Shell model Monte Carlo approaches to nuclear level densities

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Contents :

I. Introduction

Nuclear structure at finite temperature

- **properties under astrophysical environment**
  e.g. **ele.-mag. & weak responses at thermal equilibrium**
- **statistical properties at high excitation energy ($E_x \gtrsim 3\,\mathrm{MeV}$)**
  e.g. **level density — key input to low-energy nuclear reaction rates**
  (→ astrophysics)

"nuclear temperature"

microcanonical ··· $T(E) = \left[\frac{\partial}{\partial E}\ln\rho(E)\right]^{-1}$ **($\rho(E)$: level density)**

canonical ··· **saddle-point approx.** → $E(\beta) = -\frac{\partial}{\partial\beta}\ln Z(\beta)$ **($\beta = 1/T$)**

⇒ T **: external parameter controlling average excitation energy**

··· **both are treated within the same framework of thermodynamics**
(or statistical mechanics)

Nuclear level densities

- basic quantity in investigating nuclear properties at finite T

$$\rho(E) \underset{\text{Laplace transf.}}{\longleftrightarrow} Z(\beta) = \int \rho(E)\, e^{-\beta E} dE : \text{ partition fn.} \qquad \text{(in canonical formalism)}$$

e.g. exp. of $\rho(E)$ $\rightarrow$ thermal properties Ref.: A. Schiller *et al.*, P.R.C63, 021316

- relevance to astrophysics — one of the critical inputs in nucleosynthesis calculations

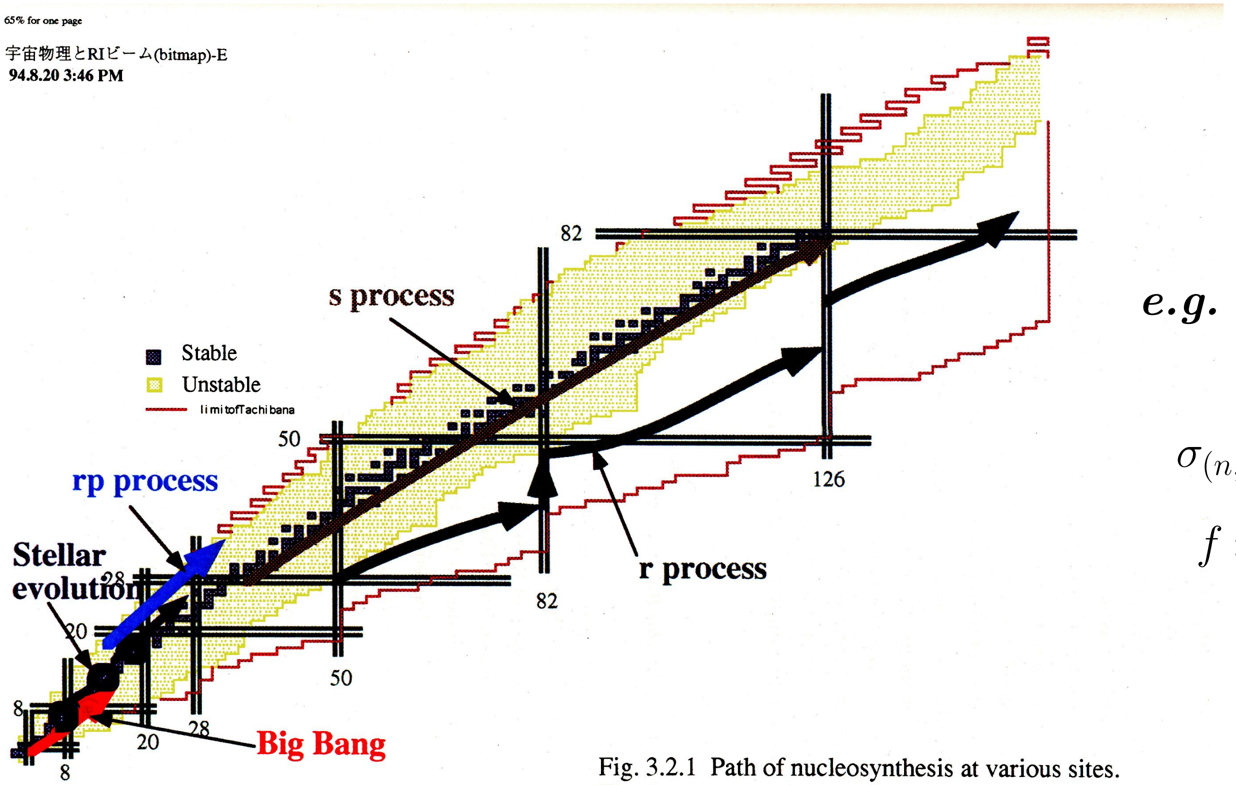


Fig. 3.2.1 Path of nucleosynthesis at various sites. The decay properties and the capture reaction rates of unstable nuclei are essential for understanding these path ways and thus the elemental abundances.

e.g. s- & r-processes

$\cdots$ (n,γ) ***vs.*** β-decay

$$\sigma_{(n,\gamma)} \propto \sum_{J\pi} \int dE\, \rho_{J\pi}(E)\, f_{J\pi}(E)$$

f : transmission coeff., *etc.* (determined fairly well)

Experimental methods to measure nuclear level densities

1. **direct counting of levels — lowest-lying states or light nuclei**
2. **level spacing among neutron resonances ($\rho \approx \bar{D}^{-1}$) — relatively small energy range**
3. **Ericson fluctuation — $E_x \sim 20$MeV**
4. **charged particle reactions**
5. **γ-strength function ($\Gamma(E_x, E_\gamma) \propto F(E_\gamma)\rho(E_x)$) $\leftarrow$ Brink-Axel hypothesis**

Previous theoretical works on nuclear level densities

- **backshifted Bethe formula (← Fermi-gas model) → next discussion**
- **distributing (spherical) s.p. levels + marginal interaction effects**

  e.g. **spectral averaging theory ··· int. → smearing**

  (treated in terms of moments)

  - **unable to constrain overall energy shift (↔ g.s. energy)**
  - **moderately good for spherical nuclei,**

    but unable to handle strong collectivity

- **finite-temperature methods**

  e.g. **mean-field approx., static-path approx. → later discussion**

II. Shell model Monte Carlo approaches to nuclear level densities

Conventional approach to nuclear level densities

Backshifted Bethe formula $\leftarrow$ **Fermi-gas model**

$$\rho_{\rm tot}(E_x) = \frac{\sqrt{\pi}}{12} a^{-1/4} (E_x - \Delta + t)^{-5/4} \exp\left[2\sqrt{a(E_x - \Delta)}\right] \qquad (E_x - \Delta = at - t^2)$$

$\cdots$ **fits well to experimental data, if the parameter a is adjusted**

(Δ: backshift, representing pairing & shell effects)

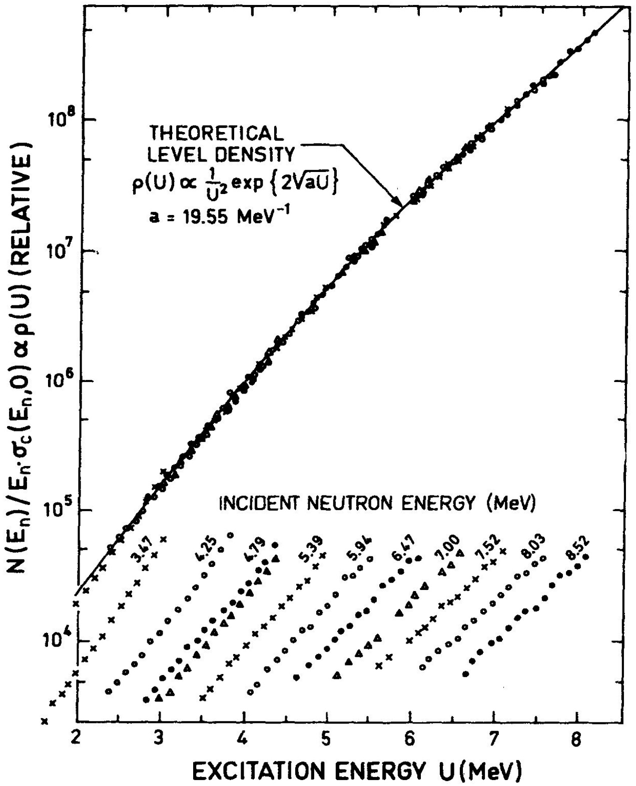
Problem $\cdots$ **value of a !** **(& sometimes Δ, also)**

1) exp. $\rightarrow a = A/6 \sim A/10\,[\mathbf{MeV}^{-1}]$ **cf. $a \approx A/15$ in Fermi-gas model**

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

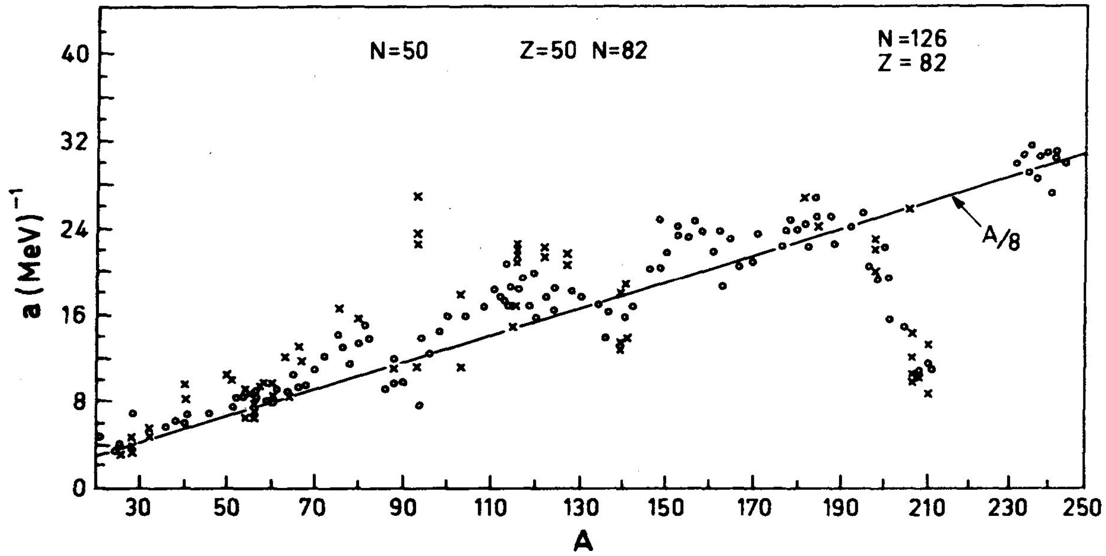
$\Rightarrow$ **predictability ?**

$\rho(E)$ **for Ag:**



$\Leftarrow (n, n')$ **at** $E_n = 3.5 - 8.5\,\text{MeV}$

A**-dep. of** a**-parameter:**



with Δ assumed from pairing gap

Ref.: Bohr-Mottelson vol.1

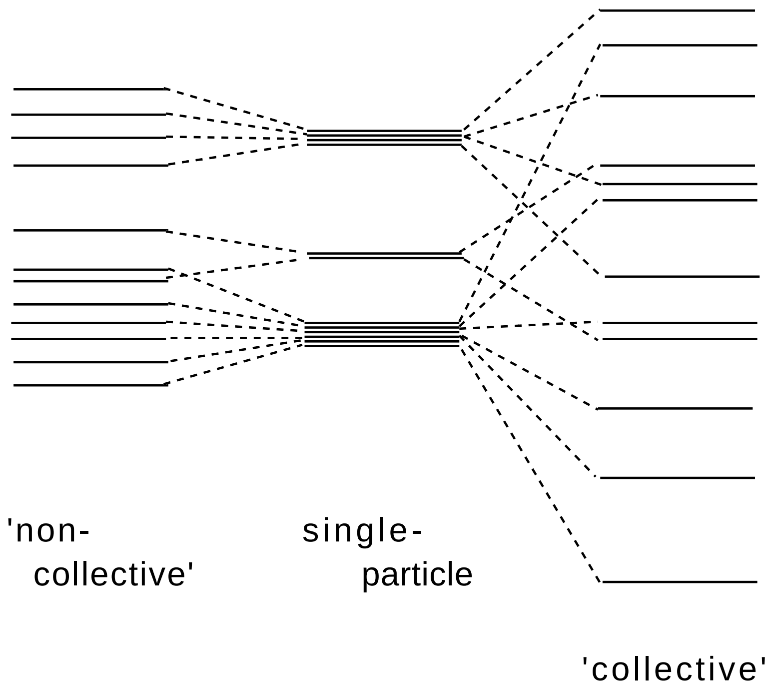
complexity due to finiteness   *e.g.* quantum fluctuation, shell effects, conservation, coexistence of collective & non-coll. d.o.f.

$\Downarrow$

Interacting shell model $\cdots$ desirable for level density calculations

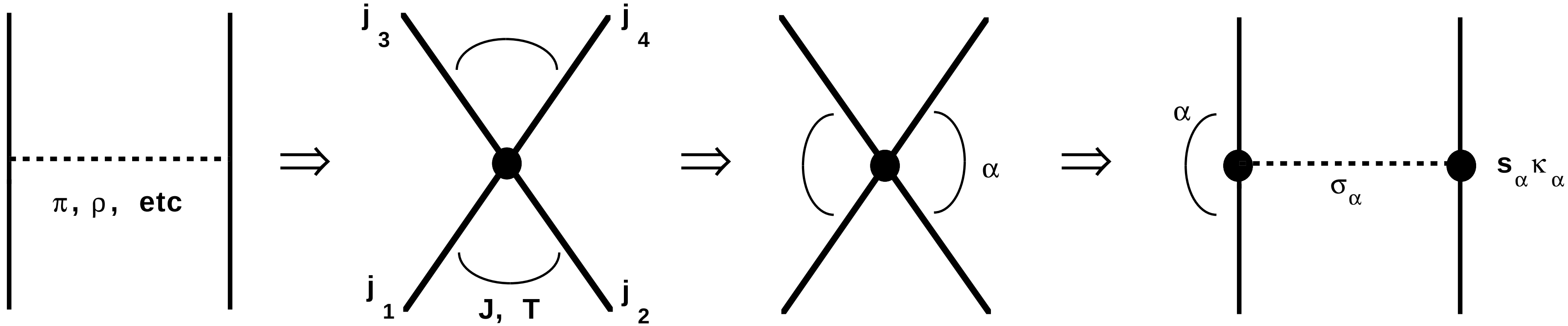
Both (1) shell effects & (2) 2-body correlations can fully be taken into account (but within finite model space)

e.g. $V = -\frac{\kappa}{2}\,\hat{\rho}^2$ ($\hat{\rho}$: 1-body op.)   typically, κ: large $\leftrightarrow$ collective



to handle sufficiently large model space
$\rightarrow$ quantum Monte Carlo method (Shell model Monte Carlo (SMMC) method)

Interacting shell model at finite T → auxiliary-fields path integral rep.



$H = \sum_j \epsilon_j \hat{N}_j + \sum_\alpha \frac{\kappa_\alpha}{2}\hat{\rho}_\alpha^2$ ← **Pandya transformation** ($\hat{\rho}_\alpha$ **: 1-body operator)**

Suzuki-Trotter decomposition : $e^{-\beta H} = \left(e^{-\Delta\beta H}\right)^{n_t}$ **with** $\beta = n_t \Delta\beta$ **;**

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

Hubbard-Stratonovich transformation :

$$\exp(-\Delta\beta\frac{\kappa_\alpha}{2}\hat{\rho}_\alpha^2) \propto \int d\sigma_\alpha \exp\left[-\Delta\beta(\frac{|\kappa_\alpha|}{2}\sigma_\alpha^2 + s_\alpha\kappa_\alpha\sigma_\alpha\hat{\rho}_\alpha)\right]; \quad s_\alpha = \begin{cases} \pm 1 & (\textbf{if } \kappa_\alpha < 0) \\ \pm i & (\textbf{if } \kappa_\alpha > 0) \end{cases}$$

$\Rightarrow$ $\mathrm{Tr}(Oe^{-\beta H}) \cong \int D[\sigma]G(\sigma)\mathrm{Tr}(OU_\sigma)$ **;** $G(\sigma) = \exp(-\Delta\beta\frac{|\kappa_\alpha|}{2}\sigma_\alpha^2)$, $U_\sigma = \Pi^{n_t}\exp(-\Delta\beta h_\sigma)$

$h_\sigma = \sum_j \epsilon_j \hat{N}_j + \sum_\alpha s_\alpha\kappa_\alpha\sigma_\alpha\hat{\rho}_\alpha$ **: (σ-dep.) s.p. Hamiltonian**

Ref. : G. H. Lang *et al.*, P.R.C 48, 1518 ('93)

SMMC: $\langle O\rangle = \dfrac{\mathrm{Tr}(Oe^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})} \cong \dfrac{1}{N_{\rm samp}}\sum_k \langle O\rangle_{\sigma(k)}$; $\langle O\rangle_{\sigma(k)} = \dfrac{\mathrm{Tr}(OU_\sigma)}{\mathrm{Tr}(U_\sigma)}$ **: measurement**

$\mathrm{Tr}_{\rm GC}(U_\sigma) = \det(1+\mathcal{U}_\sigma)$ $\mathcal{U}_\sigma$ **: s.p. matrix for** U_σ

$\cdots$ **calculable only via the s.p. matrices**

($\sigma(k) \leftarrow$ **random walk under** $W_\sigma = G(\sigma)\mathrm{Tr}(U_\sigma)$**)**

Level density calculation: $\rho(E) = \mathrm{Tr}\,\delta(E-H) \leftrightarrow Z(\beta) = \mathrm{Tr}(e^{-\beta H}) = \int dE\,\rho(E)e^{-\beta E}$

Laplace transform (Tr **: canonical trace)**

Saddle-point approx. for the inverse Laplace transformation

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

cf. thermodynamics

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

$E(\beta) = \langle H\rangle = \dfrac{\mathrm{Tr}(He^{-\beta H})}{Z(\beta)} \leftarrow$ **SMMC**

Z **&** $C \leftarrow$ **numerical integration** $\left(\ln[Z(0)/Z(\beta)] = \int d\beta' E(\beta')\right)$ **& differentiation**

$E_x = E - E_0$; $E_0 = \lim_{\beta\to\infty} E(\beta) \leftarrow E(\beta)$ **for large** β

Projections : (↔ conservation, finiteness)

- **particle-number projection** (both for protons & neutrons) → canonical

$$\mathrm{Tr}(U_\sigma) = \mathrm{Tr}_{\mathrm{GC}}(P_n U_\sigma)\,;\ P_n \propto \int d\phi\, \exp[i\phi(\hat{N} - n)]$$

ϕ : additional auxiliary field → exact integration

- **parity projection** → level densities for each parity

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

$$\mathrm{Tr}(P_\pm U_\sigma) = \tfrac{1}{2}\,\mathrm{Tr}[(1 \pm P)U_\sigma] = \tfrac{1}{2}[\,\mathrm{Tr}(U_\sigma) \pm \mathrm{Tr}(PU_\sigma)] \qquad (P:\ \text{parity op.})$$

$$\mathrm{Tr}_{\mathrm{GC}}(PU_\sigma) = \det(1 + \mathcal{P}\mathcal{U}_\sigma)\,; \quad \mathcal{P} = (-)^\ell \ \text{for each s.p. state}$$

- **isospin projection** (for T-conserved Hamiltonian & model space)

Ref.: H.N. & Y. Alhassid, Proc. of 11th Int. Symp. on Cap. γ-Ray Spec. ('03)

→ { isospin dependence of level densities
exact 'binding energy' correction (T-splitting is not necessarily reliable) }

$$\mathrm{Tr}_{\,T=T_0}(X) = \mathrm{Tr}_{\,|T_z|=T_0}(X) - \mathrm{Tr}_{\,|T_z|=T_0+1}(X) = \mathrm{Tr}_{\mathcal{A}}(X) - \mathrm{Tr}_{\mathcal{A}'}(X)$$

$$\mathcal{A} \equiv (Z, N) \cdots |T_z| = (N - Z)/2 \equiv T_0\,, \quad \mathcal{A}' \equiv (Z - 1, N + 1) \cdots |T_z| = T_0 + 1$$

random walk with $W_\sigma = G(\sigma)\mathrm{Tr}_{\mathcal{A}}(U_\sigma)$ → MC evaluation

$$\frac{Z_{T=T_0}(\beta)}{Z_{\mathcal{A}}(\beta)} = \frac{\mathrm{Tr}_{\,T=T_0}(e^{-\beta H})}{\mathrm{Tr}_{\mathcal{A}}(e^{-\beta H})} = 1 - \frac{\mathrm{Tr}_{\mathcal{A}'}(e^{-\beta H})}{\mathrm{Tr}_{\mathcal{A}}(e^{-\beta H})} \cong \frac{1}{N_{\mathrm{samp}}} \sum_k \left\{1 - \frac{\mathrm{Tr}_{\mathcal{A}'}[U_{\sigma(k)}]}{\mathrm{Tr}_{\mathcal{A}}[U_{\sigma(k)}]}\right\}$$

$$\langle O \rangle_{\mathcal{A}'} = \frac{\mathrm{Tr}_{\,T=T_0}(Oe^{-\beta H})}{Z_{T=T_0}(\beta)} = \frac{\mathrm{Tr}_{\mathcal{A}'}(Oe^{-\beta H})/Z_{\mathcal{A}}(\beta) - \mathrm{Tr}_{\mathcal{A}}(Oe^{-\beta H})/Z_{\mathcal{A}}(\beta)}{1 - Z_{\mathcal{A}'}(\beta)/Z_{\mathcal{A}}(\beta)}$$

Relation among MFA, SPA & SMMC

- **mean-field approx.** **(Hartree/Hartree-Fock)**

$$\exp(-\beta\frac{\kappa_\alpha}{2}\hat{\rho}_\alpha^2) \approx \exp\left[-\beta(\frac{|\kappa_\alpha|}{2}\sigma_\alpha^2 + s_\alpha\kappa_\alpha\sigma_\alpha\hat{\rho}_\alpha)\right]$$

$\sigma_\alpha = \langle\hat{\rho}_\alpha\rangle$ **: static mean-field (no fluctuation, no β-dependence)**

- **static-path approx.**

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

σ_α **: static auxiliary-field with fluctuation**

$\cdots$ **error of $O(\beta^2)$ in the Trotter decomp.** $\rightarrow$ **reasonable (only) for small β**

- **SMMC**

HS for $\Delta\beta$, instead of β $\rightarrow$ auxiliary-field path integral

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

σ_α **: β-dependent auxiliary-field with fluctuation**

(MC integration of the auxiliary-fields
$\rightarrow$ MC weighted sum of time-dependent 'mean-fields')

Fermion sign problem

$W_\sigma = G(\sigma)\mathrm{Tr}(U_\sigma)$ $\cdots$ **weight for the random walk of $\{\sigma\}$ in the MC calculation**

However, $\mathrm{Tr}(U_\sigma)$ is not always positive-definite $\rightarrow$ **"sign problem"**

nuclear effective interaction $\approx$ (collective part) + (non-collective perturbation)

$\uparrow$ **(almost) sign good**

$\searrow$ **unimportant for level densities ($\because$ gross property)**

$\Rightarrow$ $T=1$ **pairing +** $T=0$ **multipole interaction**

— **describes collective features well (including level densities)**

III. Spherical & nearly spherical nuclei — Fe-Ni region

Setup for $50 \lesssim A \lesssim 70$ nuclei

- **model space — full $pf + 0g_{9/2}$** (so as to cover $S_n(\lesssim 15\,\mathrm{MeV})$)
- **effective hamiltonian — T-conserving**

  s.p. energies ← Woods-Saxon potential (with LS term)

  $T=0$ surface-peaked multipole interactions ($\lambda = 2, 3, 4$)

  radial part ($\propto dV_{\mathrm{WS}}/dr$) & bare strength
  ← nuclear self-consistency (between density & s.p. potential)

  renormalization factors ↔ core-polarization effects
  ← comparison with a realistic interaction

  $\lambda = 2 \cdots \times 2,\ \ \lambda = 3 \cdots \times 1.5,\ \ \lambda = 4 \cdots \times 1$

  $T=1$ pairing interaction ← mass differences of $40 < A < 80$ spherical nuclei

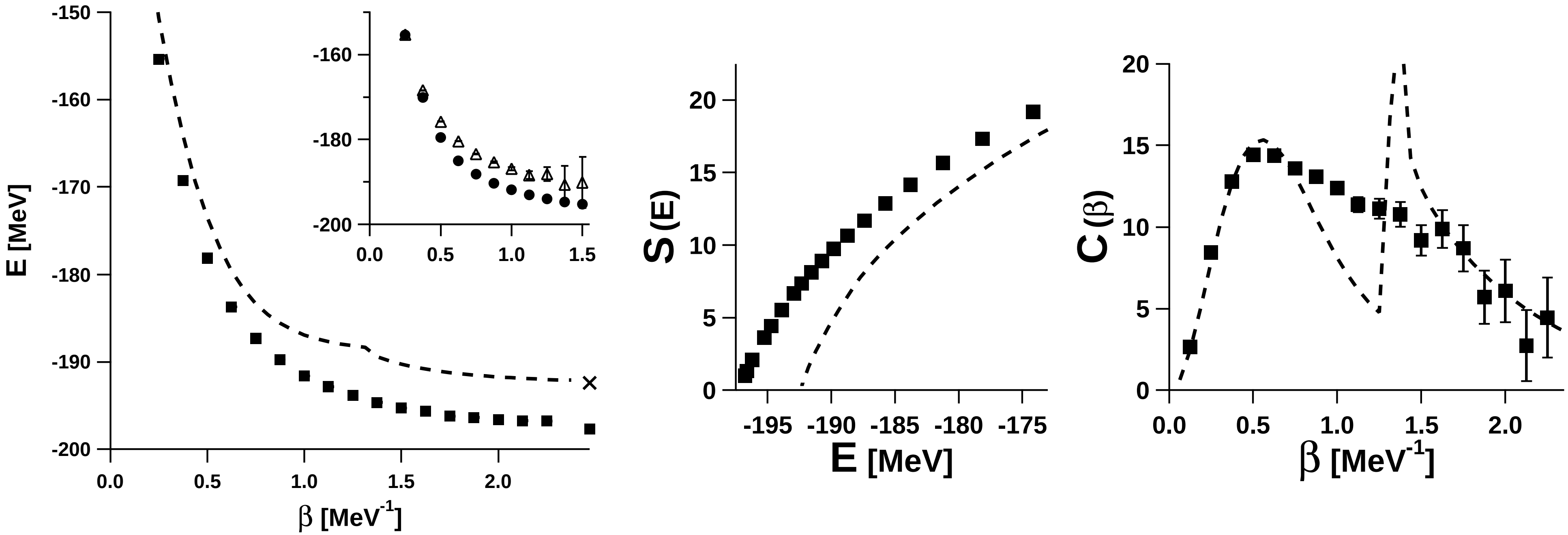
⟹ **uniquely determined for individual nucleus**

$*$ check of the hamiltonian for quadrupole collectivity in ^{56}Fe

$$E_Q \equiv \frac{\Sigma_i (E_i - E_0)|\langle 2_i^+|Q|0_g^+\rangle|^2}{\Sigma_i\,|\langle 2_i^+|Q|0_g^+\rangle|^2} \quad \rightarrow \quad \textbf{Exp. } (p,p'):\ 2.16, \quad \textbf{SMMC}: 2.12 \pm 0.11 \quad [\mathrm{MeV}]$$

- **MC** $\cdots$ $N_{\mathrm{samp}} \approx 4000$, $\Delta\beta = 1/32\,[\mathrm{MeV}^{-1}]$ (time slice)
  thermal $\cdots$ $d\beta = 1/16\,[\mathrm{MeV}^{-1}]$ (for Z & C)

Thermal properties of ^{56}Fe — SMMC *vs.* HF & exp.



- **mean-field (semi-classical) picture** → **signature to phase transition** at $\beta_c \approx 1.3\,\mathrm{MeV}^{-1}$

  $\cdots$ **deformed (low T) → spherical (high T)**

  shell model (full quantum theory) → **washed out due to quantum fluctuations !**

  ↔ **finiteness**

$E_0 \leftarrow$ **a sort of extrapolation to** $\beta = \infty$

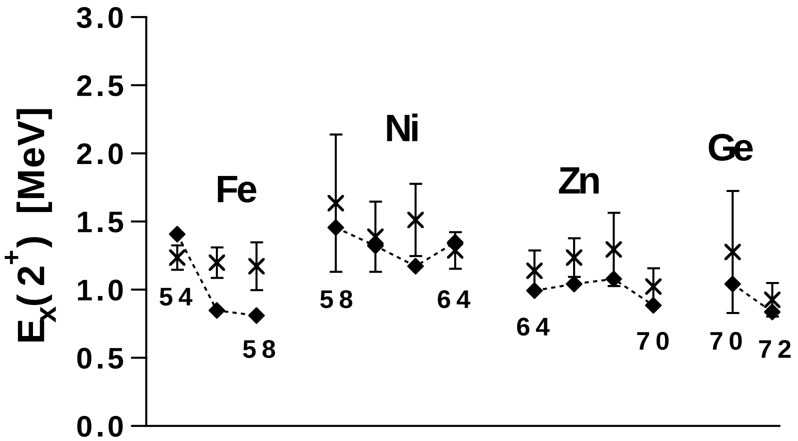
- **even-even nuclei**

  For large β, $E(\beta)$ **is slightly different from** E_0 **due to the contribution of** 2_1^+

  The amount of the 2_1^+ **contribution is estimated from** $\langle \hat{J}^2 \rangle$

  cf. **This approx. will be also good, if the influence of higher states in** $E(\beta)$ **is compensated with that in** $\langle \hat{J}^2 \rangle$

$E_x(2_1^+)$ **:**

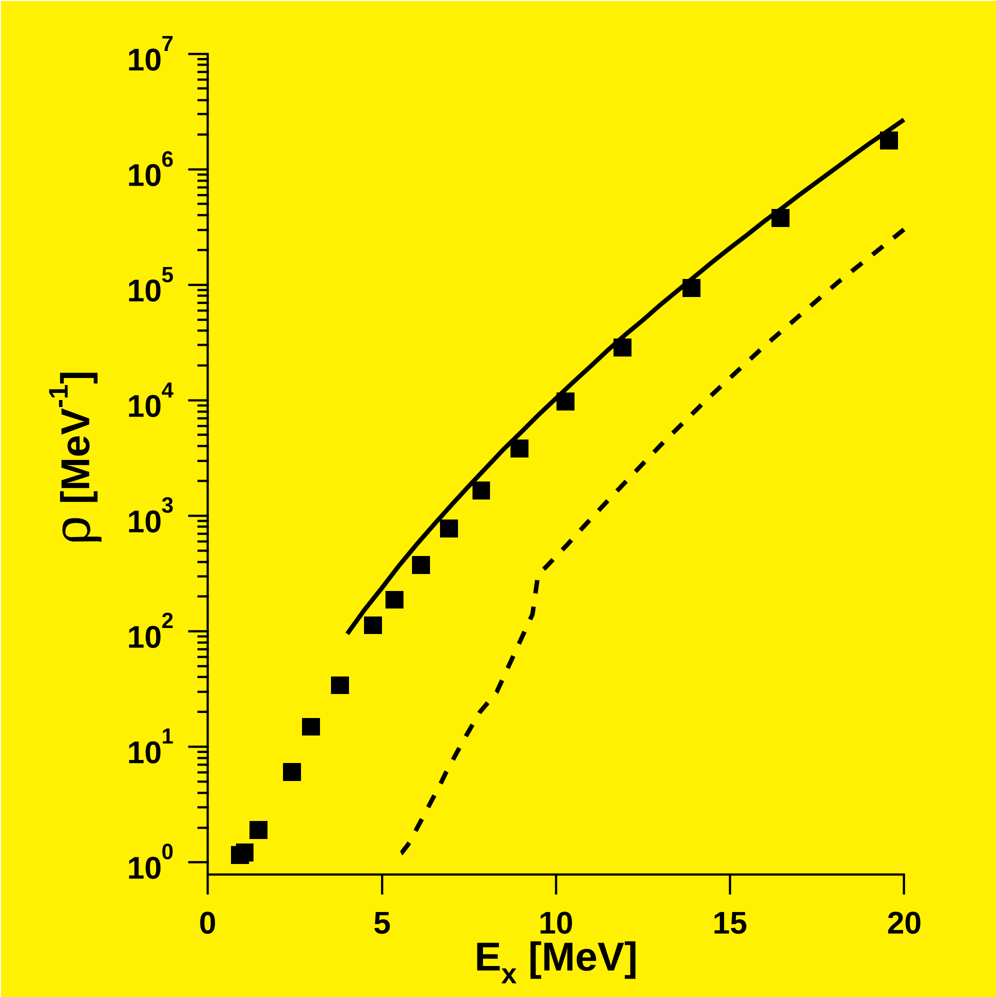


$\Rightarrow$ **check of** $\begin{cases} \text{this procedure} \\ \text{the present eff. } H \end{cases}$

- **odd-**A **& odd-odd nuclei**

  For large β, $E(\beta) \cong E_0$ **(because of higher degeneracy around** $E \cong E_0$**)**

Total level density (state density) of ^{56}Fe

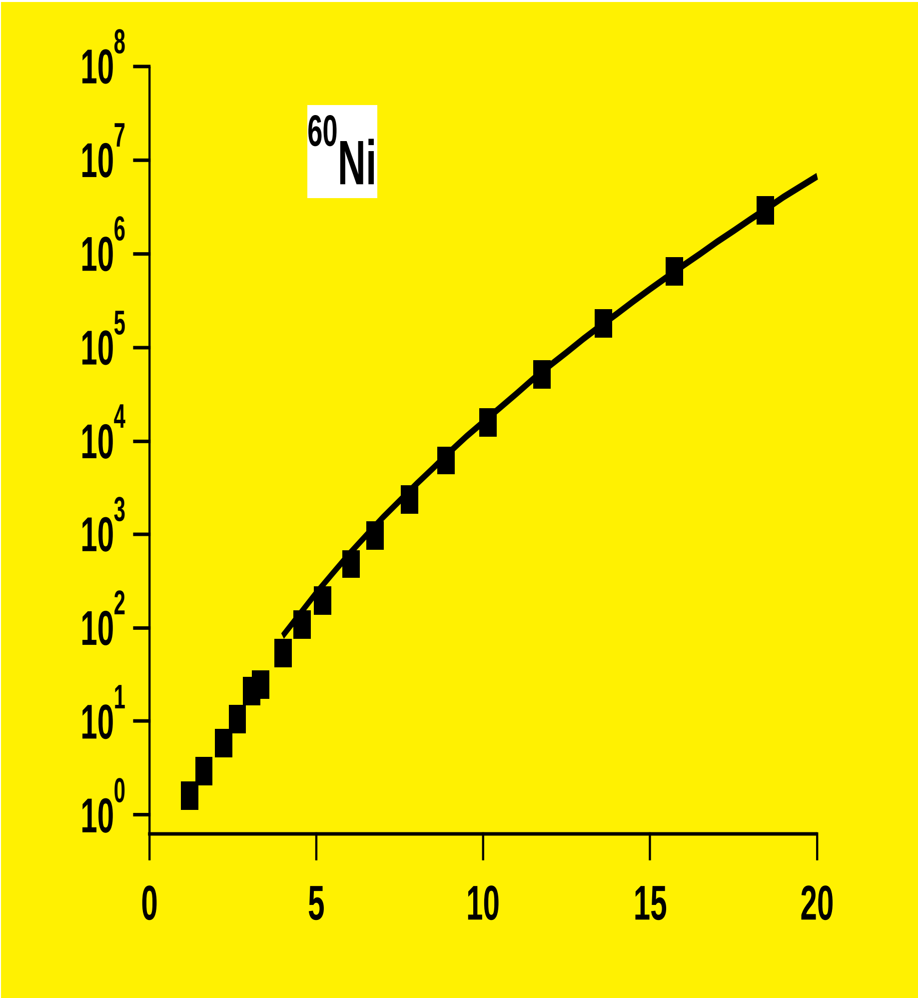


$$\left(\rho(E) = \frac{e^S}{\sqrt{2\pi\beta^{-2}C}} \quad \text{in SMMC \& HF cal.} \right)$$

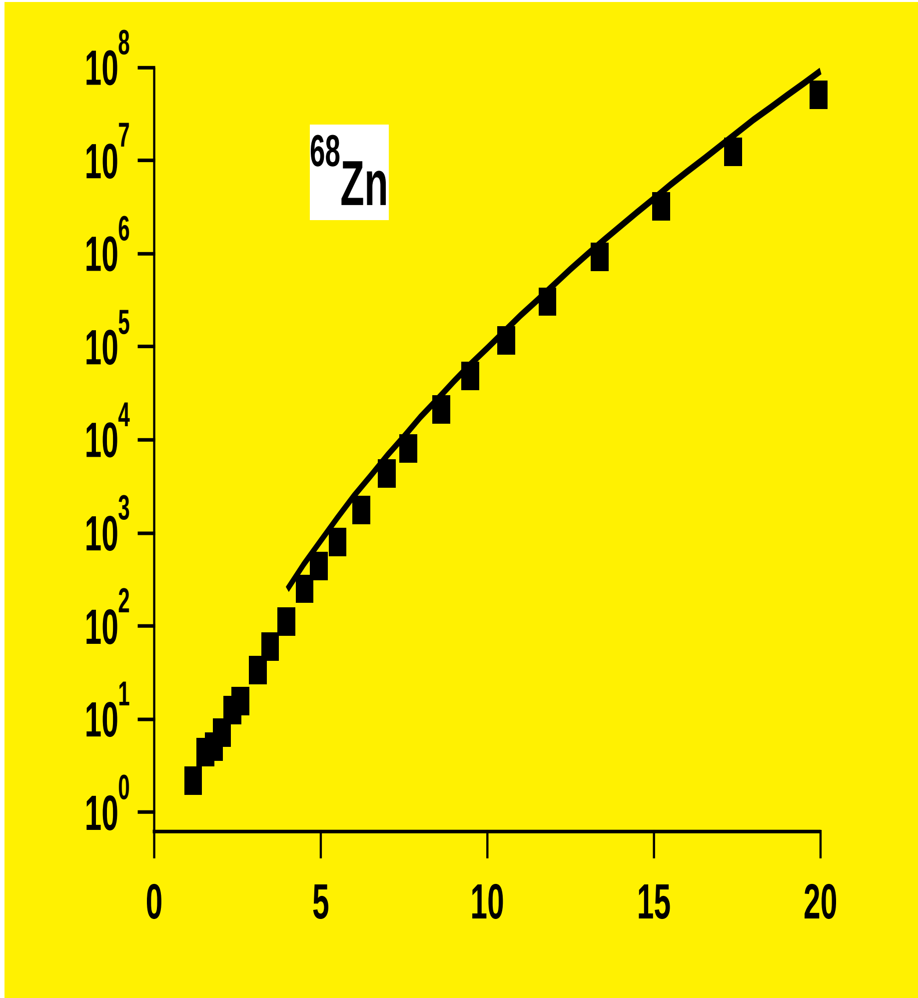
Note : Exp. total level density ← reconstructed with exp. BBF parameters

(C. C. Lu *et al.*, Nucl. Phys. A 190, 229('72))

Total level densities of other even-even nuclei

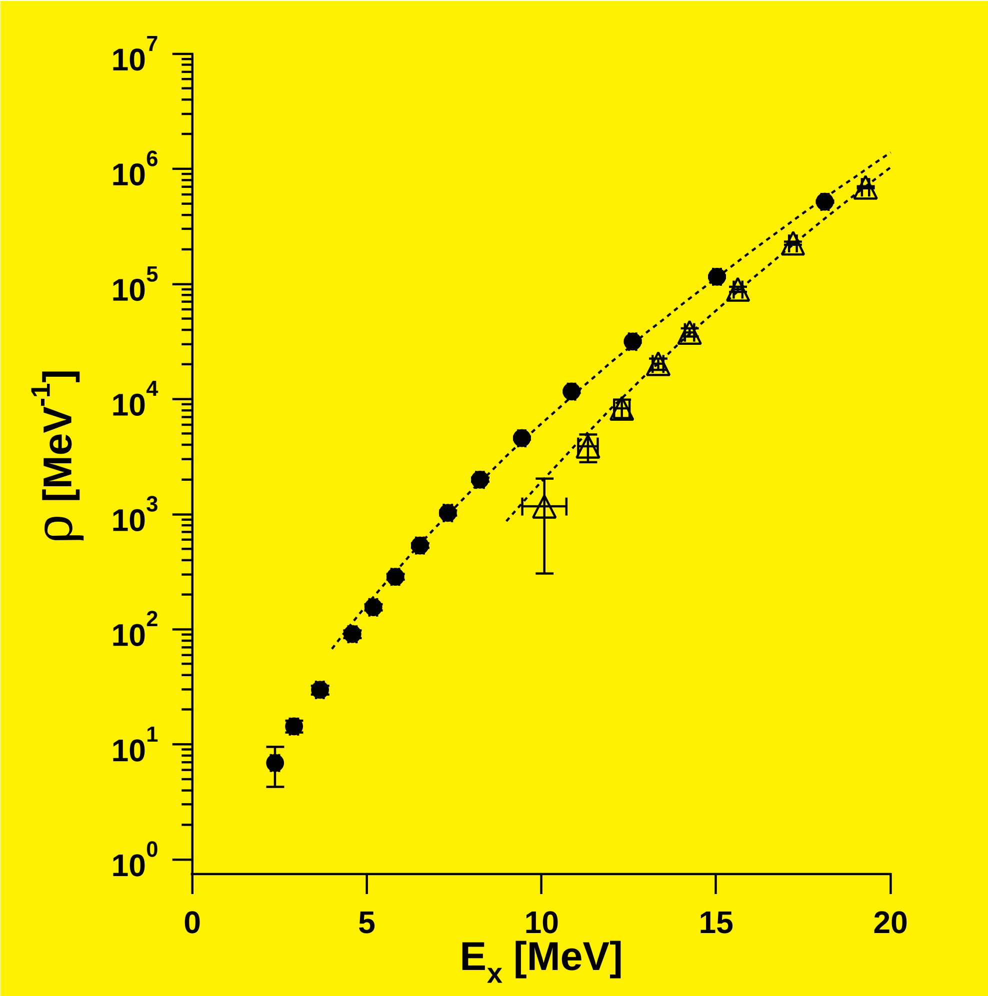


(Exp.: C. C. Lu *et al.*, N. P. A 190, 229('72))



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

Parity-projected level density of ^{56}Fe



$\Rightarrow$ **strong parity-dependence !**

— **not well considered so far**

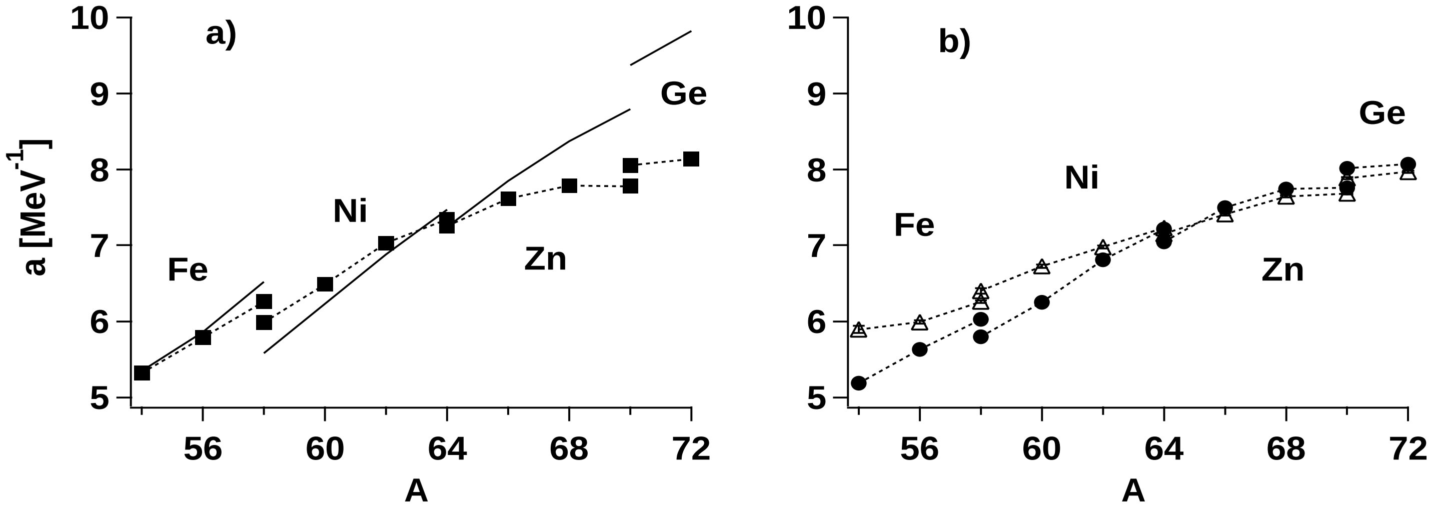
sensitive to shell structure

$\rightarrow$ **(Z- &) N-dep.**

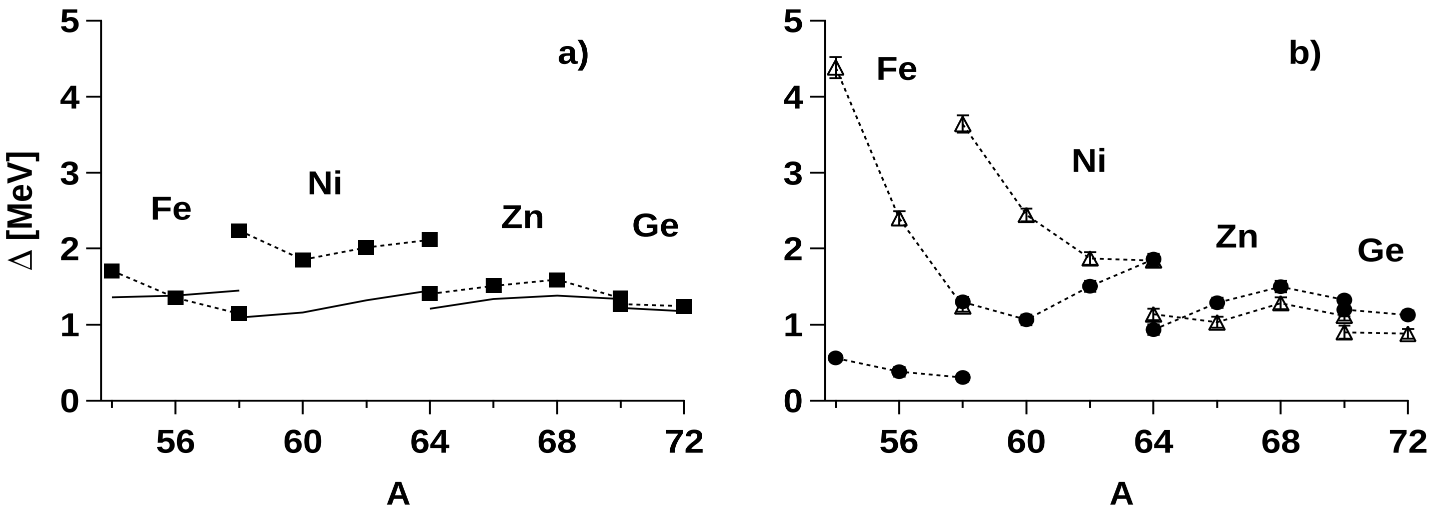
Systematics for (β-stable) even-even nuclei in the $50 \lesssim A \lesssim 70$ region

SMMC → fit to BBF **Nuclei:** $^{54-58}$**Fe,** $^{58-64}$**Ni,** $^{64-70}$**Zn,** ^{70,72}**Ge**

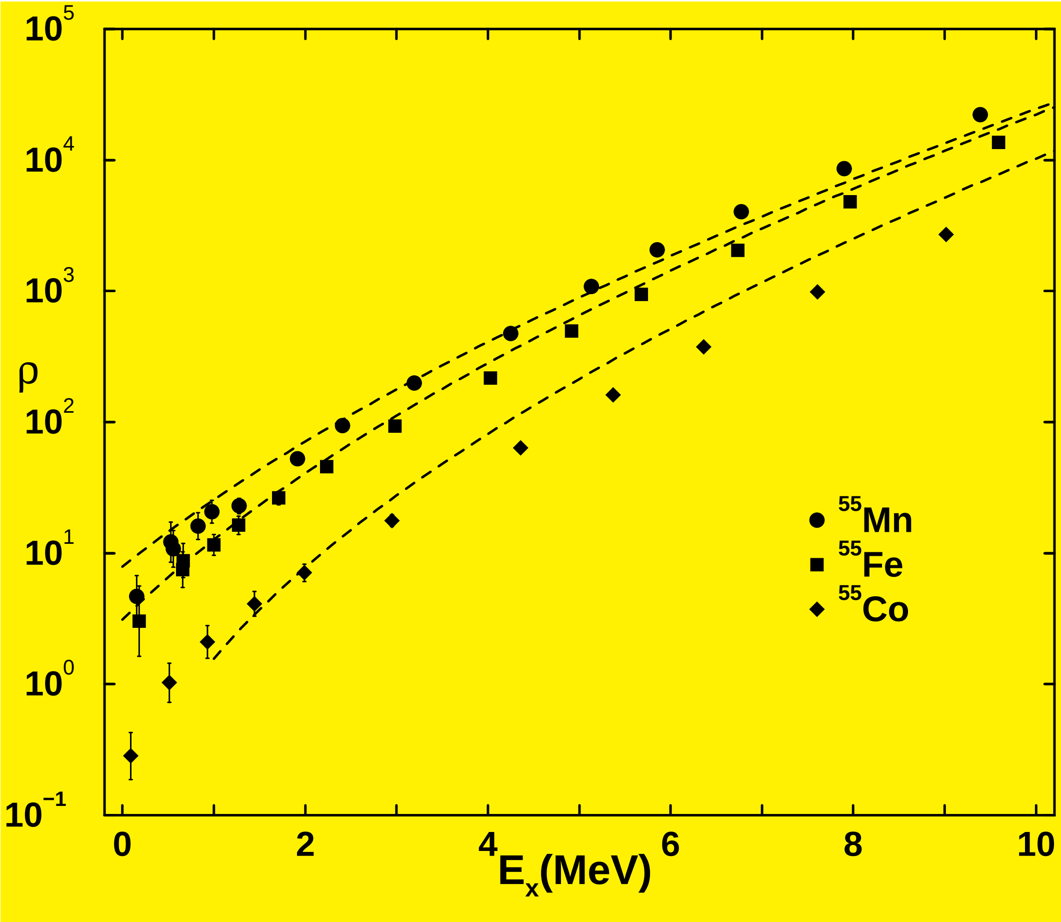
Single-particle level density parameters a:



Backshift parameters Δ:



Total level densities of $A = 55$ isobars



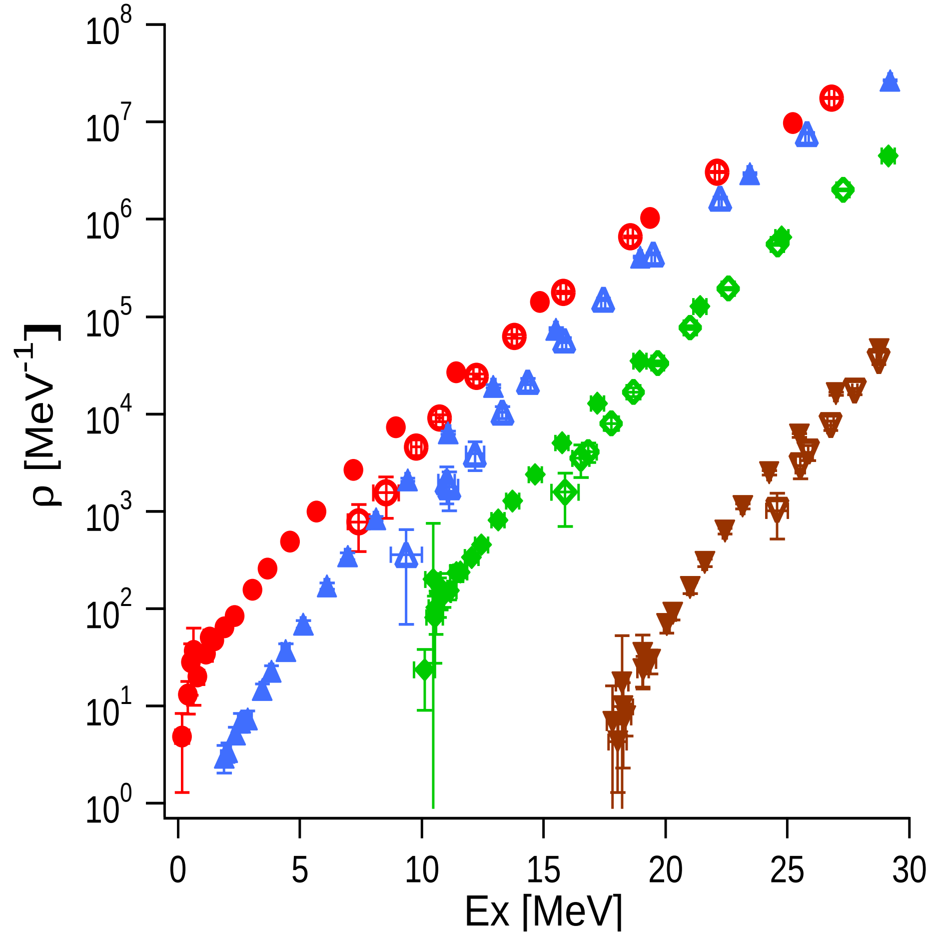
Exp. : W. Dilg *et al.*, Nucl. Phys. A217, 269 ('73)

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

— **not true !**

(← exp. & micro. cal.)

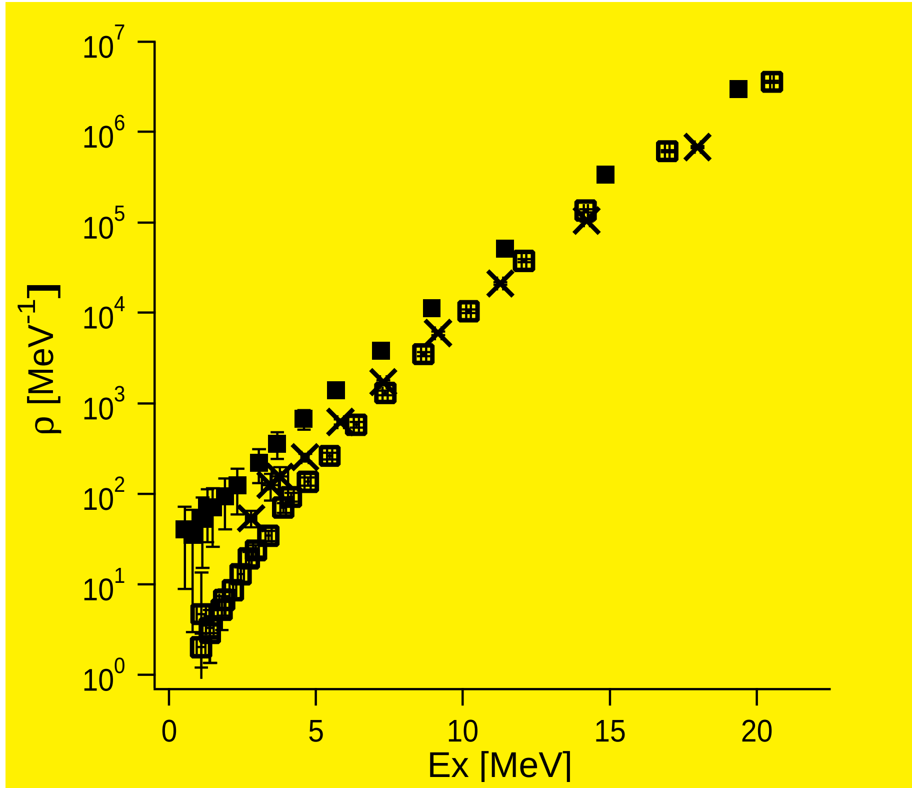
T,π-projected level densities of ^{58}Cu



Total level densities of ^{58}Cu

$$\rho_{\rm tot}(E) = \sum_{T\geq|T_z|,\pi=\pm} \rho_{T,\pi}(E)$$

(E ← **correction of** $E_T - E_{T=0}$)



■ **With T-projection** □ **Without T-projection**

× **With perturbative correction**

perturbative corr. — not so good

T-projection is important for $Z = N$ (& $Z = N \pm 1$?) nuclei

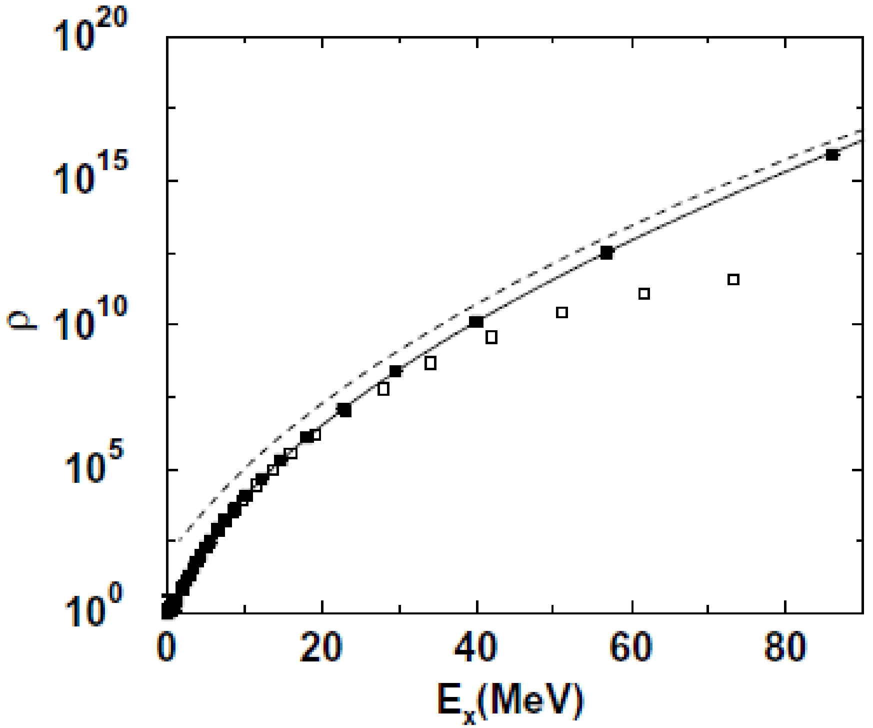
Extension to higher energy

higher energy (*i.e.* higher T) $\cdots$ size of model space is more important,

2-body correlation becomes less important

$\rightarrow$ connection to Hartree-Fock approach (without space truncation)

Total level densities of ^{56}Fe



free energy :

$$F(\beta) = F_{\rm SM,trunc}(\beta) + [F_{\rm HF,full}(\beta) - F_{\rm HF,trunc}(\beta)]$$

1st term $\leftrightarrow$ 2-body corr. at low E_x

2nd term $\leftrightarrow$ full d.o.f. at high E_x
(& subtract d.o.f. included in 1st term)

Note : in agreement with SMMC result at $E_x \lesssim 25\,{\rm MeV}$

Ref. : Y. Alhassid *et al.*, P. R. C 68, 044322 ('03)

IV. Deformed nuclei — rare-earth region

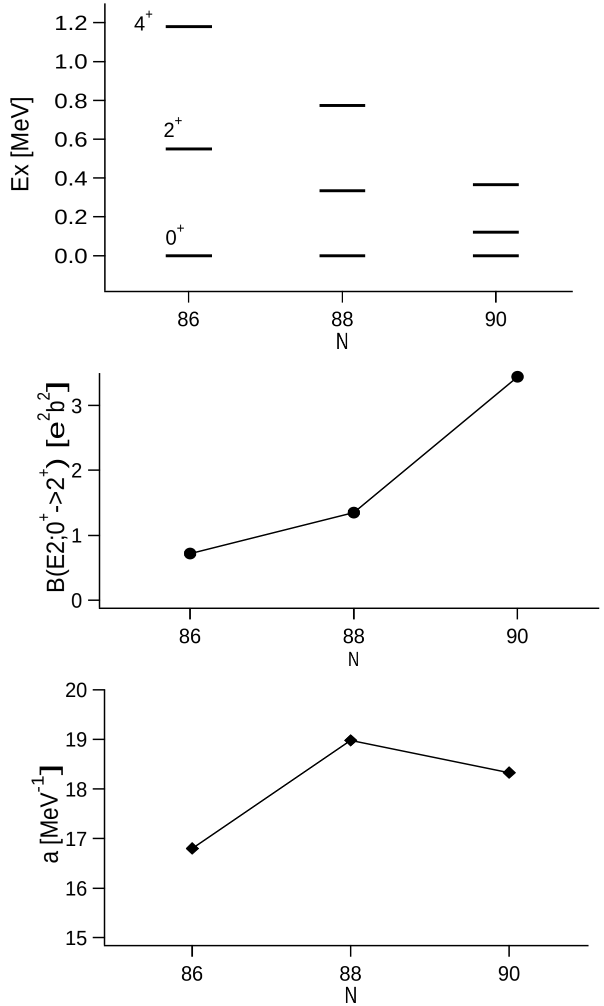
quadrupole deformation → influence level density ··· how ?

- deformation itself ?
- collective rotation ?
- influence of non-coll. d.o.f. ?

— all of them should be taken into account → shell model in large model space

Note : 'collective enhancement' ?

Sm isotopes :
(exp. data)



quadrupole collectivity
⟷̸ enhancement of ρ

What is important?

- **at high E_x ($E_x \gtrsim 5\,\mathrm{MeV}$) $\cdots$ non-coll. (*i.e.* s.p.) d.o.f. dominant**

  $\leftrightarrow$ degree of quadrupole deformation $\leftrightarrow$ strength of $Q \cdot Q$-int.

  $\leftarrow$ checked by MF approx.

- **at low E_x ($E_x \lesssim 2\,\mathrm{MeV}$) $\cdots$ $\rho(E) \propto$ (mom. of inertia $\mathcal{I}$) $\leftarrow$ single rotational band**

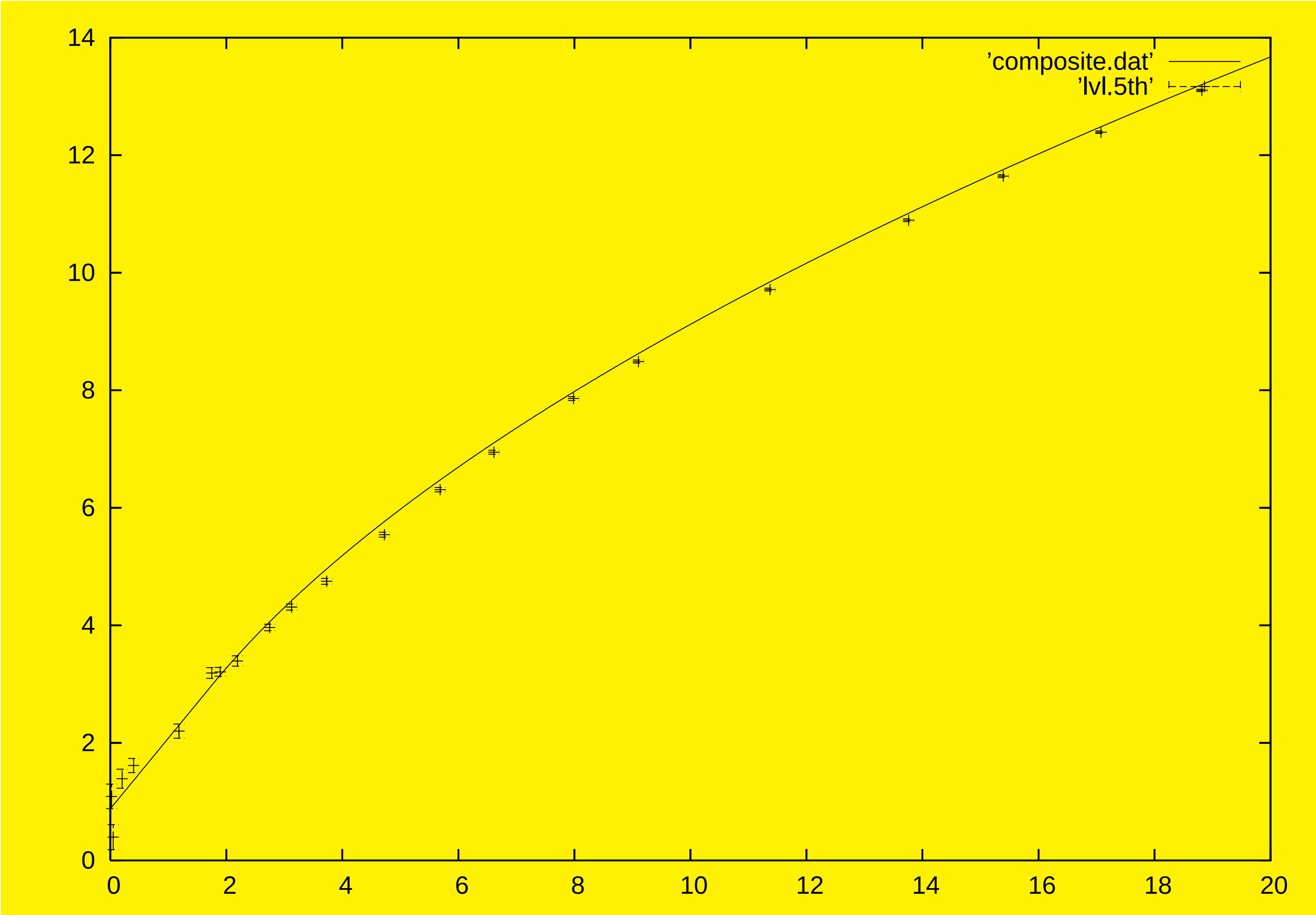
  $\leftrightarrow$ strength of pairing int. $\leftarrow$ checked from $\langle \boldsymbol{J}^2 \rangle_T \, (\approx 2\mathcal{I} \cdot T)$ for small T

  (or Thouless-Valatin estimate?)

$\Rightarrow$ preliminary result for ^{162}Dy (in collaboration with L. Fang & Y. Alhassid)

model space $\approx 1.5\,\hbar\omega$, WS s.p.e. + pairing int. + multipole int.

Total level density of ^{162}Dy — $\ln \rho(E_x)$ (preliminary)



V. Summary

1. SMMC approaches to nuclear structure at finite temperature
   → accurate microscopic calculations of nuclear level densities
   (for spherical & nearly spherical nuclei)
   ⇒ application to astrophysics ? Ref. : D. Mocelj *et al.*, N.P.A 758, 154c

2. Extensions

   higher energy ← connection to HF · · · works well

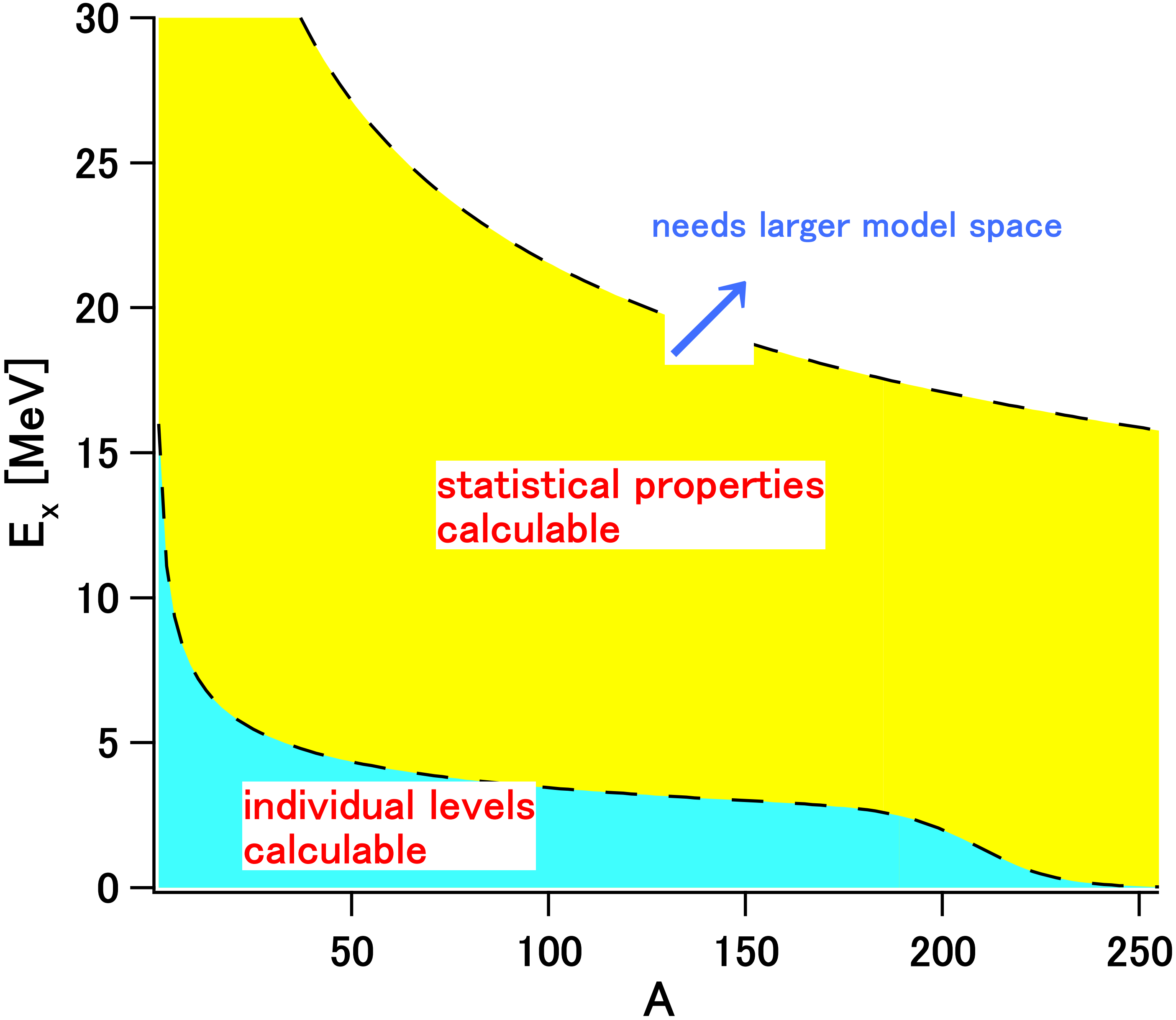
   deformed nuclei — promising (work in progress)

3. Problems

   int. parameters for deformed nuclei — systematics ? (↔ predictability)

   connection between spherical & deformed region

Crude overview of 'shell model world' at present (or in near future)



Collaborators:

Y. Alhassid, S. Liu, L. Fang (Yale Univ., U.S.A.)

G. F. Bertsch (Univ. of Washington, U.S.A.)

References:

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