

Shell Model Monte Carlo Methods and their Applications to Nuclear Level Densities

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I. Introduction

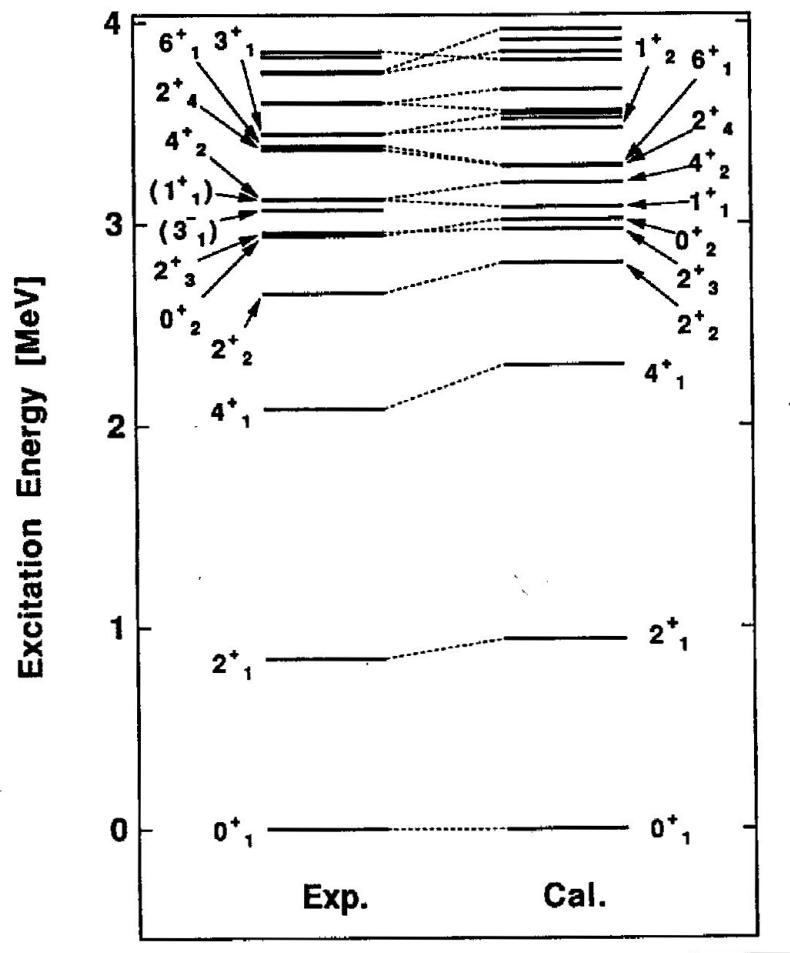
Nuclear structure

- global nature (*e.g.* saturation, binding energies, shell structure)
⇒ MF (or EDF) approaches
- 2-body correlations — often important for quantitative description
⇒ GCM, Interacting shell model (or CI), *etc.*

Advantages & disadvantages of ISM

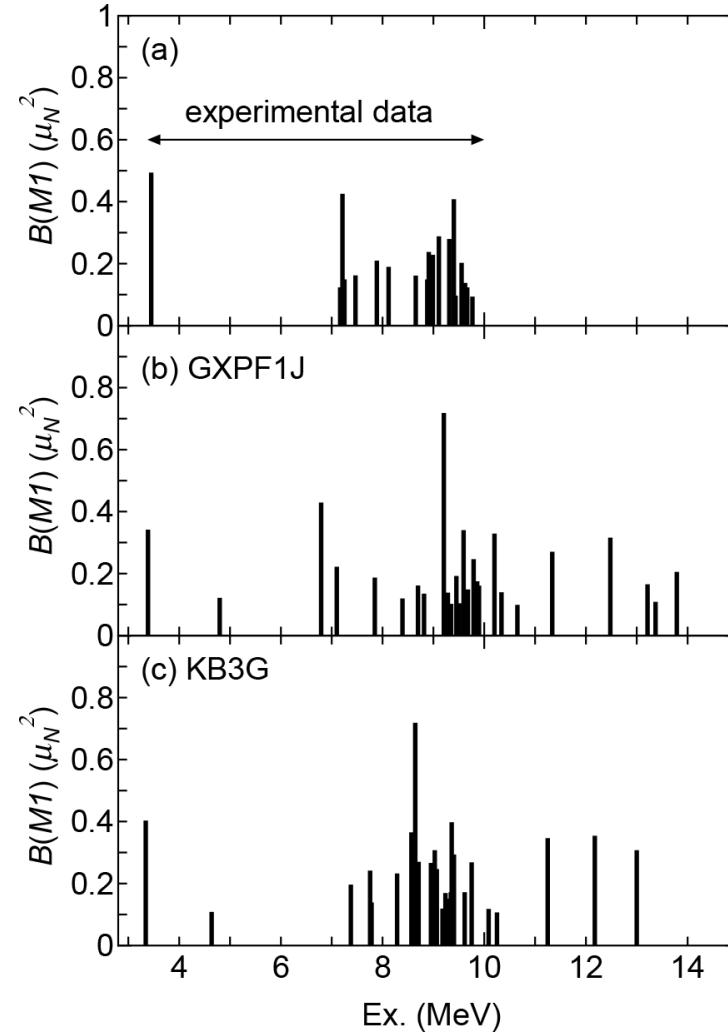
-
- A full quantum theory (→ collective + non-collective d.o.f)
good accuracy ! — up to (relatively) high excitation energies
cf. GCM
 - D model space → renormalization, energy limit
rapid increase of computational intensiveness
⇒ application & development of QMC technique (SMMC)
Ref.: G.H. Lang *et al.*, P.R.C 48, 1518 ('93)

Level scheme of ^{56}Fe :



Ref.: H.N. *et al.*,
N.P.A 571, 467 ('94)

$M1$ distribution in ^{56}Fe :



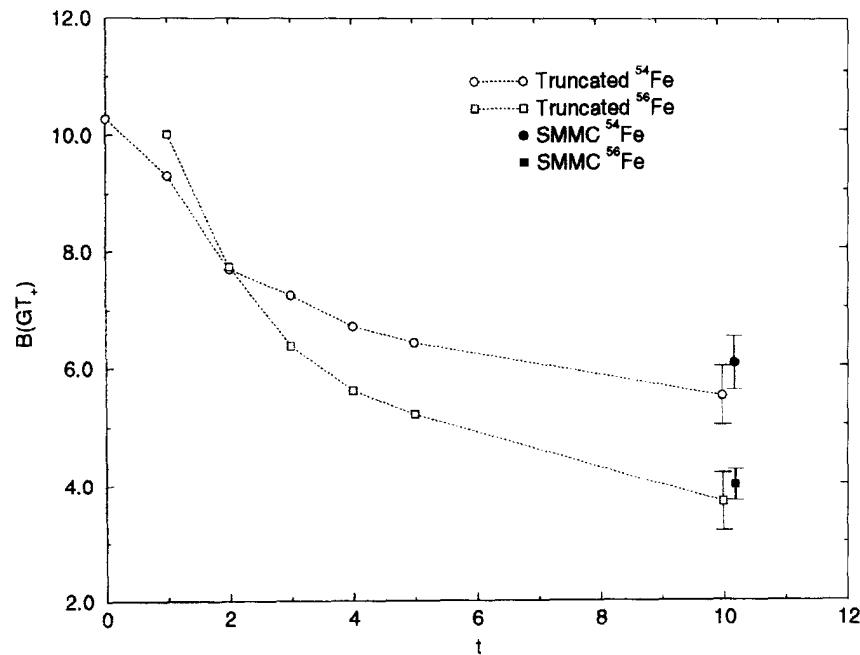
Ref.: T. Shizuma *et al.*,
P.R.C 87, 024301 ('13)

Advantages & disadvantages of SMMC

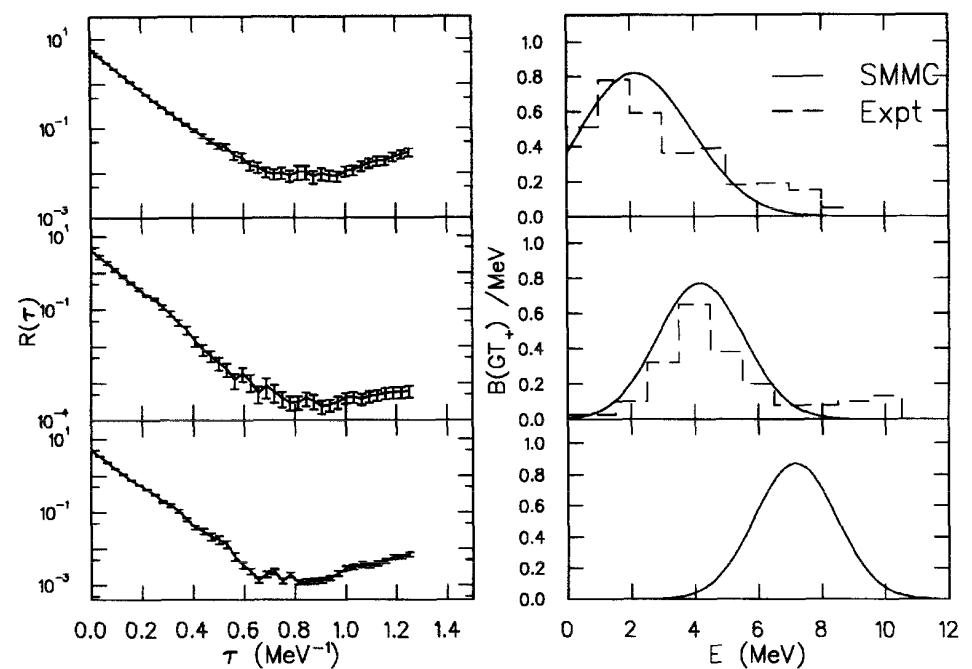
- A** implementable in large model space
‘exact’ quantum mechanical method
able to cover up to high excitation energies
including statistical properties (\leftarrow finite T)

- D** no explicit wave functions
difficult to obtain detailed spectroscopic information
statistical errors
sign problem

**Summed $B(\text{GT}_+)$:
(comparison with diag.)**



$B(\text{GT}_+)$ distribution in ^{54}Fe , $^{59,55}\text{Co}$:



Ref.: S.E. Koonin *et al.*, Phys. Rep. 278, 1 ('97)

(One of) the most successful applications of SMMC so far

... nuclear level densities

H.N. & Y. Alhassid, P.R.L. 79, 2939 ('97)

W.E. Ormand, P.R.C 56, R1678 ('97)

H.N. & Y. Alhassid, P.L.B 436, 231 ('98)

K. Langanke, P.L.B 438, 235 ('98)

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

Y. Alhassid, G.F. Bertsch, S. Liu & H.N., P.R.L. 84, 4313 ('00)

J.A. White, S.E. Koonin & D.J. Dean, P.R.C 61, 034303 ('00)

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

C. Özen *et al.*, P.R.C 75, 064307 ('07)

H.N. & Y. Alhassid, P.R.C 78, 051304(R) ('08)

A. Mukherjee & Y. Alhassid, P.R.L. 109, 032503 ('12)

+ ‘deformation’ within ISM (← certain spectroscopic information)

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

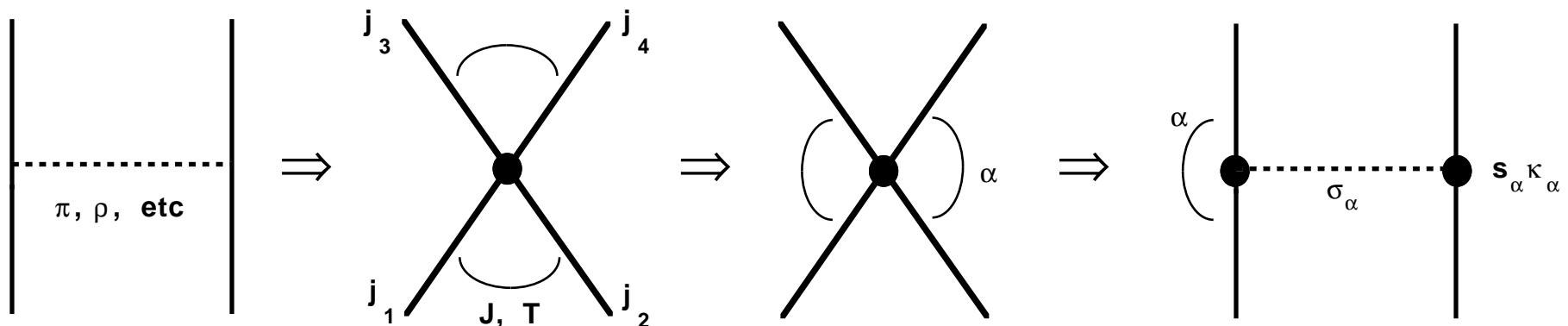
C. Özen, Y. Alhassid & H.N., P.R.L. 110, 042502 ('13)

II. Shell model Monte Carlo methods

SMMC → evaluate $\langle \mathcal{O} \rangle_\beta = \text{Tr}(\mathcal{O} e^{-\beta H})/Z(\beta)$ (e.g. $E(\beta) = \langle H \rangle_\beta$)
 H : shell model Hamiltonian (1- + 2-body)

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

$\left\{ \begin{array}{l} \text{2-body int.} \rightarrow \text{Pandya transform.} \\ e^{-\beta H}: \text{Suzuki-Trotter decomp.} \\ \qquad \qquad \qquad \rightarrow \text{Hubbard-Stratonovich transform.} \end{array} \right.$



$$e^{-\beta H} = (e^{-\Delta\beta H})^{n_t}; \quad e^{-\Delta\beta H} \approx \prod_j \left[\exp(-\Delta\beta \epsilon_j \hat{N}_j) \right] \prod_\alpha \left[\exp(-\Delta\beta \frac{\kappa_\alpha}{2} \hat{\rho}_\alpha^2) \right] + O((\Delta\beta)^2)$$

HS transform. : $\exp(-\Delta\beta \frac{\kappa_\alpha}{2} \hat{\rho}_\alpha^2) \propto \int d\sigma_\alpha \exp \left[-\Delta\beta \left(\frac{|\kappa_\alpha|}{2} \sigma_\alpha^2 + s_\alpha \kappa_\alpha \sigma_\alpha \hat{\rho}_\alpha \right) \right]$

$s_\alpha = \pm 1$ (if $\kappa_\alpha < 0$) or $\pm i$ (if $\kappa_\alpha > 0$)

$$\Rightarrow \text{Tr}(\mathcal{O} e^{-\beta H}) \approx \int \mathcal{D}[\sigma] G(\sigma) \text{Tr}(\mathcal{O} U_\sigma) \quad (\text{AF path integral})$$

$$G(\sigma) = \exp(-\Delta\beta \frac{|\kappa_\alpha|}{2} \sigma_\alpha^2), \quad U_\sigma = \prod \exp(-\Delta\beta \mathbf{h}_\sigma);$$

$$\mathbf{h}_\sigma = \sum_j \epsilon_j \hat{N}_j + \sum_\alpha s_\alpha \kappa_\alpha \sigma_\alpha \hat{\rho}_\alpha$$

$$\text{Tr}_{\text{gc}}(U_\sigma) = \det(1 + \mathcal{U}_\sigma) \quad \mathcal{U}_\sigma: \text{s.p. matrix for } U_\sigma$$

... **calculable only via the s.p. matrices**

σ_α : auxiliary field \leftrightarrow ‘mean field’

cf. **Mean-field approx.** — $\sigma_\alpha = \langle \hat{\rho}_\alpha \rangle \cdots$ static mean-field
 (no fluctuation, no τ -dependence)

Static-path approx. — $\exp(-\beta \frac{\kappa_\alpha}{2} \hat{\rho}_\alpha^2) \propto \int d\sigma_\alpha \exp \left[-\beta \left(\frac{|\kappa_\alpha|}{2} \sigma_\alpha^2 + s_\alpha \kappa_\alpha \sigma_\alpha \hat{\rho}_\alpha \right) \right]$
 $\sigma_\alpha \cdots$ static auxiliary-field with fluctuation

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)
 ↑ random walk of $\{\sigma_\alpha(\tau)\}_k$
 Metropolis algorithm (& amendment) → detailed balance
 cf. $N_k \gtrsim 4000$ in practical SMMC calculations

- advantage: easier to handle large model space
CPU time $\propto M_{\text{s.p.}}^3 \times n_t$, suitable for parallel computing
- finite- T method → suitable for statistical properties
(but not for distinguishing discrete levels)
- conservation laws → projections
 - Z & N proj. → canonical ens. ($\text{Tr}_{\text{gc}} \rightarrow \text{Tr}$)
 - π , J (J_z), isospin proj.
- $E_0 = \lim_{\beta \rightarrow \infty} \langle H \rangle_\beta$ … evaluated also by SMMC
(stabilization method required for heavy nuclei)
- disadvantage: sign problem
 - propagator $\text{Tr}(e^{-\beta h(\sigma_k)})$: not necessarily positive-definite
 - dominant part of nuclear int. — sign good!

III. Brief survey of nuclear level densities

Nuclear level densities (\leftrightarrow partition fn.)

— one of the key inputs

in calculations of low-energy nuclear reactions

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

\leftrightarrow Hauser-Feshbach formula

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

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

\Rightarrow application to nuclear-astrophysics

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

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

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

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

Experimental methods to measure nuclear level densities

1. Direct counting of levels — lowest-lying states or light nuclei
 $(E_x \lesssim 2 - 3 \text{ MeV})$
2. Level spacing among neutron resonances ($\rho = \bar{D}^{-1}$)
— small energy range around $E_x = S_n \sim 8 \text{ MeV}$, restricted to *s*-wave
3. Ericson fluctuation — $E_x \sim 20 \text{ MeV}$
4. Charged particle reactions (\leftarrow reaction model)
5. ‘Oslo method’ ··· γ -ray matrix $P(E_x, E_\gamma) = C(E_x) T^{(\gamma)}(E_\gamma) \rho(E_x - E_\gamma)$
 $(\leftarrow \text{Brink-Axel hypothesis})$
— $E_x \sim 3 - 7 \text{ MeV}$

Conventional approach to nuclear level densities

★ Backshifted Bethe's formula (\leftarrow Fermi-gas model)

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

… fits well to experimental data (except at very low E_x),
if the parameter $\textcolor{brown}{a}$ (& Δ) is adjusted
(Δ : backshift \leftrightarrow pairing & shell effects)

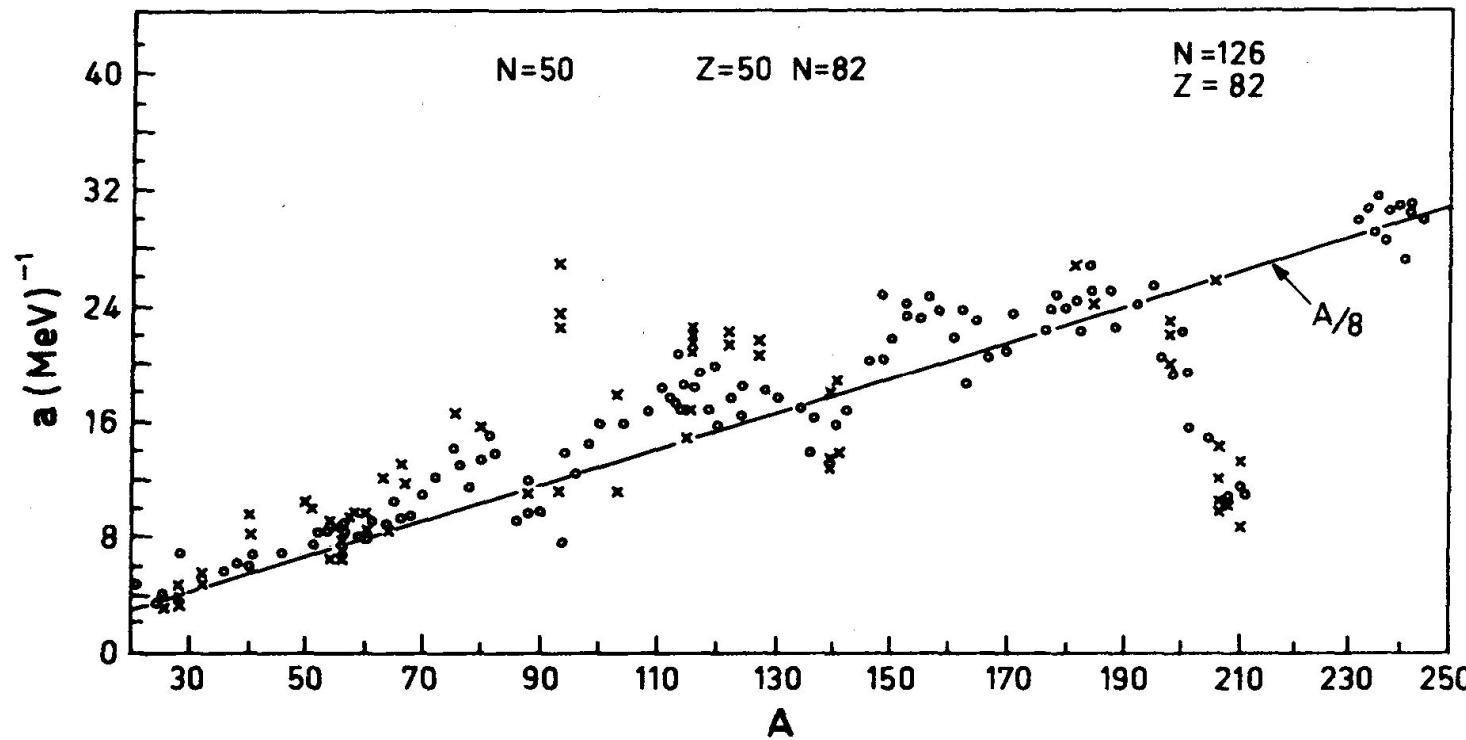
$$\rho_{J,\pi}(E_x) = \rho(E_x) \frac{2J+1}{4\sqrt{2\pi}\textcolor{violet}{\sigma}^3} \exp\left[-J(J+1)/2\textcolor{violet}{\sigma}^2\right]; \quad \sigma = \mathcal{L} \sqrt{(E_x - \Delta)/\textcolor{brown}{a}}$$

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

However,

- 1) $\textcolor{brown}{a} = A/6 \sim A/10 \text{ MeV}^{-1}$,
in contrast to the Fermi-gas prediction $a \approx A/15$
- 2) $\textcolor{brown}{a}$: 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 $A \sim 150$, $E_x \sim 8$ MeV)

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

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

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

→ matching to BBF at $E_x = E_M$

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

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

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

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

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

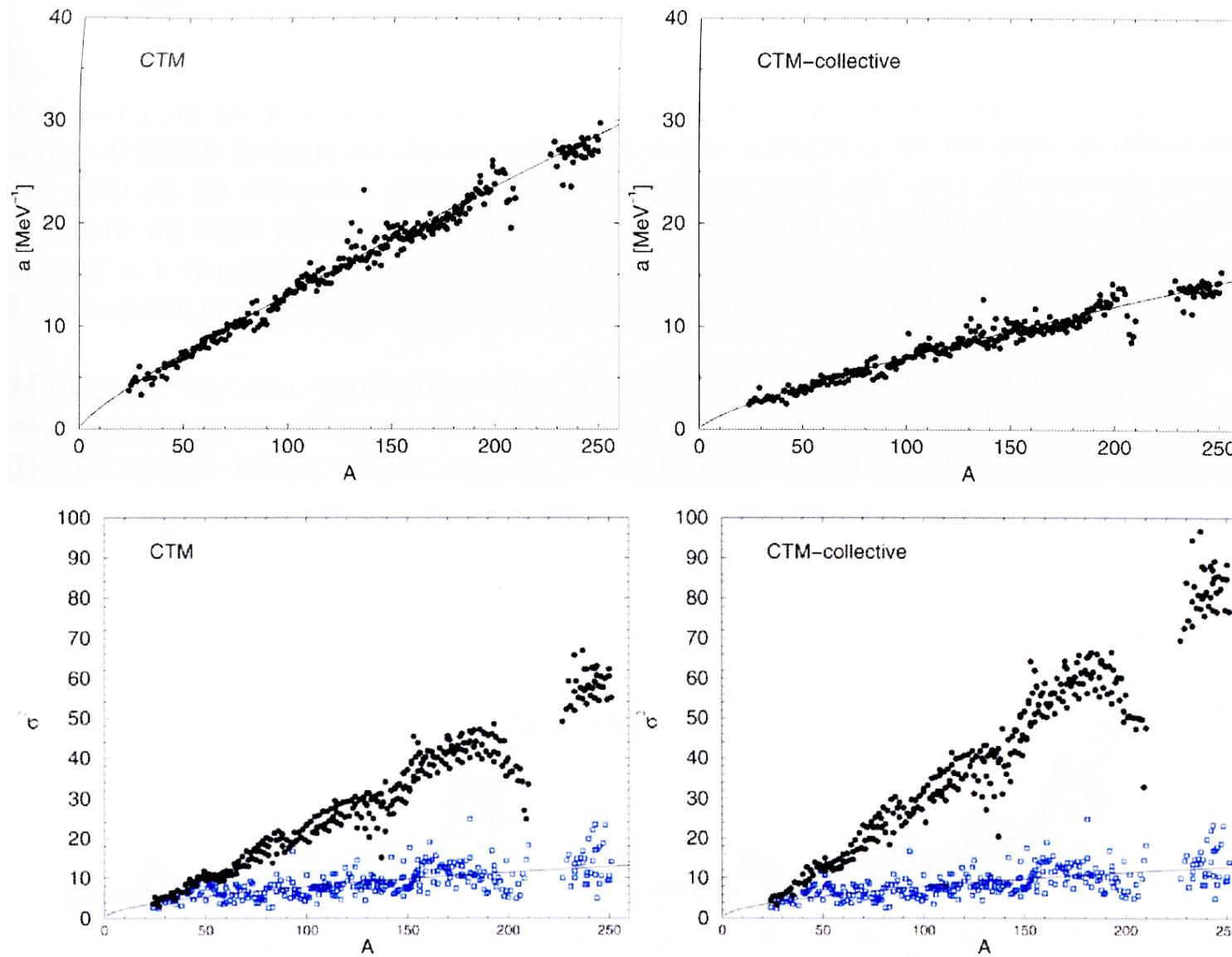
→ can be harmonious with $a \approx A/15 \text{ MeV}^{-1}$ (Fermi-gas value)

- 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.*, N.P.A 810, 13 ('08)

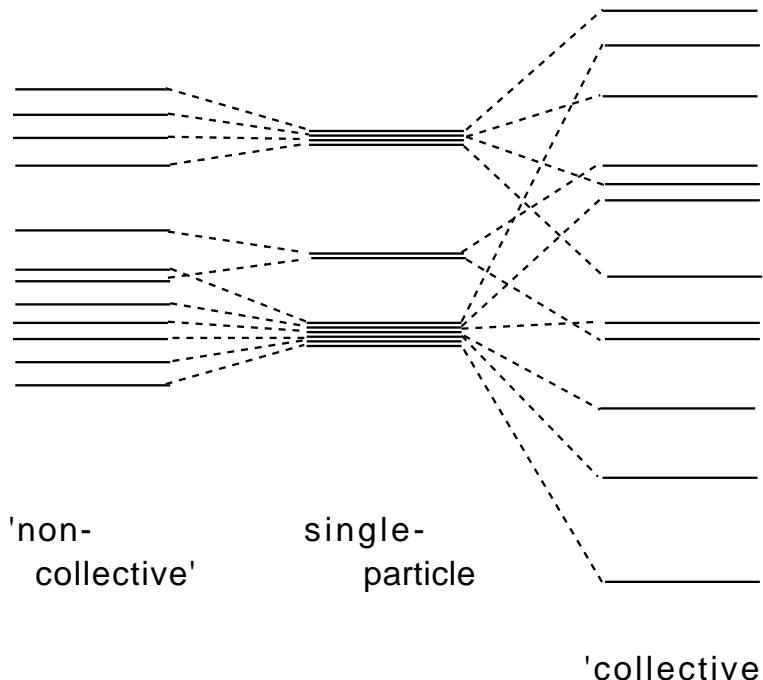
⇒ It has been difficult to predict nuclear level densities
to good accuracy

What is needed?

(1) shell effects (2) ‘collective’ 2-body correlations

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

typically, κ : large \leftrightarrow collective



(Both coll. & non-coll. d.o.f. relevant !)

full shell model \rightarrow Both (1) & (2) are fully taken into account
within the model space

... large model space required \longrightarrow SMMC (H.N. & Y. Alhassid)

IV. SMMC level densities (in medium-mass nuclei)

‘Nuclear temperature’ \leftrightarrow (average) excitation energy

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

\rightarrow statistical properties — thermodynamics in finite systems

state density

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

Laplace transform.

(Tr : can. trace)

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

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

(S : entropy, C : heat capacity)

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

★ Nuclei around Fe-Ni region

- setup

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

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

int. $\left\{ \begin{array}{l} \text{monopole pairing (SE channel)} \\ \text{strength} \leftarrow \text{even-odd mass difference} \\ \text{surface-peaked multipole (isoscalar, } \lambda = 2, 3, 4) \\ \text{strength} \leftarrow \text{self-consistency + renorm.} \\ \text{renorm. factor} \leftarrow \text{realistic int.} \end{array} \right.$

no adjustable parameters !

... sign good (for even-even nuclei) \rightarrow small stat. error

- applications

$\rho(E_x)$ \rightarrow $\left\{ \begin{array}{l} \text{comparison to BBF} \\ \text{extension to higher } E_x \text{ (via connection with HF)} \end{array} \right.$

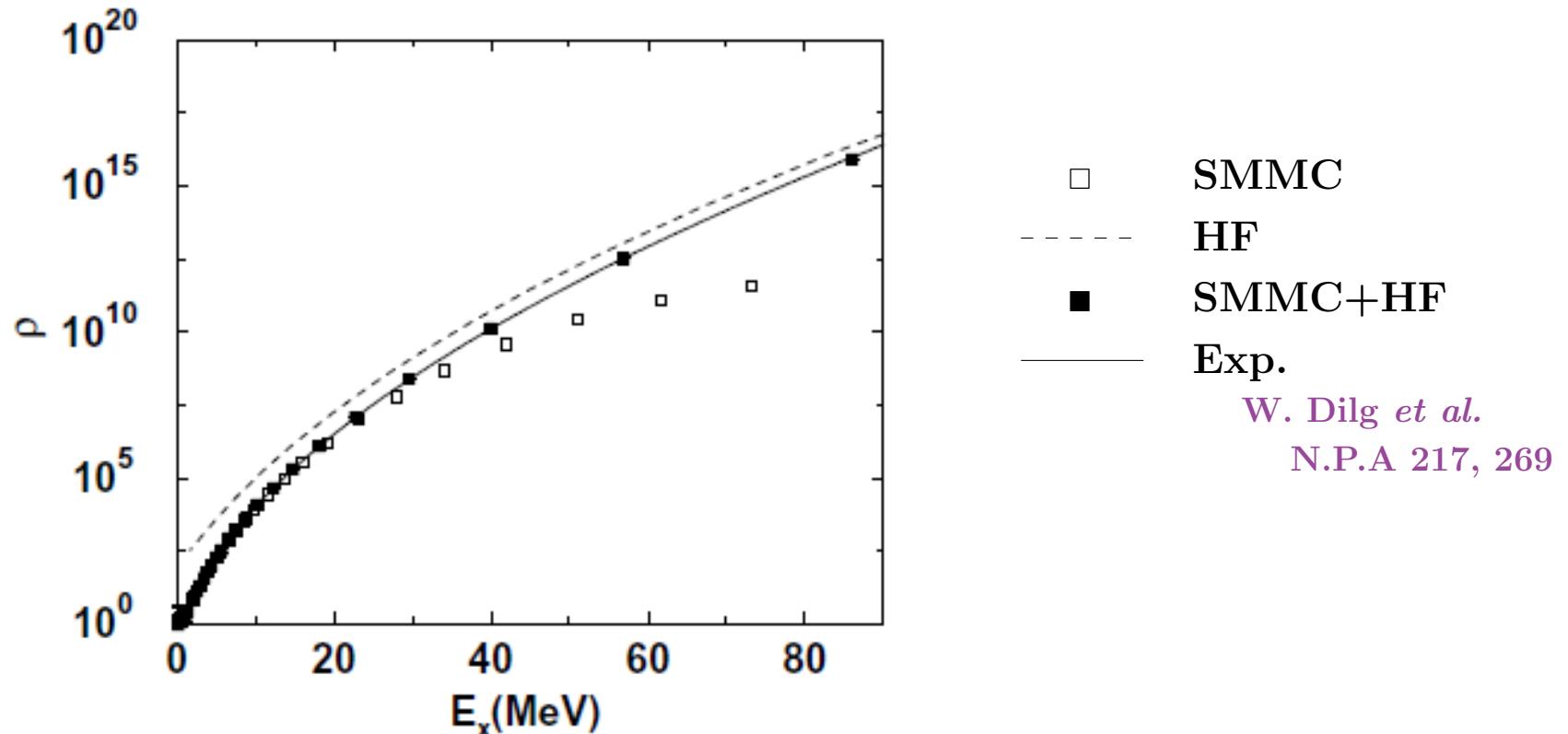
$\rho_\pi(E_x)$ ($\leftarrow \pi$ proj.)

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

$\rho_T(E_x)$ (\leftarrow isospin proj.) \rightarrow correction subject to $Z \approx N$ nuclei

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

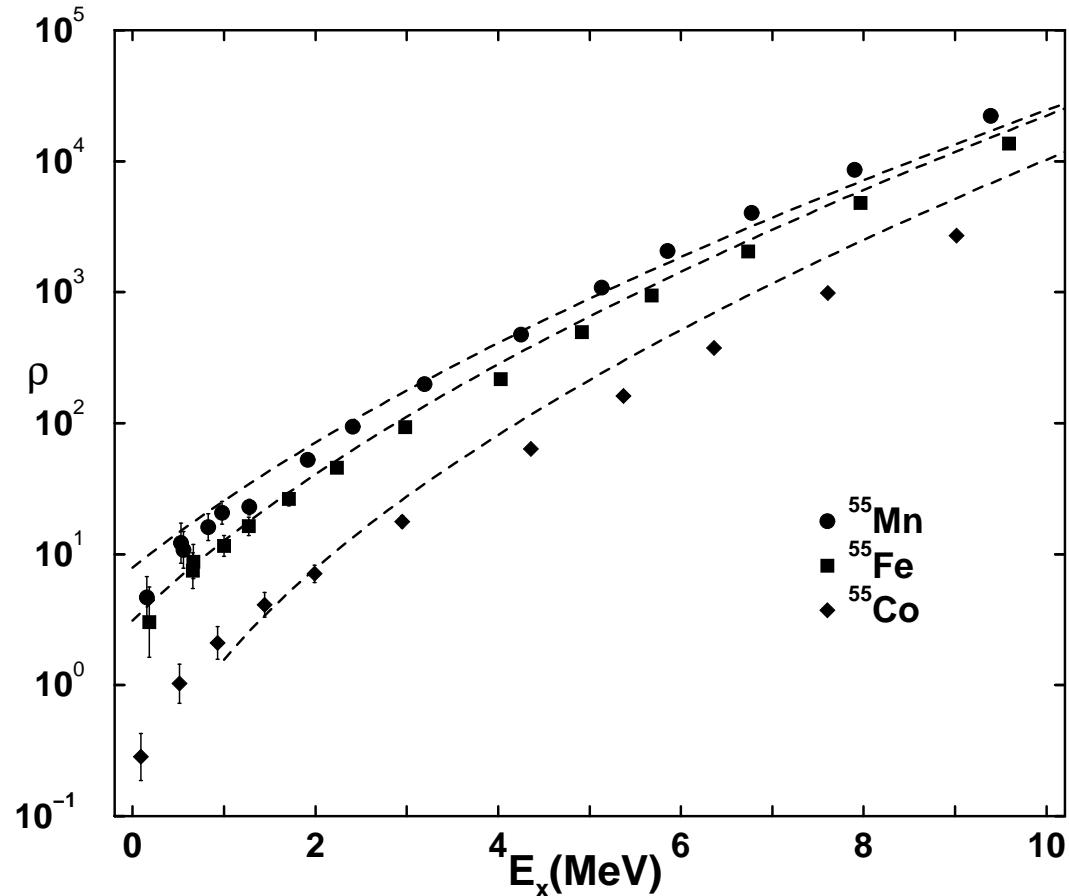
SMMC for $pf + g_{9/2}$
finite- T HF } → connection of $F(\beta) \rightarrow \rho(E)$



$\left\{ \begin{array}{ll} E_x \lesssim 10 \text{ MeV} & \text{— strong correlations inside } pf + g_{9/2} \text{ shell} \\ E_x \gtrsim 25 \text{ MeV} & \text{— weak correlation, s.p. d.o.f. is essential} \end{array} \right.$

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

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

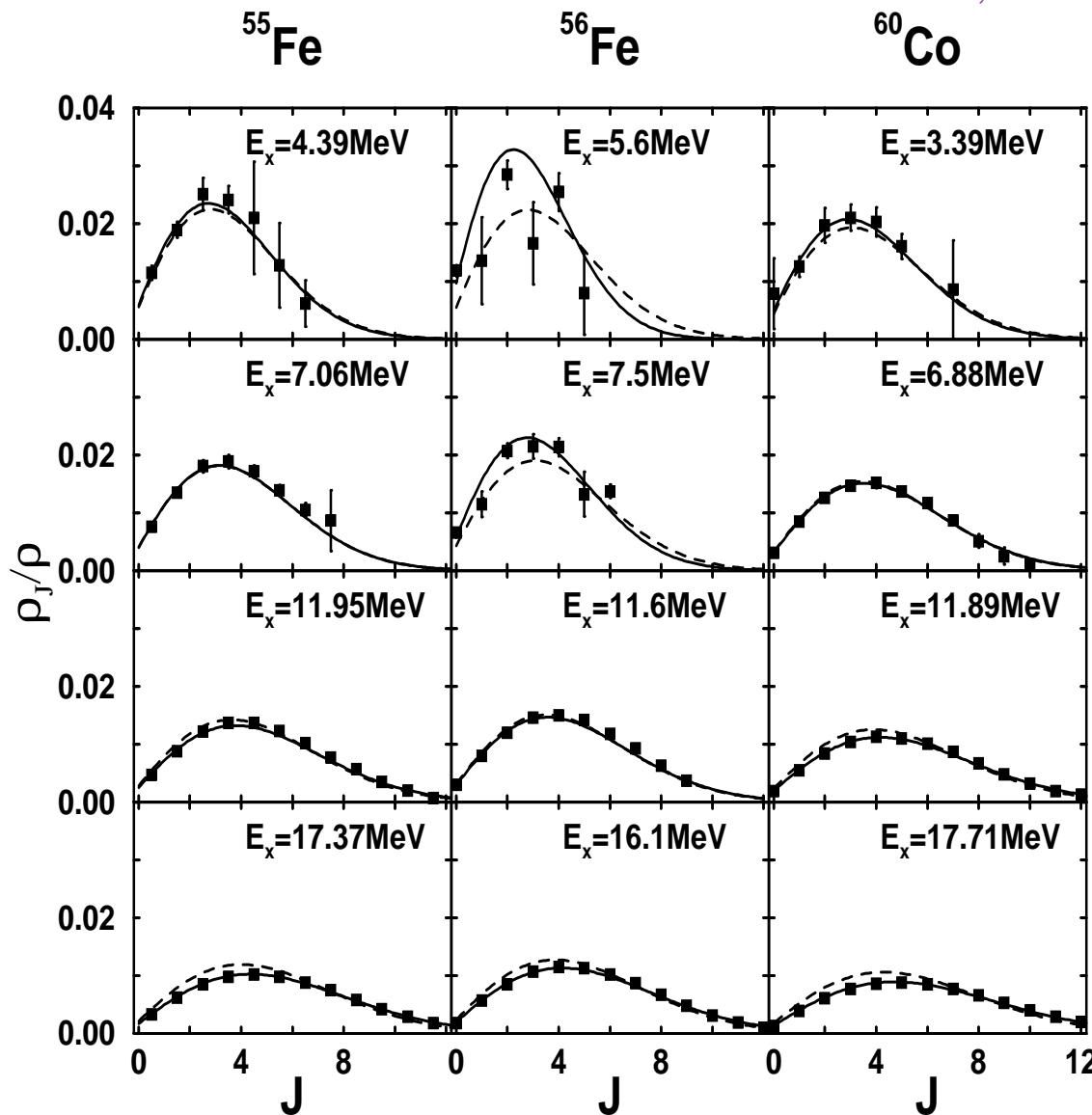


Many empirical formulas
predict equal $\rho(E_x)$
among odd- A isobars
— not true !
(← exp. & micro. cal.)

Exp.: W. Dilg *et al.*, N.P.A 217, 269 ('73)

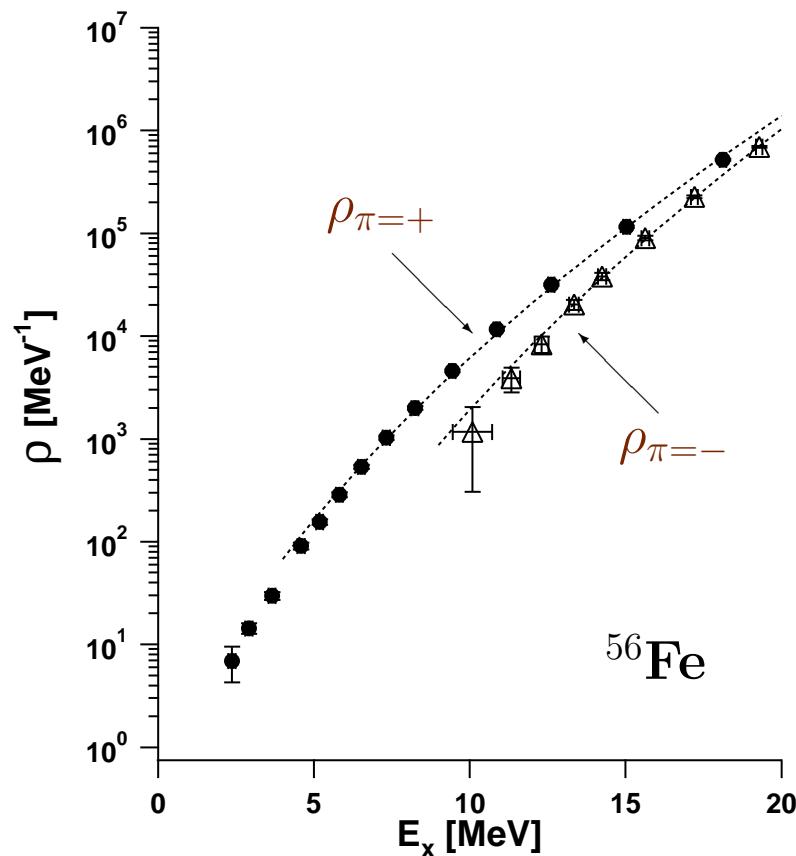
J -dep. level density $\rho_{J\pi}(E_x)$ of ^{56}Fe :

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

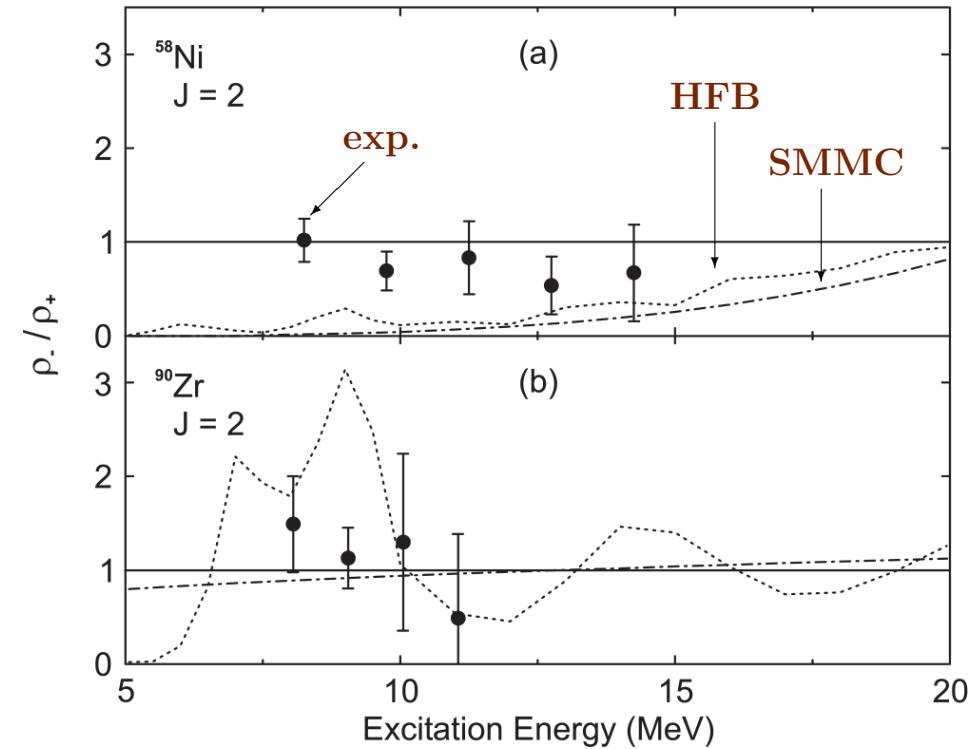


- SMMC results
- spin-cutoff model with σ
- { — fitted to SMMC
--- from rigid-body \mathcal{I}
- significant deviation
from spin-cutoff model
- { at low E_x &
in even-even nuclei
- ↔ influence of pairing

π -dep. state density $\rho_\pi(E_x)$:
SMMC



Exp.



Ref.: Y. Kalmykov *et al.*

P.R.L. 99, 202502 ('07)

— exc. out of *sd*-shell plays a role

→ C. Özen, E. Akyüz & H.N., work in progress

V. SMMC in rare-earth nuclei

★ Questions

- rotational (*i.e.* well-deformed) nuclei
 - · · described within spherical shell model ?
with how large model space ?
- crossover transition from vibrational to rotational nuclei ?
- how to identify vibrational / rotational characters in SMMC ?
- nuclear shape & level densities ?
- micro. understanding of $K_{\text{vib}}(E_x)$, $K_{\text{rot}}(E_x)$ (for level density)

★ Nuclides: ^{162}Dy , even- N Nd-Sm isotopes

Ref: Y. Alhassid, L. Fang & H.N., P.R.L. 101, 082501 ('08)
 C. Özen, Y. Alhassid & H.N., P.R.L. 110, 042502 ('13)

★ Setup

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

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

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

... biggest SMMC calculations to date!

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

int. $\begin{cases} pp \text{ & } nn \text{ monopole pairing } (g_0 = \gamma g_0^{\text{BCS}}) \\ \text{strength} \leftarrow \text{even-odd mass difference} \\ \quad \quad \quad + \text{fit to } \mathcal{I}_g \\ (p + n) \text{ surface-peaked multipole } (\lambda = 2, 3, 4) \\ \text{strength} \leftarrow \text{self-consistency + renorm.} \\ \text{renorm. factor for } \lambda = 2 \ (k_2) \leftarrow \text{fit} \\ \text{adjust. parameters — smooth function of } N \end{cases}$

★ Technical developments for SMMC calculations

1) **Proton-neutron formalism** $\leftarrow p \& n$ occupying different shell

2) **Stabilization of canonical propagator**

$E_g, \mathcal{I}_g \dots$ needs calculations at $\beta \gtrsim 10 \text{ MeV}^{-1}$
for heavy well-deformed nuclei

propagator $U_\sigma (\leftrightarrow e^{-\beta H}) \dots$ ill-behaved at large β

\Rightarrow stabilization for canonical propagator ($\leftarrow n\text{-proj.}$)

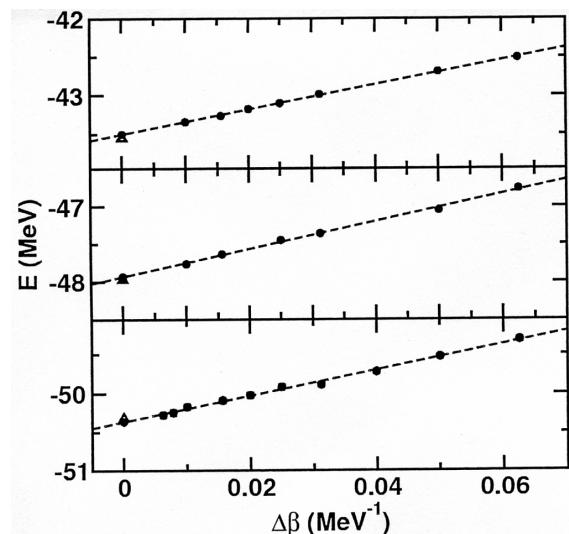
3) **Assessment of discretization effects** — extrapolation to $\Delta\beta = 0$

test case: ^{22}Ne

for ^{162}Dy

$\dots \Delta\beta = 1/32 \& 1/64 \text{ MeV}^{-1}$

$\rightarrow \begin{cases} \text{linear extrapolation} & \text{for } \beta \leq 3.25 \text{ MeV}^{-1} \\ \text{average} & \text{for } \beta > 3.25 \text{ MeV}^{-1} \end{cases}$



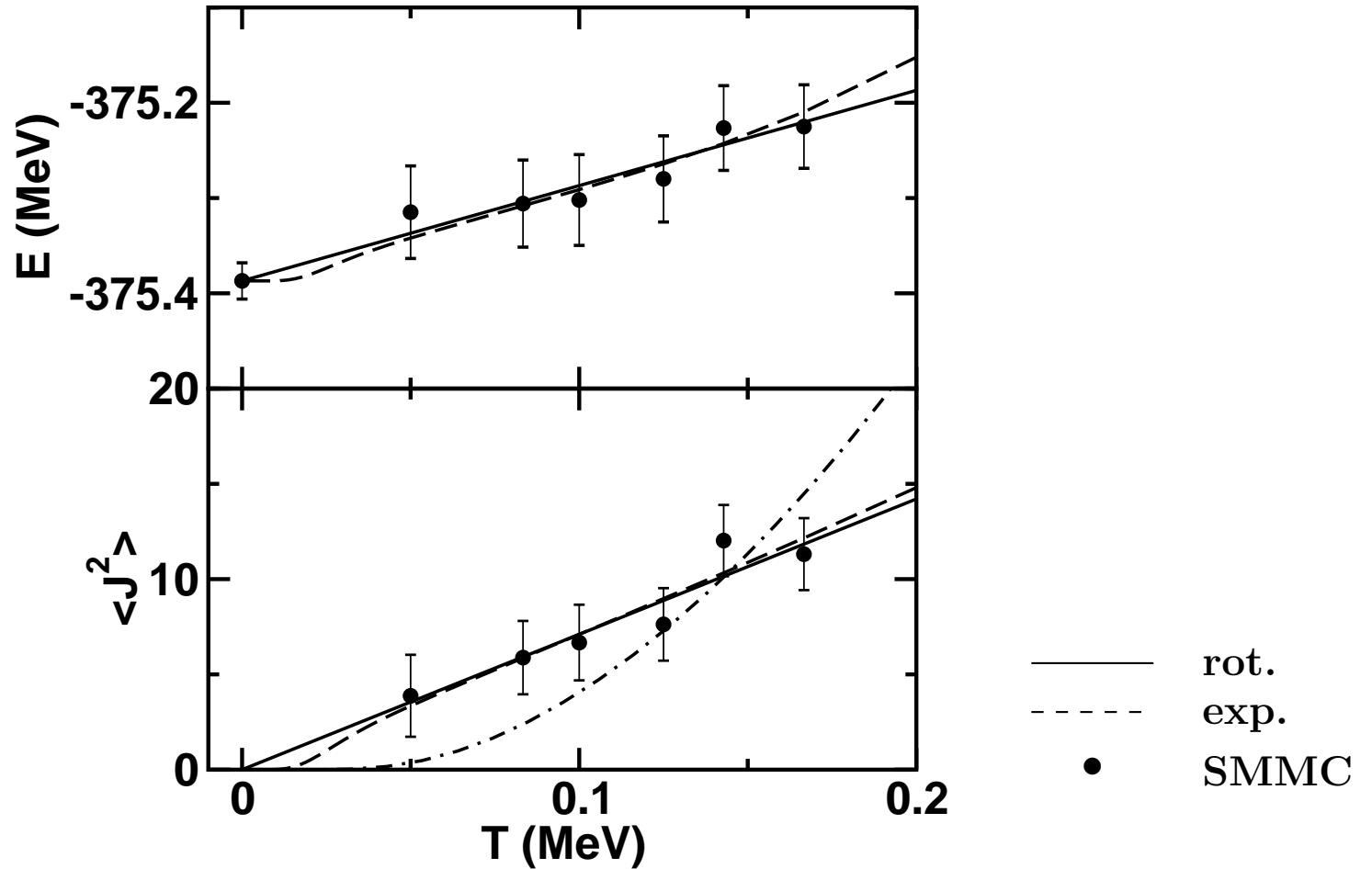
$(\beta = 0.5, 0.75, 1 \text{ MeV}^{-1})$

★ Rotational character? ... ^{162}Dy

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

$\rightarrow E(T) \approx E_0 + T$, $\langle \mathbf{J}^2 \rangle_T \approx 2\mathcal{I}_g T$ cf. $\langle \mathbf{J}^2 \rangle_T \propto e^{-E_x(2^+)/T}$ for vib.

SMMC:

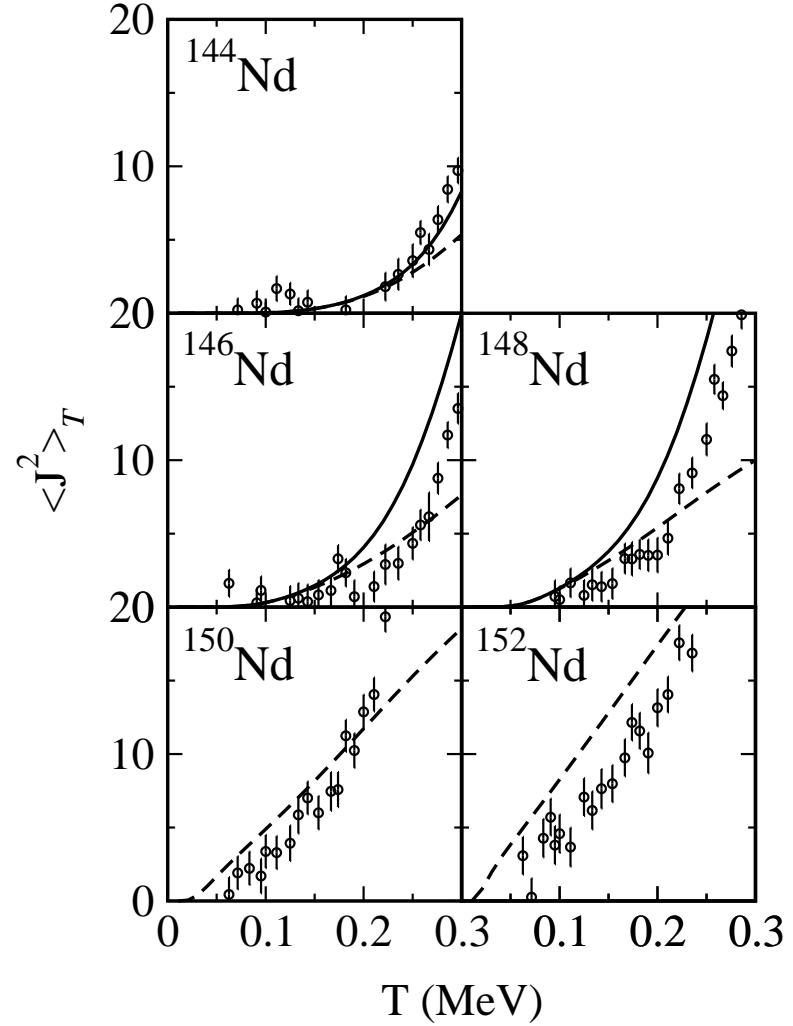
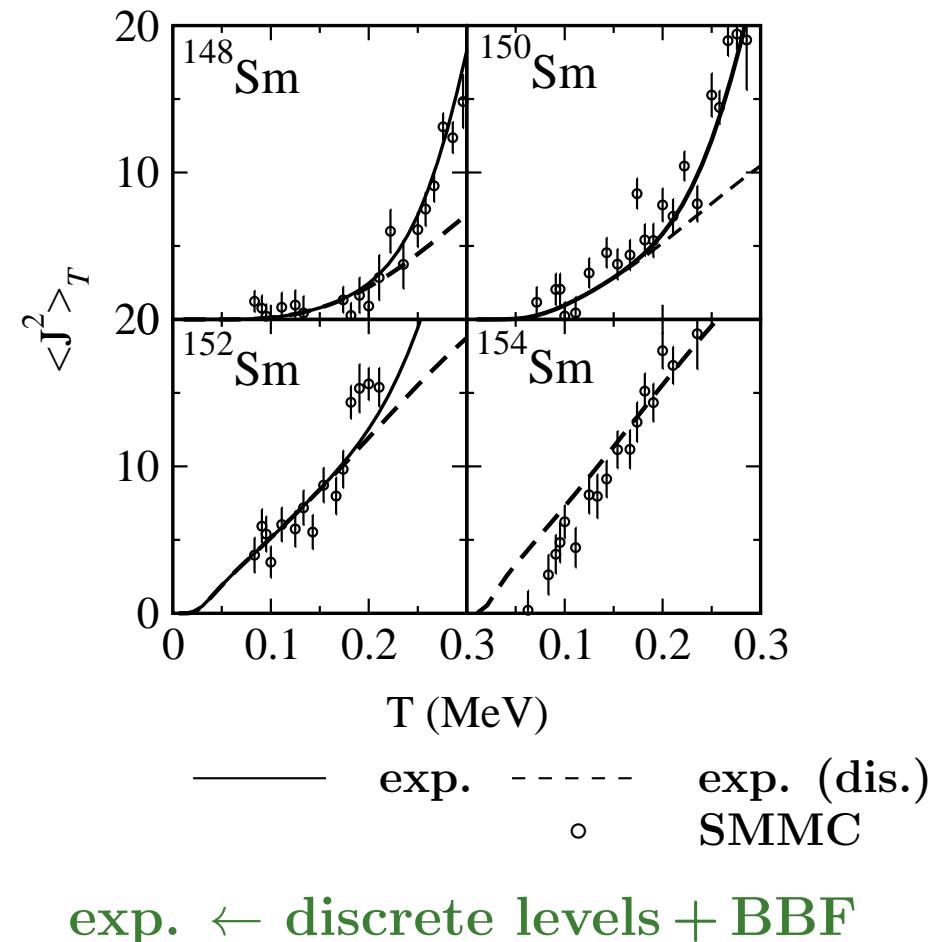


$\rightarrow \mathcal{I}_g = 35.8 \pm 1.5 \text{ MeV}^{-1}$ vs. $\mathcal{I}_g = 37.2$ (exp.)

★ Crossover from vibrational to rotational nuclei ?

... even- N Nd-Sm isotopes

$$\langle J^2 \rangle_T \approx \begin{cases} 30 e^{-E_x(2^+)/T} / (1 - e^{-E_x(2^+)/T})^2 & (\text{vib.}) \\ 6 T / E_x(2^+) & (\text{rot.}) \end{cases} \quad (\text{at low } T) \quad \Rightarrow \text{vib. / rot.}$$



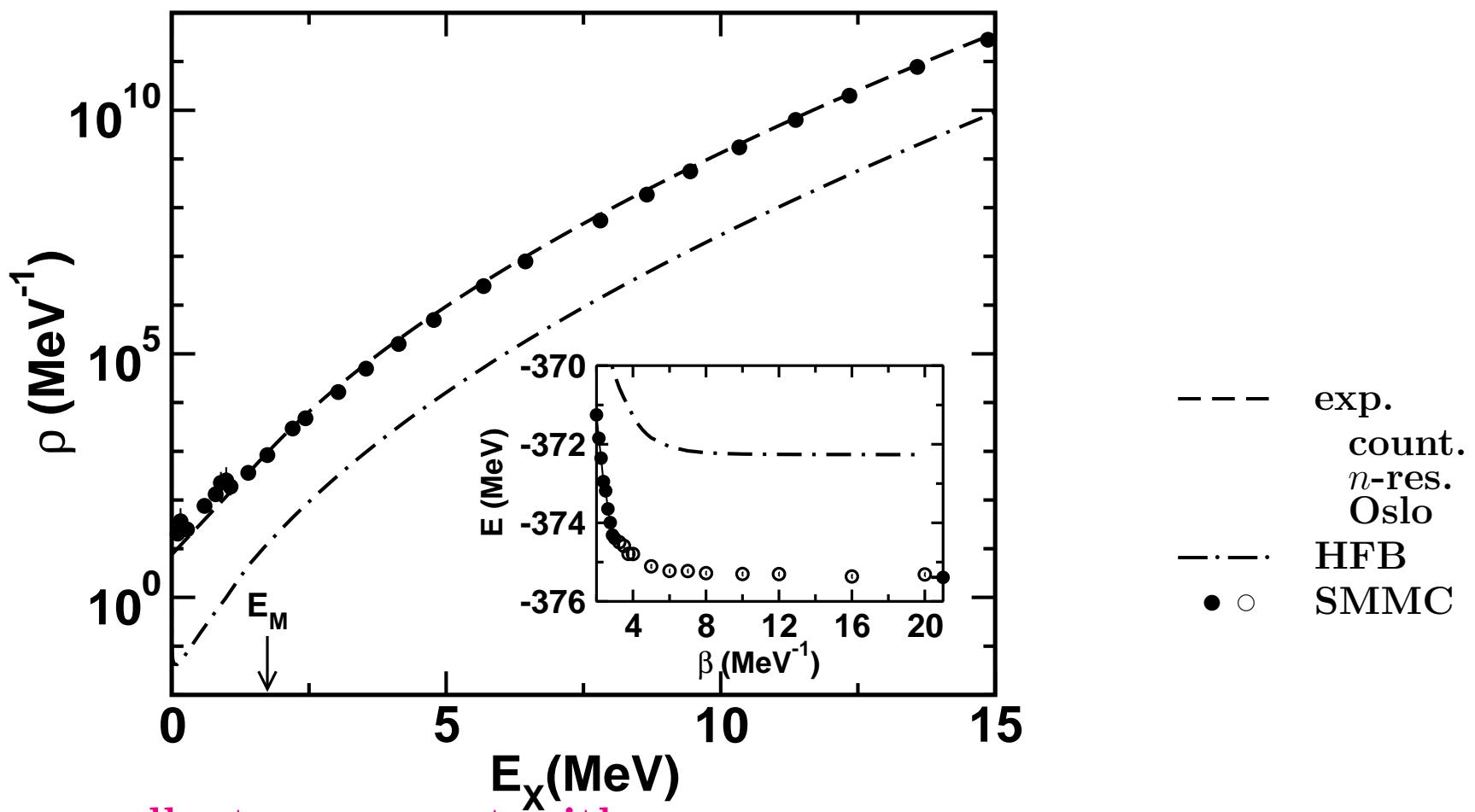
crossover from vib. to rot. well reproduced! (within shell model)

fit to $\langle J^2 \rangle_T \rightarrow$
$$\begin{cases} {}^{148}\text{Sm} : E_x(2^+) = 0.538 \pm 0.031 \text{ MeV } vs. 0.550 \text{ MeV (exp.)} \\ {}^{154}\text{Sm} : 0.087 \pm 0.006 \text{ MeV} \\ {}^{144}\text{Nd} : 0.702 \pm 0.062 \text{ MeV} \\ {}^{150}\text{Nd} : 0.132 \pm 0.012 \text{ MeV} \\ {}^{152}\text{Nd} : 0.107 \pm 0.006 \text{ MeV} \end{cases}$$

★ SMMC state densities

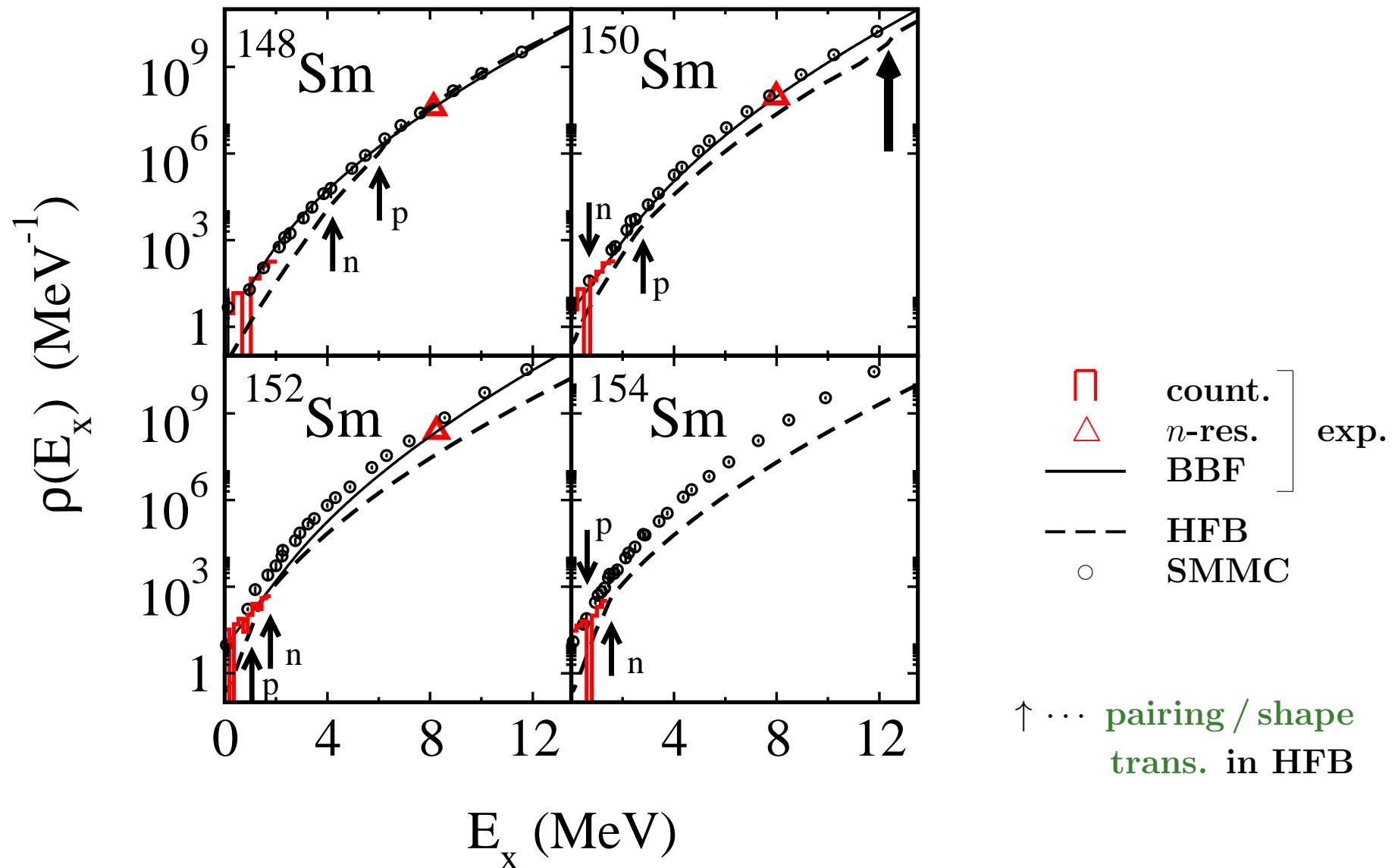
(vs. exp. & finite- T HFB)

^{162}Dy :



- excellent agreement with exp.
- almost equal “slope” at high E_x , but factor 10² enhancement from finite- T HFB \leftrightarrow collective rotation

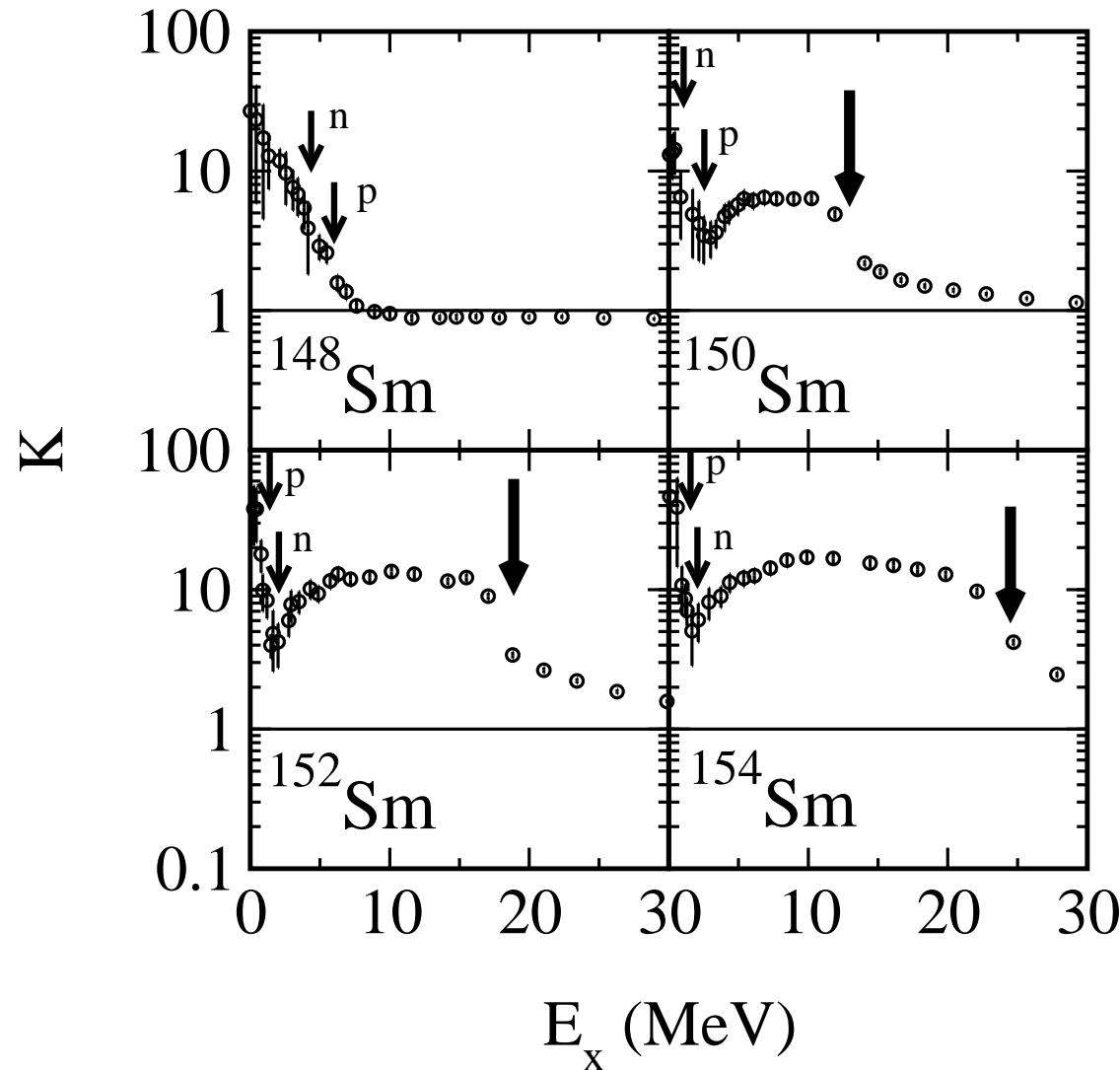
$^{148-154}\text{Sm}$:



★ Collective enhancement

$$K(E_x) := \rho_{\text{SMMC}}(E_x) / \rho_{\text{HFB}}(E_x)$$

$$\xleftrightarrow[?]{} K_{\text{vib}}(E_x), K_{\text{rot}}(E_x)$$



“decay” of K

\leftrightarrow losing collectivity

{

 pairing

 rotation

VI. Summary & future prospect

Summary

- SMMC methods reviewed briefly
projections ← isolated finite system
- Applications to level densities — successful
rotational properties & crossover — O.K.
collective enhancement — obtained microscopically

Future prospect

- 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)
- Quantitative derivation of collective enhancement factor ?