殻模型モンテカルロ法による
核準位密度の微視的計算

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原子核の準位密度 — 原子核の統計的性質

$\left\{\begin{array}{l}\text{有限量子多体系の統計力学}\\ \text{低エネルギー核反応 — 宇宙・天体における核反応}\end{array}\right.$

- Bethe, *et al.*

  $\left\{\begin{array}{l}\text{‘温度’の導入, grand-canonical formalism, etc.}\\ \qquad\qquad\qquad\longleftarrow \text{saddle-point 近似}\\ \text{Fermi-gas model に基づく議論}\end{array}\right.$

  ··· 比較的高いエネルギー ($E_x \gtrsim$ 20MeV?) で有効

  ∵ 量子効果が小さい

- 低エネルギーでは？

  Parameter を導入 → fit できる

  しかし，parameter の値の予言は困難

  (理論的根拠不十分，核種依存性大)

  ··· エネルギー依存性に対する関数形を与えただけ

  問題点 — 量子効果！

  Fermi-gas model, grand-can. formalism (↔ 保存則)

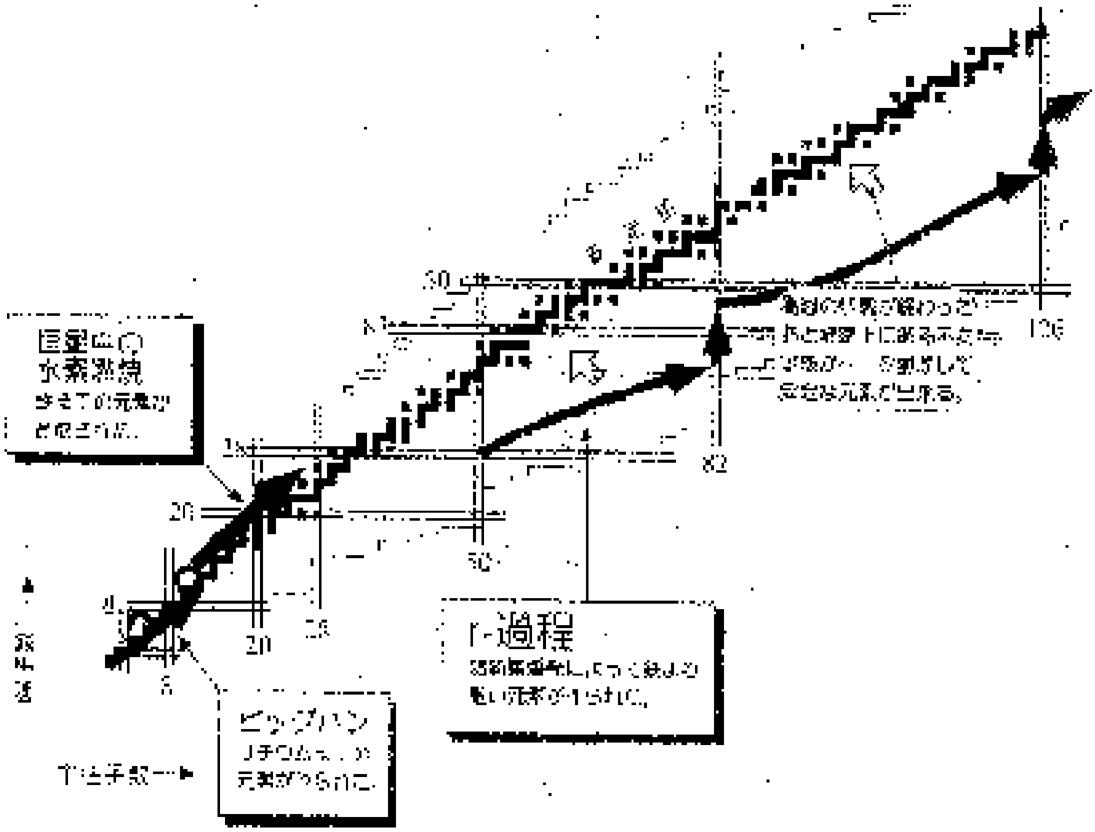
  ··· 妥当か？ — maybe not

  Note : Astrophysical importance — $E_x \lesssim$ 15MeV

⇒ 量子効果を正確に扱う理論の必要性

→ (interacting) shell model

但し，model space を限定 → $E_x \lesssim$ 20MeV



Nuclear level densities — one of the critical inputs in nucleosynthesis calculations

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

$$\sigma_{(n,\gamma)} \propto \sum_{J_i\pi_i J_f\pi_f} \int \frac{dE_f}{E_i}\, T^{(n)}_{J_i\pi_i}(E_i)\, T^{(\gamma)}_{J_f\pi_f}(E_f)\, \rho_{J_f\pi_f}(E_f)\, e^{-E_i/T}$$

$\cdots$ Hauser-Feshbach formula

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

$T^{(n/\gamma)}_{J\pi}(E)$: transmission coefficient from compound state

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

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

Conventional approach to nuclear level densities

Backshifted Bethe formula ← Fermi-gas model

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

$$(E_x - \Delta = at - t^2)$$

$\cdots$ fits well to exp. data, if the parameters (a & Δ) are adjusted

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)

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

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What should we take into consideration to describe nuclear level densities?

(1) shell effects

(2) 'collective' 2-body correlations

(Interacting) Shell model $\cdots$ desirable for level density calculations

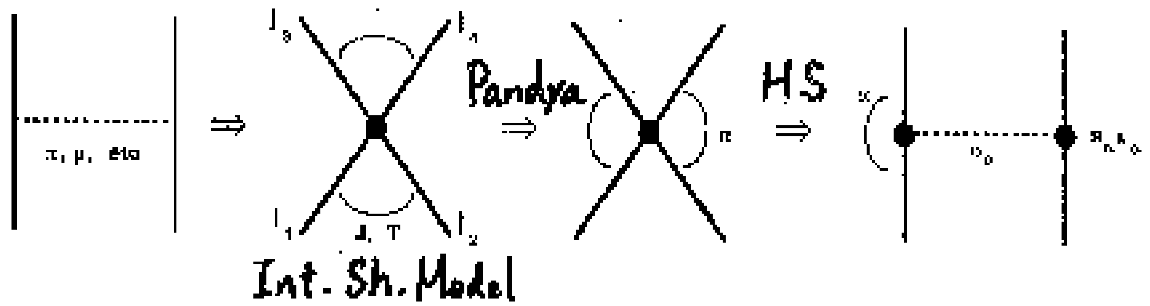
Both (1) shell effects & (2) 2-body correlations are fully taken into account within the model space

Large model space is required to describe the $E_x \approx S_n$ region

$\longrightarrow$ Shell model Monte Carlo (SMMC) method

Auxiliary-fields path integral for shell model (at finite temperature)

$\longrightarrow$ SMMC Ref.: S. E. Koonin *et al.*, Phys. Rep. 278, 1



$H = \sum_i \epsilon_i \hat{n}_i + \sum_\alpha \frac{\kappa_\alpha}{2} \hat{\rho}_\alpha^2$ ← Pandya transformation

($\hat{\rho}_\alpha$: 1-body operator)

(imaginary-)time evolution operator : $e^{-\beta H} = \left(e^{-\Delta\beta H}\right)^{n_t}$ $\beta = 1/T$

$\tau_0 \to \tau_1 \to \cdots \to \tau_{n_t} = \beta$ ($\tau_m = m\Delta\beta$)

Trotter decomposition + Hubbard-Stratonovich transformation

(at each time step $\tau_m \to \tau_{m+1}$)

$\Rightarrow e^{-\beta H} = \int \mathcal{D}[\sigma] G_\sigma U_\sigma + O\left((\Delta\beta)^2\right)$ (AF path integral)

$\sigma_\alpha(\tau)$: auxiliary-field ($\leftrightarrow$ mean-field)

$G_\sigma = \exp\left[-\frac{1}{2}\Delta\beta \sum_{\alpha,m} |\kappa_\alpha| \sigma_\alpha^2(\tau_m)\right]$ ⋯ self-energy of σ

$U_\sigma = \exp[-\Delta\beta h_\sigma(\tau_{n_t})] \cdots \exp[-\Delta\beta h_\sigma(\tau_1)]$

with $h_\sigma(\tau) = \sum_i \epsilon_i \hat{n}_i + \sum_\alpha s_\alpha |\kappa_\alpha| \sigma_\alpha(\tau) \hat{\rho}_\alpha$

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

$$\langle \mathcal{O} \rangle = \frac{\mathrm{Tr}(\mathcal{O} e^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})} = \frac{\int \mathcal{D}[\sigma] G_\sigma \langle \mathcal{O} \rangle_\sigma \mathrm{Tr} U_\sigma}{\int \mathcal{D}[\sigma] G_\sigma \mathrm{Tr} U_\sigma} \cong \frac{1}{N_{\mathrm{samp}}} \sum_k \langle \mathcal{O} \rangle_{\sigma(k)} ;$$

$$\langle \mathcal{O} \rangle_\sigma = \frac{\mathrm{Tr}(\mathcal{O} U_\sigma)}{\mathrm{Tr} U_\sigma}$$ ⋯ calculable only via the s.p. matrices

$\{\sigma_\alpha(\tau_m)_k\}$ sampled via a random walk under $W_\sigma = G_\sigma \mathrm{Tr} U_\sigma$

(quantum Monte Carlo method)

SMMC

$$\langle O\rangle = \frac{\mathrm{Tr}(Oe^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})} \simeq \frac{1}{N_{\rm samp}} \sum_k \langle O\rangle_{\sigma(k)}\,; \quad \text{by Monte Carlo}$$

$$\langle O\rangle_{\sigma(k)} = \frac{\mathrm{Tr}(OU_\sigma)}{\mathrm{Tr}(U_\sigma)} : \text{measurement}$$

(computed for fixed $\{\sigma_\alpha\}_k$, which is chosen

via a 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

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

cf. thermodynamics S : entropy, C : specific heat

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

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

& differentiation

$$E_x = E - E_0\,; \quad E_0 = \lim_{\beta\to\infty} E(\beta) \leftarrow E(\beta) \text{ for large } \beta$$

cf. Grand-canonical case

$$\rho_{\rm GC}(E) \cong \frac{e^{S_{\rm GC}}}{\sqrt{(2\pi)^3(\Delta N_\pi)^2(\Delta N_\nu)^2\beta^{-2}C_{\rm GC}}}$$

昨年度までの成果

1. 原子核の準位密度の microscopic でかつ realistic な理論計算に初めて成功した (← 殻模型モンテカルロ法)。

   ⟶ 微視的で高精度の理論に基づく systematic な計算,
   astrophysics への応用の端緒

2. 有限多体系の有限温度での量子効果の発現の様子と重要性，及び保存則 (*e.g.* parity, isospin) の影響を明らかにした。

   (← 量子モンテカルロ計算における projection 法の開発)

課題

1. Deformation of nuclear shape ⇒ heavier nuclei

   Model space more than 1 major-shell required

   e.g. rare-earth region — accurate data available

   低温 ($T \lesssim 0.4$MeV) での計算に改良が必要

2. Spin projection ⇒ 核準位密度の角運動量 (J) 依存性?

   Astrophysical importance

   spin dep. of thermonuclear reactions

   J-projection ⋯ not yet available

   M-projection は (ある程度) 実行可能

Setup for Fe-region nuclei $S_n \lesssim 15\text{MeV}$

- model space — full $pf + 0g_{9/2}$ (so as to cover S_n)
- effective hamiltonian

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

common between protons & neutrons

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

radial part ($\propto dV_{\rm WS}/dr$) & bare strength

← nuclear self-consistency

(between density & s.p. potential)

renormalization factors ↔ core-polarization effects

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

← comparison with a realistic interaction (by Kuo)

$T = 1$ pairing interaction

← so as to reproduce

mass differences of $40 < A < 80$ spherical nuclei

⟶ uniquely determined for individual nucleus,

and sign good (for even-even nuclei)

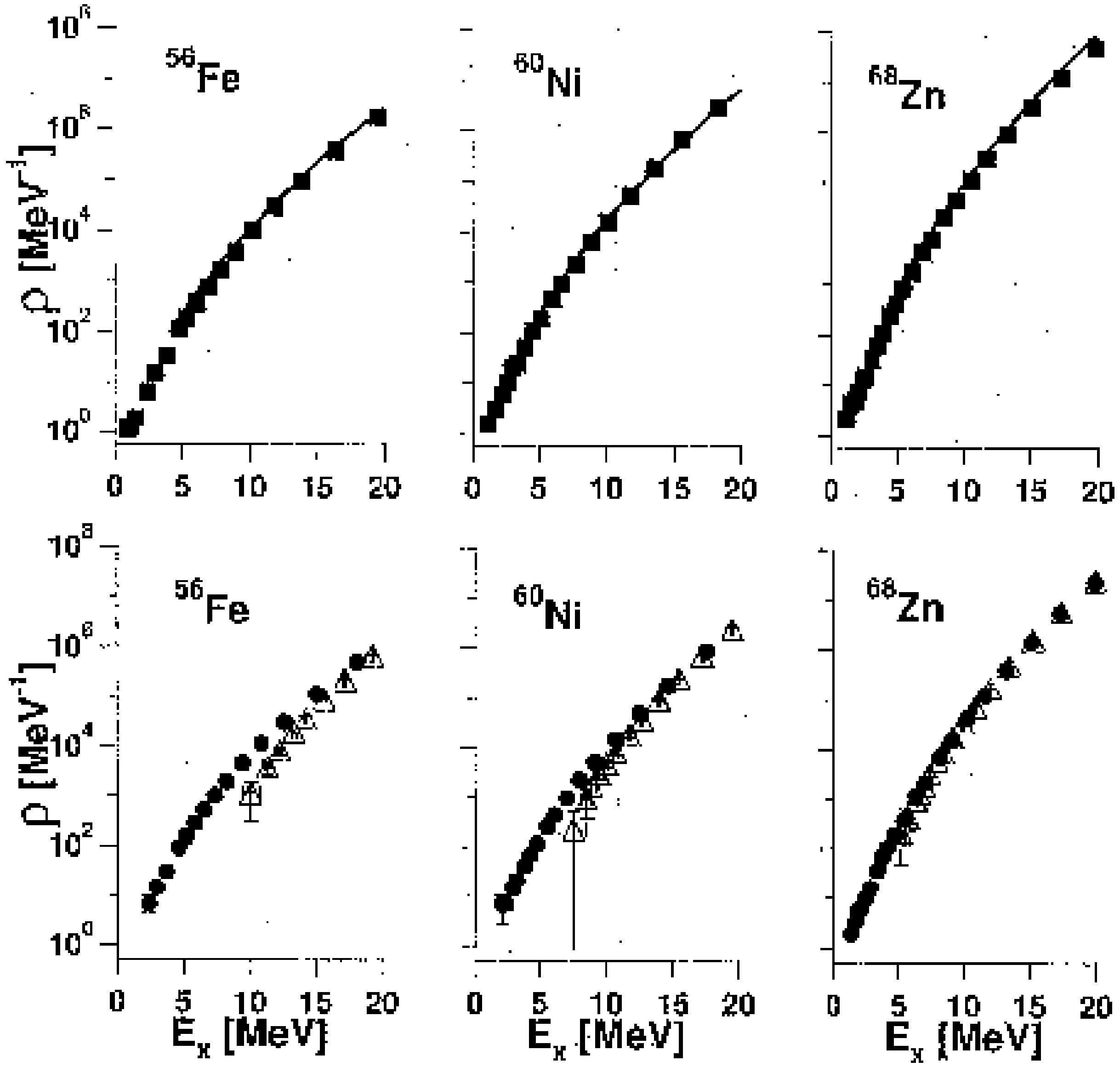
* Check of the hamiltonian for quadrupole collectivity in ^{56}Fe

$$E_Q \equiv \frac{\Sigma_i (E_i - E_0) |\langle 2_i^+ Q | 0_g^+ \rangle|^2}{\Sigma_i |\langle 2_i^+ | Q | 0_g^+ \rangle|^2}$$

→ Exp. (p, p') : 2.16, SMMC : 2.12±0.11 [MeV]

- MC ⋯ $N_{\rm samp} \approx 4000$, $\Delta\beta = 1/32$ [MeV^{-1}] (time slice)

thermal ⋯ $d\beta = 1/16$ [MeV^{-1}] (for Z & C)



56Fe
60Ni
68Zn
ρ [MeV-1]
10^0
10^2
10^4
10^6
10^8
0 5 10 15 20
Ex [MeV]

M projection

$$\mathrm{Tr}_M(U_\sigma) = \mathrm{Tr}(P_M U_\sigma)\,;\; P_M \propto \int d\varphi \exp[i\varphi(\hat{J}_z - M)]$$

φ : additional auxiliary field → exact integration

- Exp. data　M に関する degeneracy が不明

$$\rho'_{\rm tot}(E) = \sum_J \rho_J(E) \qquad \longleftarrow \text{実験値}$$

$$\rho_{\rm tot}(E) = \sum_J (2J+1)\rho_J(E)\,:\ \text{total level density}$$

← 実験値 + model (Bethe, Feshbach, Bloch, ⋯)

$$\cdots\quad \rho'_{\rm tot}(E) = \frac{1}{\sqrt{2\pi}\sigma_J}\rho_{\rm tot}(E)$$

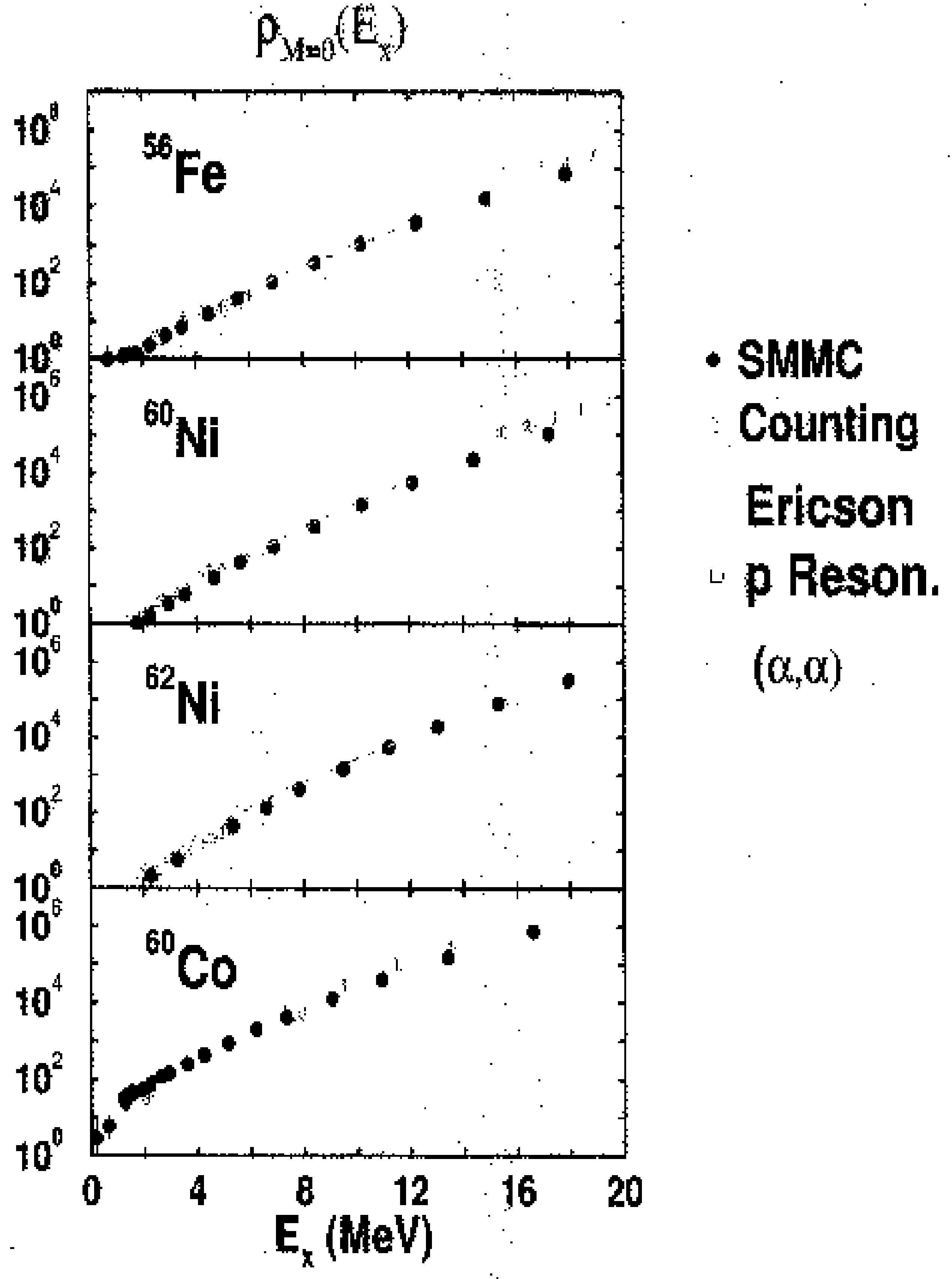
$$\sigma_J^2 = \mathcal{I}\sqrt{(E-\Delta)/a}\,:\ \text{spin cut-off factor}$$

($\mathcal{I}$: mom. of inertia　a, Δ ← E-dep. of $\rho_{\rm tot}$)

今までの計算 → $\rho_{\rm tot}$ の比較 ⋯ $\mathcal{I}$ の ambiguity ($\sim$ factor of 2)

$$\rho'_{\rm tot}(E) = \begin{cases} \rho_{M=0}(E) \\ \rho_{M=1/2}(E) \end{cases} \qquad \longleftarrow M\text{ projection}$$

⇒ 実験値との直接的な比較



$\rho_{M=0}(E_x)$
^{56}Fe
^{60}Ni
^{62}Ni
^{60}Co
E_x (MeV)
SMMC
Counting
Ericson
p Reson.
(α,α)

- 核準位密度の spin distribution ：

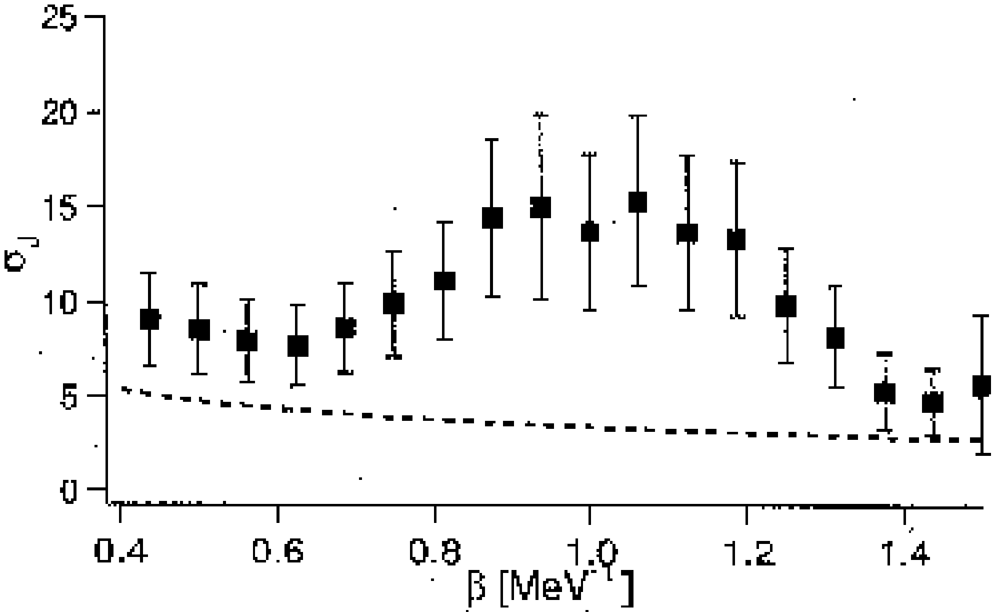
← Spin cut-off factor の T-dep. ← ρ'_{tot}/ρ_{tot}

$$\rho'_{tot}(E) \quad \frac{1}{\sqrt{2\pi}\sigma}\rho_{tot}(E)$$

$$\sigma_J^2 = \mathcal{I}/\beta \quad (\because \ \beta = 1/T = \sqrt{a/(E-\Delta)})$$

$$\mathcal{I} \sim \mathcal{I}_{\rm rig.} = \tfrac{2}{5}AMR^2 \simeq \tfrac{2}{5}Mr_0^2A^{5/3} \qquad \leftarrow \text{剛体球 model}$$

For positive-parity levels of ^{56}Fe :



(preliminary)

Spin cut-off factor の強い T-dependence

↔ 核準位密度の non-trivial な spin distribution

(従来の model の破綻)

$\mathcal{I}$ の温度依存性？ — 不十分 $(\because \mathcal{I} > \mathcal{I}_{\rm rig.})$

⇒ Model-indep. な解析が望まれる

(Error bar を小さくする工夫も必要)

今年度の成果

- M-projection 法の開発・実行
- 核準位密度の実験値との直接的な比較

  → 計算の信頼性さらに up

- Spin distribution について　従来の model に基づく解析

  Spin cut-off factor の異常な T-dependence

  → 従来の model の問題点？

今後の課題

- Deformed nuclei, 特に low T ($\beta \gtrsim 2.5\mathrm{MeV}^{-1}$) での計算
- J-projection　各 sample に対して 3-dim. integration

  → model-indep. な spin distribution の研究

  Note : T-proj. との違い　$[\hat{h}_\sigma, \hat{\mathbf{J}}] \neq 0$

共に，program の本格的な再 coding が必要　- 2003 年度

(→ test run, CPU time の評価)