
    (in the fixed model space)

strength of quadrupole int. ↔ distribution of q.p. levels

··· { deformation / (+ non-coll. d.o.f.) }

↔ "slope" of $\ln\rho(E_x)$ — can be adjusted in HFB

strength of pairing int. ↔ $\mathcal{I}_g$ ··· rotation

↔ $\rho(E_x)$ at $E_x \lesssim 2\,\mathrm{MeV}$

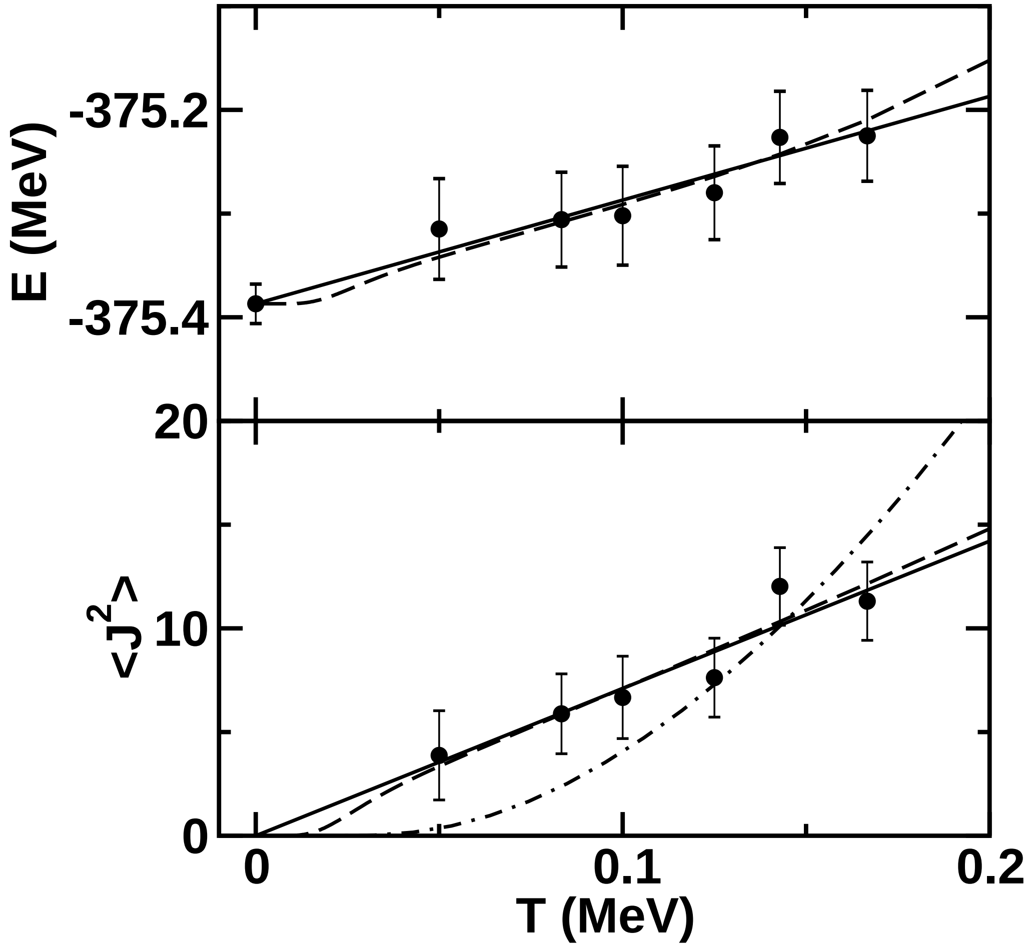
— needs to be confirmed !

★ **Rotational levels ?**

$E_x \lesssim 1\,\mathrm{MeV}$ ($\leftrightarrow T \lesssim 0.2\,\mathrm{MeV}$) $\cdots$ **g.s. band only**

$\rightarrow E(T) \approx E_0 + T$, $\langle \boldsymbol{J}^2 \rangle \approx 2\mathcal{I}_g T$ **cf. if vibrational,** $\langle \boldsymbol{J}^2 \rangle \propto T^2$

SMMC :



$\rightarrow \mathcal{I}_g = 35.8 \pm 1.5\,\mathrm{MeV}^{-1}$ ***vs.*** $\mathcal{I}_g = 37.2$ **(exp.)**