Spin- and isospin-projected nuclear level densities in the shell model Monte Carlo methods

@ Oslo (May 11 – 15, 2009)

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I. Introduction

Nuclei — isolated system with various conservation laws (π, J, T)

$\cdots$ statistical properties ? — challenging problem !

important pieces : • shell effects • 2-body correlations

Level densities (↔ partition function)

— most basic physical quantity for statistical properties of nuclei

I. Introduction

Nuclei — **isolated system with various conservation laws** (π, J, T)

$\cdots$ **statistical properties ?** — **challenging problem !**

important pieces : • **shell effects** • **2-body correlations**

Level densities (↔ **partition function**)
— **most basic physical quantity for statistical properties of nuclei**

SMMC approach to nuclear level densities

$\cdots$ **successful for medium-mass** ($A \sim 50 - 70$) **& rare-earth** (***e.g.*** ^{162}**Dy**) **nuclei**

- **state densities — good agreement with exp.**
- π **projection** → π**-dep. of level densities (?)**
- J **projection** → J**-dep. of level densities ?**
- T **projection** → **correction of** T**-dep.** (T **: isospin**)

Why SMMC ?

- interacting shell model (with spherical bases)

$$\rightarrow \begin{cases} \text{shell effects} \quad \rightarrow \text{nucleus-dep.} \\ \text{(collective) 2-body correlations} \\ \qquad \text{conservation laws} \leftrightarrow \text{correlations via NG mode} \\ \text{g.s. energy} \rightarrow \text{excitation energies} \end{cases}$$

size of model space ?

- model space — can be large (much larger than diagonalization)
- finite temp. formalism (→ not constrained to lowest states)

  n proj. → canonical ensemble

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⇒ microscopic framework suitable to investigate nuclear statistical properties !

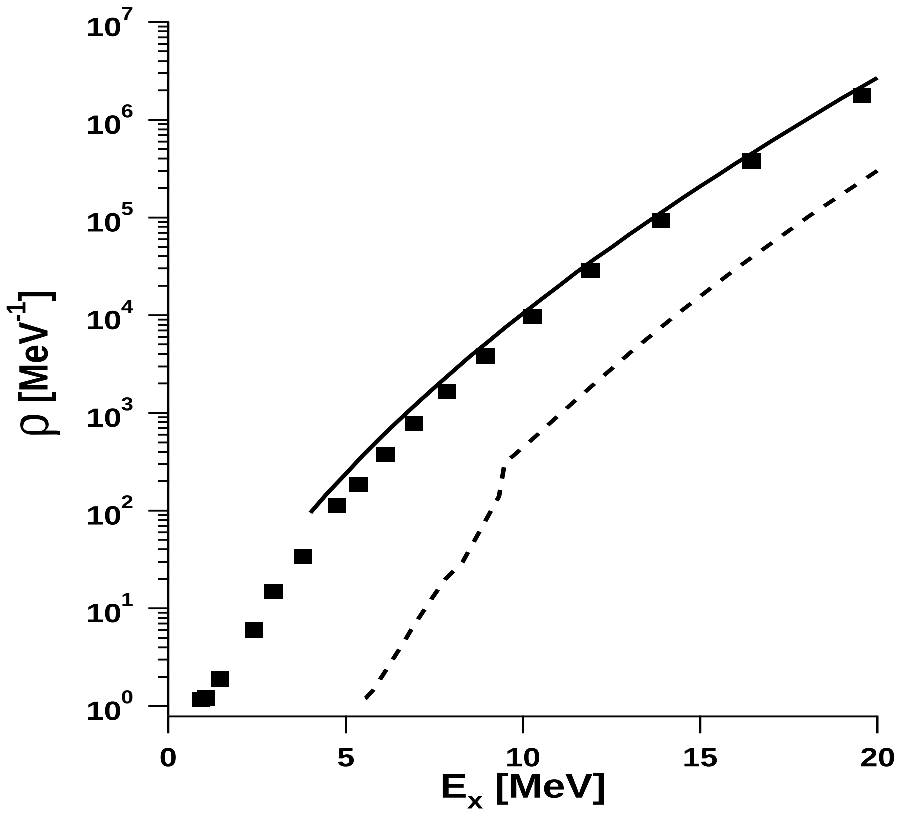
(→ predictability)

SMMC $\rightarrow E(\beta) = \langle H \rangle_\beta$ **(**β**: inverse temp.)** $\rightarrow Z$**,** S**,** C

$\rightarrow$ **state density** $\rho(E) = \sum_{J\pi}(2J+1)\rho_{J\pi}(E_x) \approx \dfrac{e^S}{\sqrt{2\pi\beta^{-2}C}}$

(saddle-point approx.)

State density of ^{56}**Fe:** **Ref.: H.N. & Y. Alhassid, P.R.L. 79, 2939 ('97)**



$\left(E_x \gtrsim 25\,\mathrm{MeV} \cdots \right.$ **s.p. d.o.f. is essential** $\rightarrow$ **connection to HF**

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

★ J-projected level densities

- significance — important input in astrophysics !

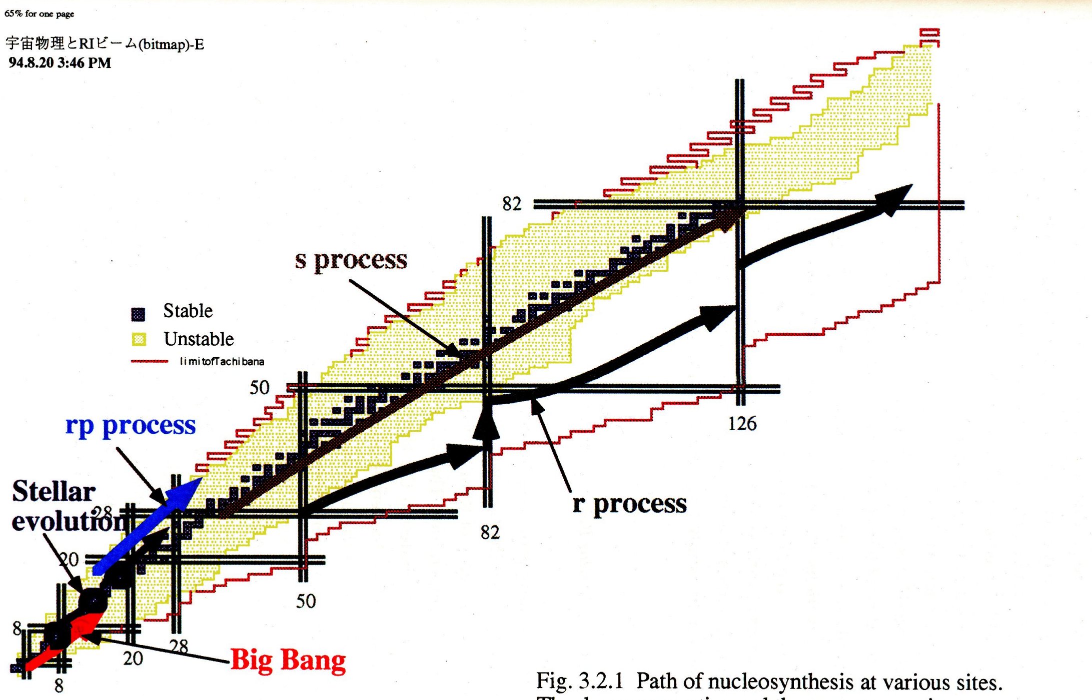


Fig. 3.2.1 Path of nucleosynthesis at various sites. The decay properties and the capture reaction rates of unstable nuclei are essential for understanding these path ways and thus the elemental abundances.

nucleosynthesis

s & r-process
— (n,γ) ***vs.*** β-decay

rp-process
— (p,γ) ***vs.*** β-decay

e.g. $\sigma_{fi}^{(n,\gamma)} \propto \int \frac{dE_x}{E_n} \sum_{J,\pi} (2J+1)\, \rho_{J\pi}(E_x)\, \frac{\mathcal{T}_{J\pi}^{(\gamma)}(E_\gamma)\mathcal{T}_{J\pi}^{(n)}(E_n)}{\mathcal{T}_{\rm tot}}$

($\mathcal{T}$: transmission coef.)

$\cdots$ **Hauser-Feshbach formula**

- **conventional approach — spin cutoff model**

$$\rho_J(E_x) = \rho(E_x)\,\frac{2J+1}{2\sqrt{2\pi}\sigma^3}\,e^{-J(J+1)/2\sigma^2} \qquad (\textbf{\textit{e.g.}}\ \sigma = \sqrt{\mathcal{I}/\beta}\,)$$

$\cdots$ **how good ?**

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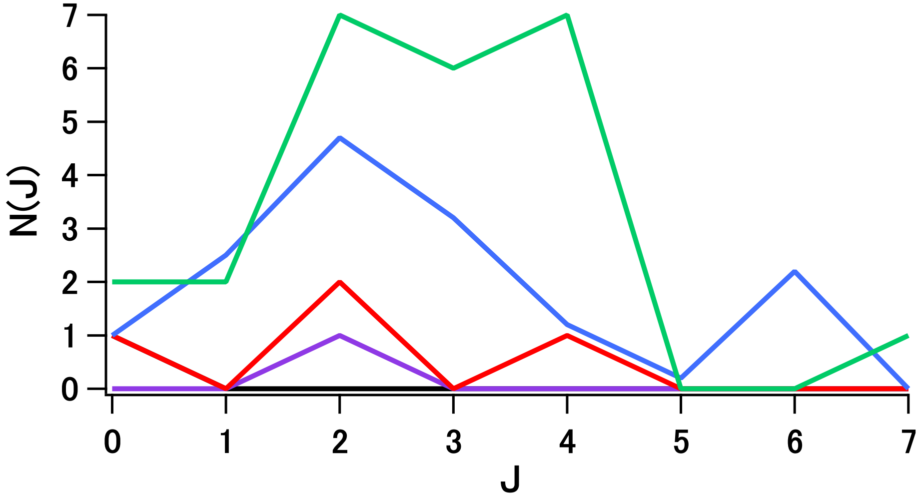
cf. number of levels up to $E_x = 5\,\mathrm{MeV}$ in ^{56}Fe : (in each $1\,\mathrm{MeV}$ bin)



— **significant deviation from Gaussian** (at low E_x)

- **conventional approach — spin cutoff model**

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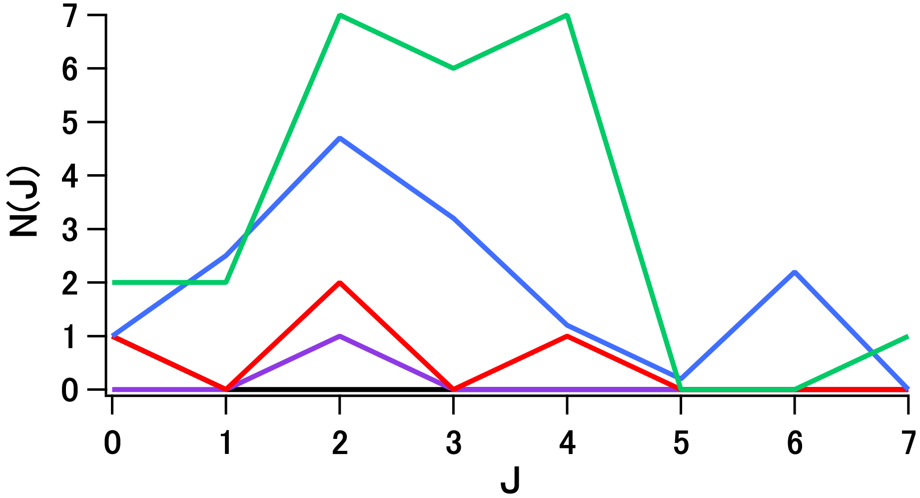

— **significant deviation from Gaussian (at low E_x)**

$\Rightarrow$ **detailed microscopic study via SMMC**

★ **T-projected level densities** — **important in $Z \sim N$ nuclei**

(as discussed later)

II. Setup

0) **Fe-region nuclei** $\cdots$ **successful SMMC description for state density**

$\rightarrow$ **extensive study using the same setup**

1) **Model space — complete $pf + g_{9/2}$ shell**

2) **Effective Hamiltonian** $(\cdots$ **isoscalar)**

$$H = \sum_a \varepsilon_a \hat{n}_a + g_0 P^{(0,1)\dagger} \cdot \tilde{P}^{(0,1)} - \sum_\lambda \chi_\lambda : O^{(\lambda,0)} \cdot O^{(\lambda,0)} :$$

($\leftrightarrow$ **dominating collective features**)

$$P^{(0,1)\dagger} = \tfrac{1}{2} \sum_a (-)^\ell \, [a_a^\dagger \times a_a^\dagger]^{(\lambda=0,T=1)},$$

$$O^{(\lambda,T)} = \frac{1}{\sqrt{2\lambda+1}} \sum_{ab} \langle a || \tfrac{dV_{\rm WS}}{dr} Y_\lambda || b \rangle \, [a_a^\dagger \times \tilde{a}_b]^{(\lambda,T)}$$

- ε_a **: s.p. energy** $\leftarrow$ **Woods-Saxon (+ ℓs) pot.**
- **(surface-peaked) multipole-multipole interaction**

  $\chi_\lambda = \chi \, k_\lambda$ **;** $\begin{cases} \chi \textbf{: self-consistent value} \\ k_\lambda \textbf{: renormalization factor} \leftrightarrow \textbf{core pol. effects} \end{cases}$

  $\lambda = 2, 3, 4$ **;** $k_2 = 2$, $k_3 = 1.5$, $k_4 = 1$ **($\leftarrow$ fit to realistic int.)**
- **($T = 1$) monopole pairing interaction**

  $g_0 = 0.212\,\mathrm{MeV}$ **($\leftarrow$ fit to systematics of even-odd mass difference)**

III. J-projected level densities

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

★ J projection in SMMC

- **J_z projection** $\cdots$ **1-dim. integral**

$$\mathrm{Tr}_M \hat{X} = \sum_{\alpha, J \geq |M|} \langle \alpha J M | \hat{X} | \alpha J M \rangle$$

$$= \int \frac{d\varphi}{2\pi} \mathrm{Tr}\big[e^{i\varphi(\hat{J}_z - M)} \hat{X}\big] \left(= \int \frac{d\varphi}{2\pi} \sum_{M'} \mathrm{Tr}_{M'}\big[e^{i\varphi(M'-M)} \hat{X}\big] \right)$$

$$= \frac{1}{2J_s + 1} \sum_{k=-J_s}^{J_s} e^{-i\varphi_k M}\, \mathrm{Tr}\big[e^{i\varphi_k \hat{J}_z} \hat{X}\big]\,; \quad \varphi_k = \frac{2\pi k}{2J_s + 1}$$

(J_s: max. value of J)

Tr: **canonical trace → triple proj. with respect to** (Z, N, M)

- **J projection** $\cdots$ **3-dim. integral? (with respect to Euler angles)**

$\hat{X}$: **scalar operator** (***e.g.*** **Hamiltonian)**

$$\mathrm{Tr}_J \hat{X} = \sum_{\alpha} \langle \alpha J | \hat{X} | \alpha J \rangle = \sum_{\alpha, J' \geq J} \langle \alpha J' J | \hat{X} | \alpha J' J \rangle - \sum_{\alpha, J' \geq J+1} \langle \alpha J'\, J{+}1 | \hat{X} | \alpha J'\, J{+}1 \rangle$$

$$= \mathrm{Tr}_{M=J} \hat{X} - \mathrm{Tr}_{M=J+1} \hat{X}$$

→ **3-dim. integral may be avoidable**

- **incorporation into SMMC**

  — **combination with Hubbard-Stratonovich representation**

$$\textbf{HS rep.}: \; e^{-\beta H} = \int D[\sigma]\, G_\sigma U_\sigma \qquad \left(\begin{array}{l} \sigma \;: \textbf{ auxiliary field} \\ G_\sigma : \textbf{ Gaussian weight} \\ U_\sigma : \textbf{ s.p. propagator under } \sigma \textbf{ fields} \end{array} \right)$$

$$\to \langle O \rangle_\beta \equiv \frac{\mathrm{Tr}(O e^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})} = \frac{\int D[\sigma]\, G_\sigma \mathrm{Tr}(O U_\sigma)}{\int D[\sigma]\, G_\sigma \mathrm{Tr}\, U_\sigma} = \frac{\left\langle \frac{\mathrm{Tr}(O U_\sigma)}{\mathrm{Tr}\, U_\sigma} \Phi_\sigma \right\rangle_W}{\langle \Phi_\sigma \rangle_W} \; ;$$

$$\langle X_\sigma \rangle_W \equiv \frac{\int D[\sigma]\, W(\sigma)\, X_\sigma}{\int D[\sigma]\, W(\sigma)}, \quad W(\sigma) \equiv G_\sigma \, |\mathrm{Tr}\, U_\sigma| \, , \quad \Phi_\sigma \equiv \frac{\mathrm{Tr}\, U_\sigma}{|\mathrm{Tr}\, U_\sigma|}$$

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$$\frac{Z_M(\beta)}{Z(\beta)}\left(= \frac{\mathrm{Tr}_M(e^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})}\right) = \frac{\left\langle \frac{\mathrm{Tr}_M\, U_\sigma}{\mathrm{Tr}\, U_\sigma}\Phi_\sigma\right\rangle_W}{\langle\Phi_\sigma\rangle_W}\,,$$

$$\frac{Z_J(\beta)}{Z(\beta)}\left(= \frac{\mathrm{Tr}_J(e^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})}\right) = \frac{\left\langle \left(\frac{\mathrm{Tr}_{M=J}\, U_\sigma}{\mathrm{Tr}\, U_\sigma} - \frac{\mathrm{Tr}_{M=J+1}\, U_\sigma}{\mathrm{Tr}\, U_\sigma}\right)\Phi_\sigma\right\rangle_W}{\langle\Phi_\sigma\rangle_W}\,,$$

$$\langle O\rangle_{\beta,J}\left(\equiv \frac{\mathrm{Tr}_J(Oe^{-\beta H})}{Z_J(\beta)}\right) = \frac{\left\langle \left(\frac{\mathrm{Tr}_{M=J}(OU_\sigma)}{\mathrm{Tr}\, U_\sigma} - \frac{\mathrm{Tr}_{M=J+1}(OU_\sigma)}{\mathrm{Tr}\, U_\sigma}\right)\Phi_\sigma\right\rangle_W}{\left\langle \left(\frac{\mathrm{Tr}_{M=J}\, U_\sigma}{\mathrm{Tr}\, U_\sigma} - \frac{\mathrm{Tr}_{M=J+1}\, U_\sigma}{\mathrm{Tr}\, U_\sigma}\right)\Phi_\sigma\right\rangle_W} \quad (O: \textbf{scalar})$$

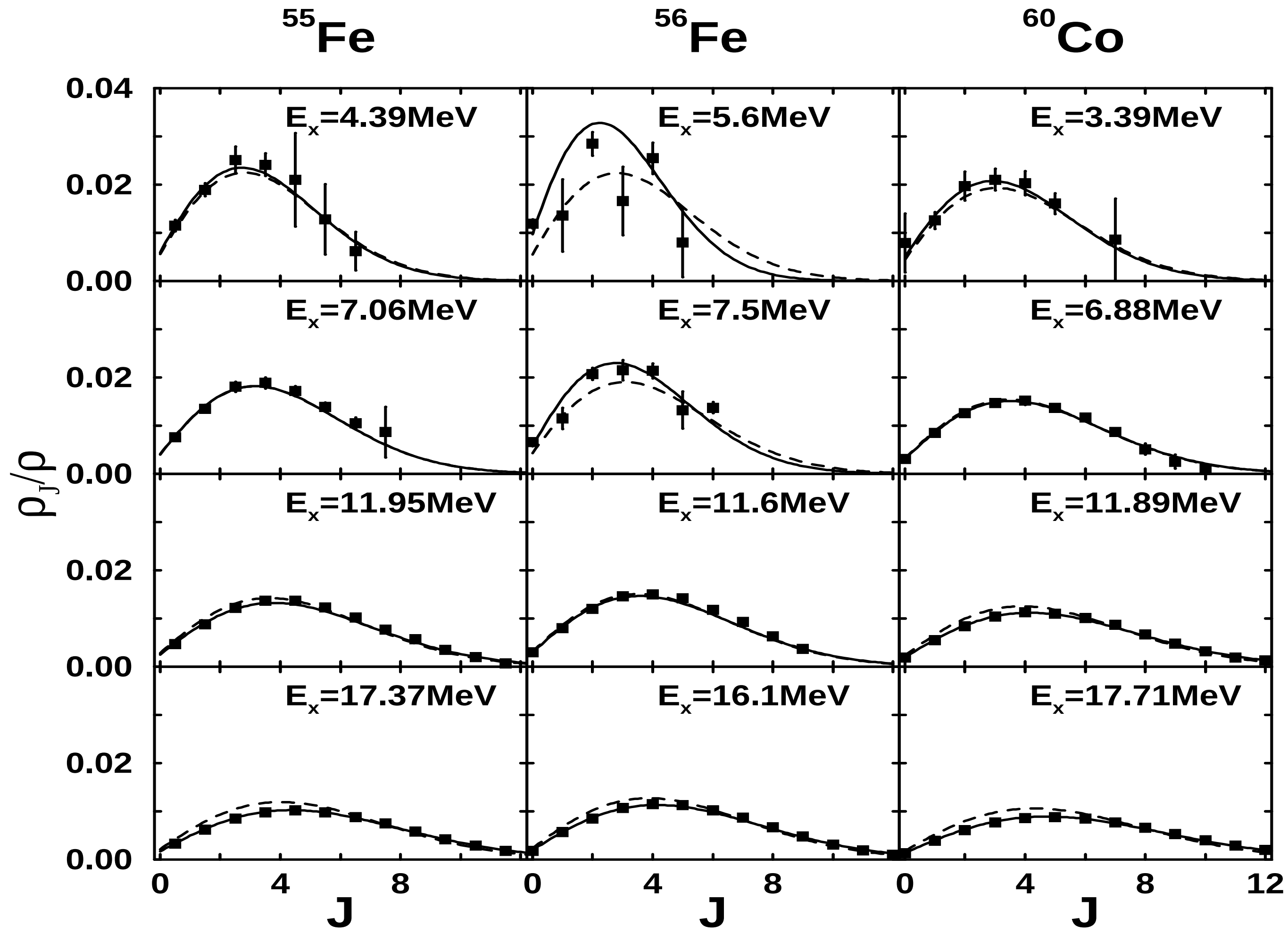
MC sampling of σ **according to** $W(\sigma)$ $\rightarrow$ **evaluate** $\langle O\rangle_{\beta,J}$

★ J-projected level densities

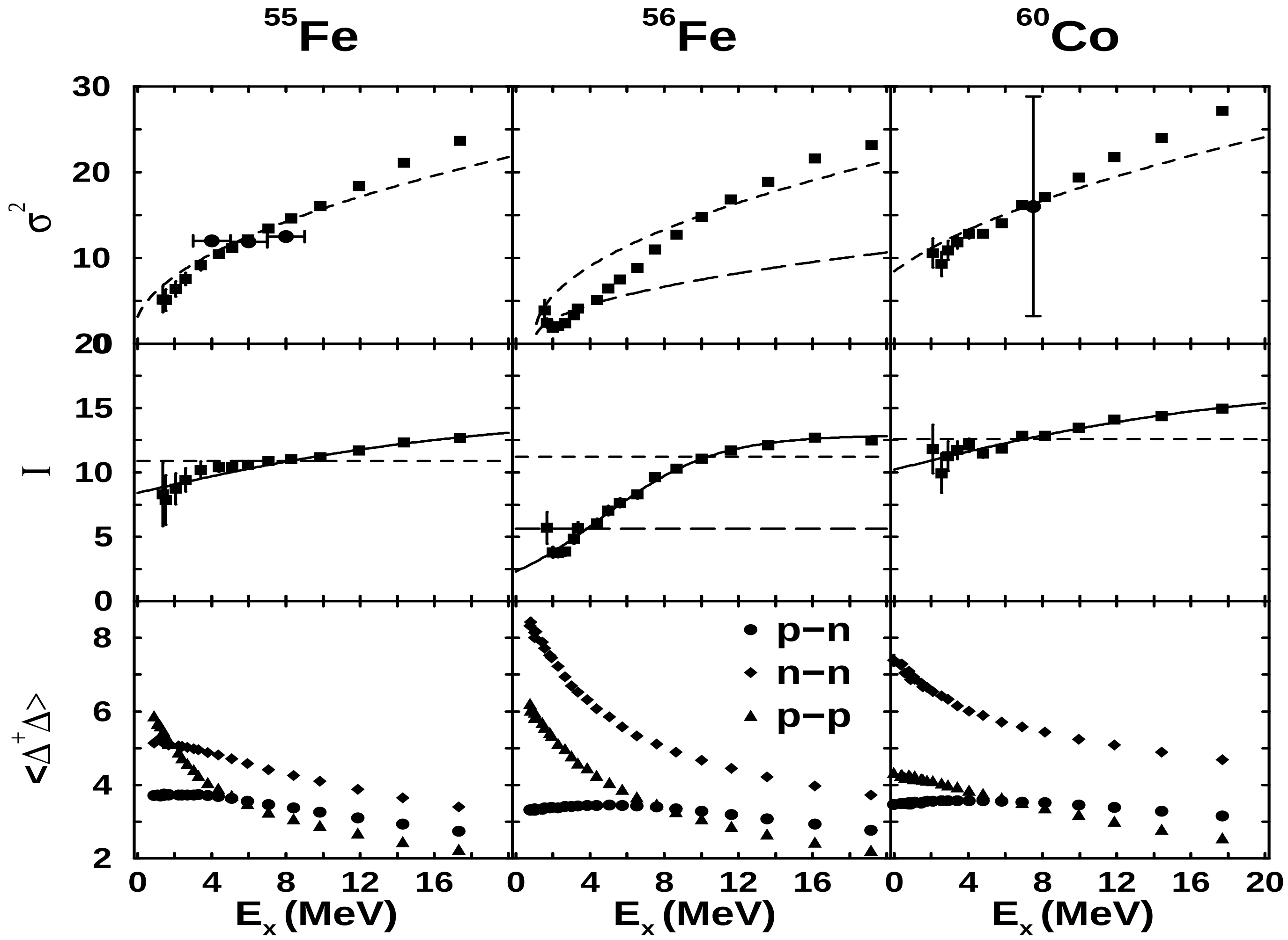
$$\text{SMMC} \rightarrow E_J(\beta) = \langle H \rangle_{\beta,J} \rightarrow Z_J,\ S_J,\ C_J \rightarrow \rho_J \approx \frac{e^{S_J}}{\sqrt{2\pi\beta^{-2}C_J}}$$

^{56}Fe (even-even), ^{55}Fe (odd-A) & ^{60}Co (odd-odd)

— comparison to spin cutoff model



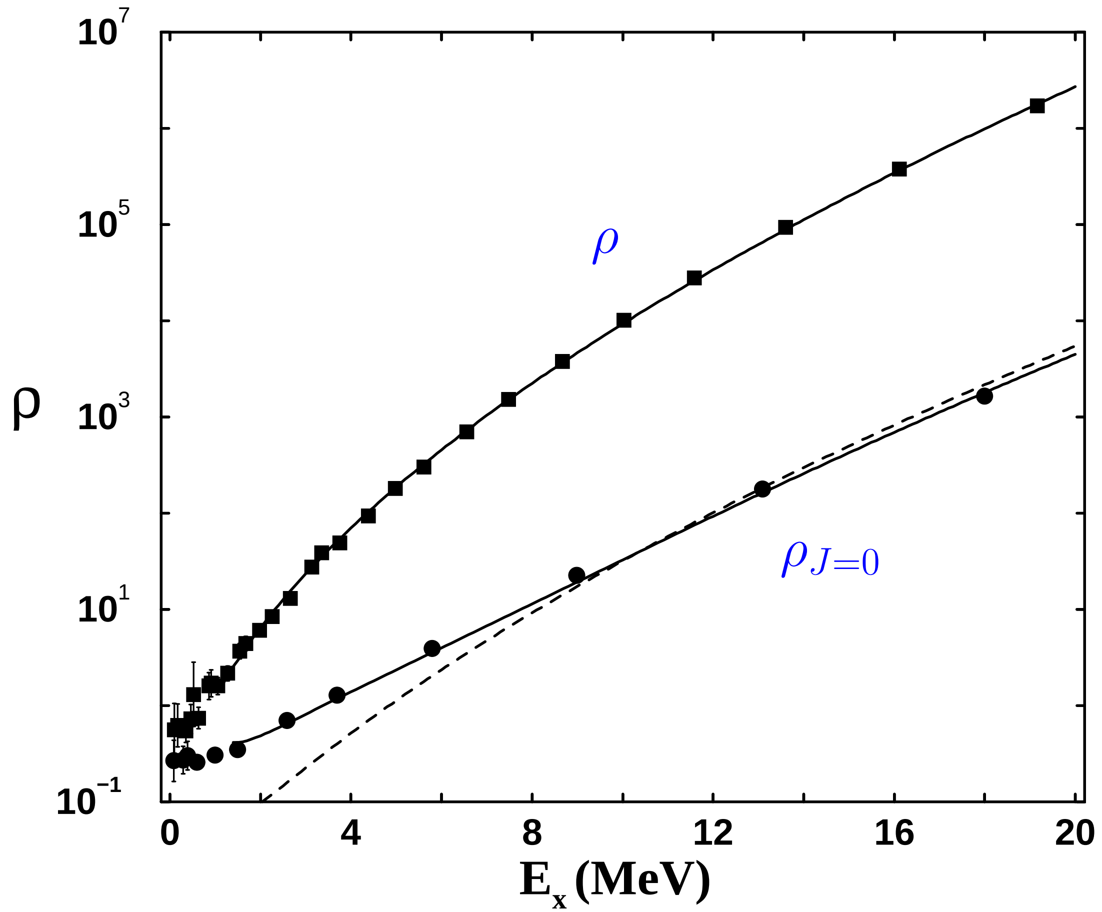
if fitting the spin cutoff parameter $\sigma \cdots$



- ○ significant deviation from spin cutoff model (even-odd staggering)
- ○ reduction of $\mathcal{I}$ from $\mathcal{I}_{\rm rig.}$ value ($\leftrightarrow$ pairing)

at low E_x in even-even nuclei !

$\rho_{J=0}(E_x)$ in ^{56}Fe :



enhancement at $E_x \lesssim 8\,\mathrm{MeV}$ $\leftrightarrow$ **reduction of** $\mathcal{I}$

IV. T-projected level densities

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

★ **Present effective Hamiltonian** $\cdots$ **good sign** $\rightarrow$ **errors kept small**

— **good for each T, but T-dep. ?** (cf. "modified SDI" : $V_{\rm SDI} + \alpha \boldsymbol{T}^2$)

$$E_T^{(0)} \equiv \lim_{\beta\to 0} E_T(\beta)\,; \quad \begin{cases} E_T(\beta) - E_T^{(0)} & \cdots \ \textbf{reasonable} \\ E_T^{(0)} - E_{T_0}^{(0)} & \cdots \ \textbf{?} \quad (T_0 \equiv (N-Z)/2) \end{cases}$$

$\rightarrow$ **desired to correct** $[E_T^{(0)} - E_{T_0}^{(0)}]$

T-dep. could be important in $Z \sim N$ nuclei !

($\because$ $T=0$ & $T=1$ **states lie closely**)

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T-dep. could be important in $Z \sim N$ nuclei!

($\because$ $T = 0$ & $T = 1$ states lie closely)

- perturbative correction

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

assume $H' = H + \alpha \boldsymbol{T}^2 \rightarrow \langle H' \rangle_\beta \approx \langle H \rangle_\beta + \Delta E_{\mathrm{pert.}}(\beta)$

$\Delta E_{\mathrm{pert.}}(\beta)$: perturbative corr. due to $\alpha \boldsymbol{T}^2$

$\rightarrow \rho(E_x)$

— $\begin{cases} \alpha \boldsymbol{T}^2 \text{ correction appropriate? (estimate of } \alpha\text{?)} \\ \text{perturbative regime?} \end{cases}$

- **T projection** $\rightarrow \rho_T$

  $\rightarrow$ **correction to** $[E_T^{(0)} - E_{T_0}^{(0)}]$ **(energy shift using exp. data)**

  $\left\{ \begin{array}{l} \textbf{beyond perturbative regime} \\ \textbf{not constrained to } \alpha \boldsymbol{T}^2 \textbf{ form} \cdots \; H' = H + f(\boldsymbol{T}^2) \end{array} \right.$

★ T **projection in SMMC** (**$\cdots$ analogous to J projection**)

$\hat{X}$ **: isoscalar operator** $\mathrm{Tr}_{A,T=T_0}\hat{X} = \mathrm{Tr}_{A,T_z=T_0}\hat{X} - \mathrm{Tr}_{A,T_z=T_0+1}\hat{X}$

T_z **projection** $\leftrightarrow$ **number (re-)projection**

HS-rep. $\rightarrow$ $$\frac{Z_{A,T=T_0}(\beta)}{Z_{A,T_z=T_0}(\beta)} = \frac{\langle(1 - \frac{\mathrm{Tr}_{A,T_z=T_0+1}U_\sigma}{\mathrm{Tr}_{A,T_z=T_0}U_\sigma})\Phi_\sigma\rangle_W}{\langle\Phi_\sigma\rangle_W},$$

$$\langle O\rangle_{\beta,T} \left(\equiv \frac{\mathrm{Tr}_{A,T}(Oe^{-\beta H})}{Z_{A,T}(\beta)}\right)$$

$$= \frac{\langle(\frac{\mathrm{Tr}_{A,T_z=T_0}(OU_\sigma)}{\mathrm{Tr}_{A,T_z=T_0}U_\sigma} - \frac{\mathrm{Tr}_{A,T_z=T_0+1}(OU_\sigma)}{\mathrm{Tr}_{A,T_z=T_0+1}U_\sigma} \cdot \frac{\mathrm{Tr}_{A,T_z=T_0+1}U_\sigma}{\mathrm{Tr}_{A,T_z=T_0}U_\sigma})\Phi_\sigma\rangle_W}{\langle(1 - \frac{\mathrm{Tr}_{A,T_z=T_0+1}U_\sigma}{\mathrm{Tr}_{A,T_z=T_0}U_\sigma})\Phi_\sigma\rangle_W}, \textit{etc.}$$

(**O : isoscalar**)

MC sampling of σ for $(A, T_z = T_0) = (Z, N)$ $\rightarrow$ evaluate $\langle O\rangle_{\beta,T}$

$\cdots$ **exact T-proj. sample by sample**

★ T**-projected level densities**

SMMC $\rightarrow E_T(\beta) = \langle H\rangle_{\beta,T} \rightarrow Z_T$, S_T, $C_T \rightarrow \rho_T \approx \dfrac{e^{S_T}}{\sqrt{2\pi\beta^{-2}C_T}}$

(**$T\pi$-proj. densities by combining with π-proj.**)

★ E_T **correction**

exp. data of $[E_T^{(0)} - E_{T_0}^{(0)}]\cdots$ $\left\{\begin{array}{l} E_x \textbf{ of lowest } T(\neq T_0) \textbf{ state} \\ \qquad\qquad\textbf{(\textit{e.g.} } T=1 \textbf{ state of } {}^{58}\textbf{Cu)} \\ \textbf{mass difference (with } E_{\rm Coul} \textbf{ correction)} \end{array}\right.$

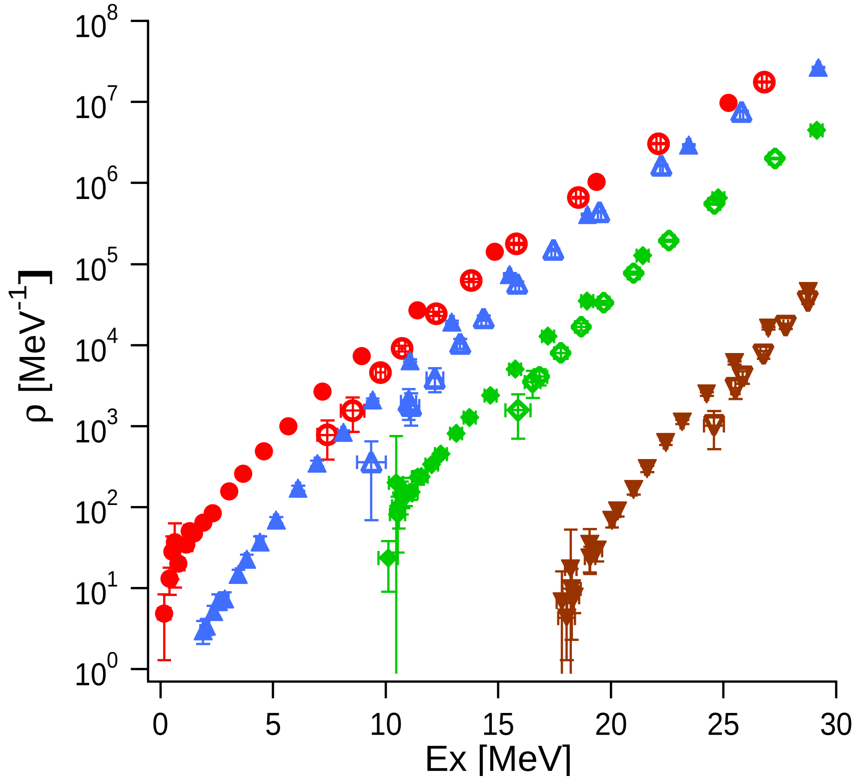
$\longrightarrow$ **overall shift of** E_T**:** $E'_T = E_T + \delta E_T$

$$\delta E_T = [E_T^{(0)} - E_{T_0}^{(0)}]_{\rm exp.} - [E_T^{(0)} - E_{T_0}^{(0)}]_{\rm cal.}$$

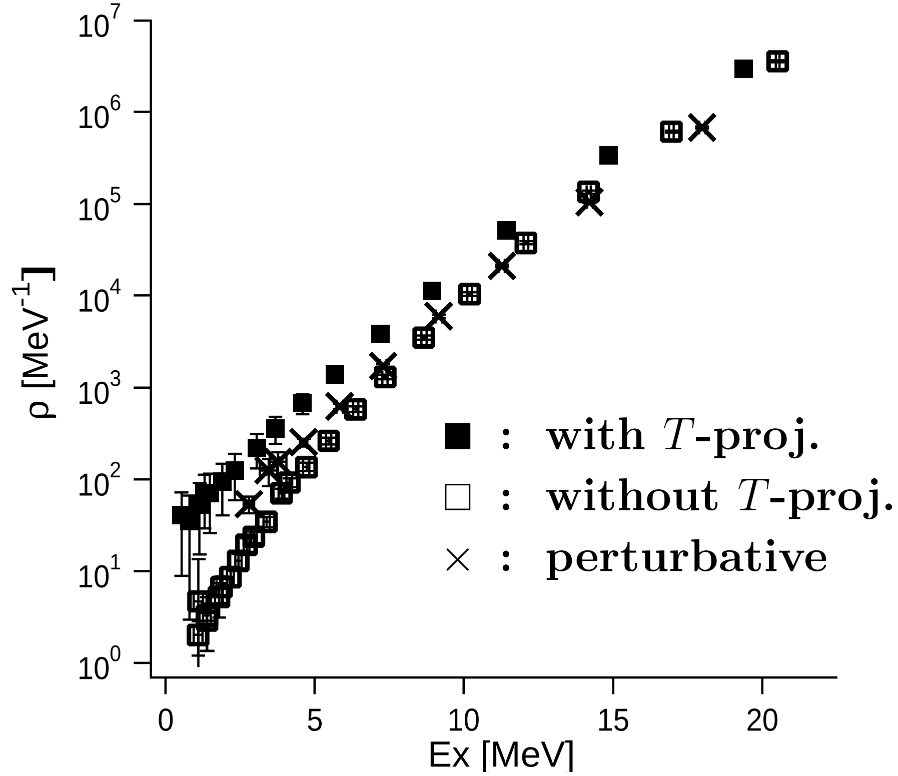
$\longrightarrow \rho_T(E_x) \longrightarrow \rho(E_x) = \sum_T \rho_T(E_x)$

^{58}**Cu** $(Z = N = \mathrm{odd})$

$\rho_{T\pi}(E_x)$ **:**



$\rho(E_x)$ **:**



○ **T-proj. $\rightarrow$ E_T corr.**

$\cdots$ **important**

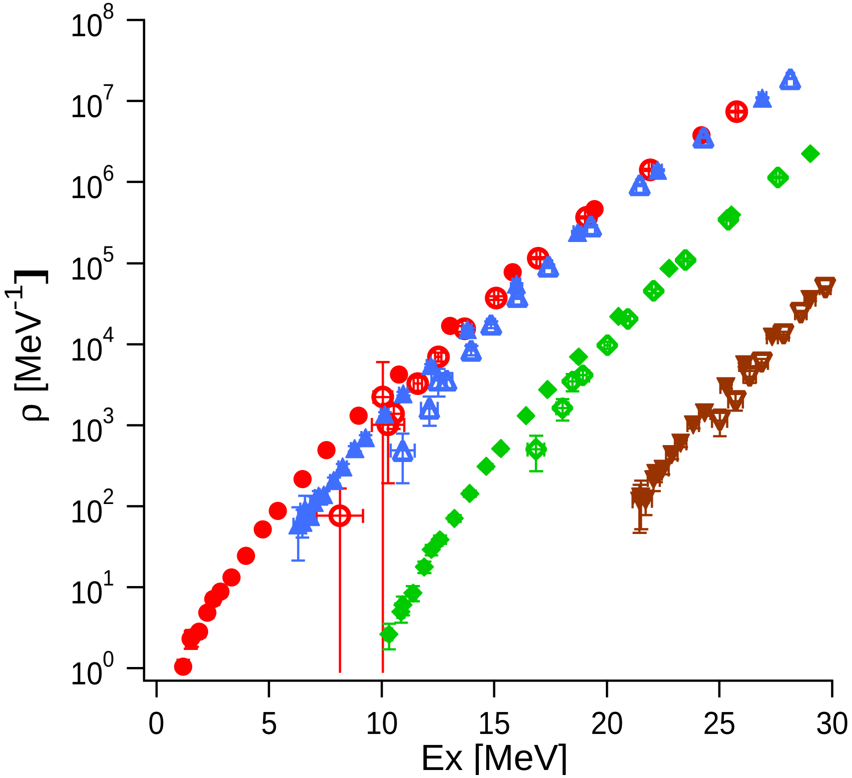
○ **perturbative corr.**

$\cdots$ **not good**

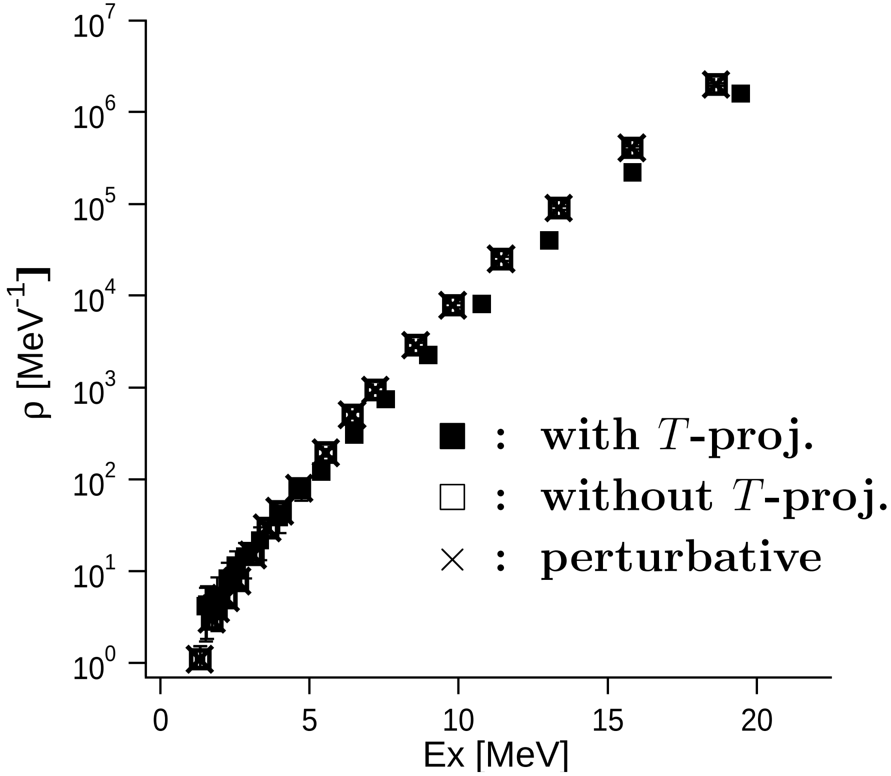
(cf. $[E^{(0)}_{T=1} - E^{(0)}_{T=0}]_{\mathrm{exp.}} = 0.2\,\mathrm{MeV}$**)**

^{60}**Zn** $(Z = N = \text{even})$

$\rho_{T\pi}(E_x)$:



$\rho(E_x)$:



V. Summary

1. **Introducing J projection in SMMC**

   → **fully microscopic study on J distribution of level densities**

   - **even-odd staggering**
   - **suppression of $\mathcal{I}$** **(in terms of spin cutoff model)**

   } **at low E_x for even-even nuclei**

2. **Introducing T projection in SMMC**

   → **reliable correction to E_T with good-sign interaction**

   → **reliable microscopic calculation of level densities in $Z \sim N$ nuclei**

   (cf. perturbative correction — not good enough)