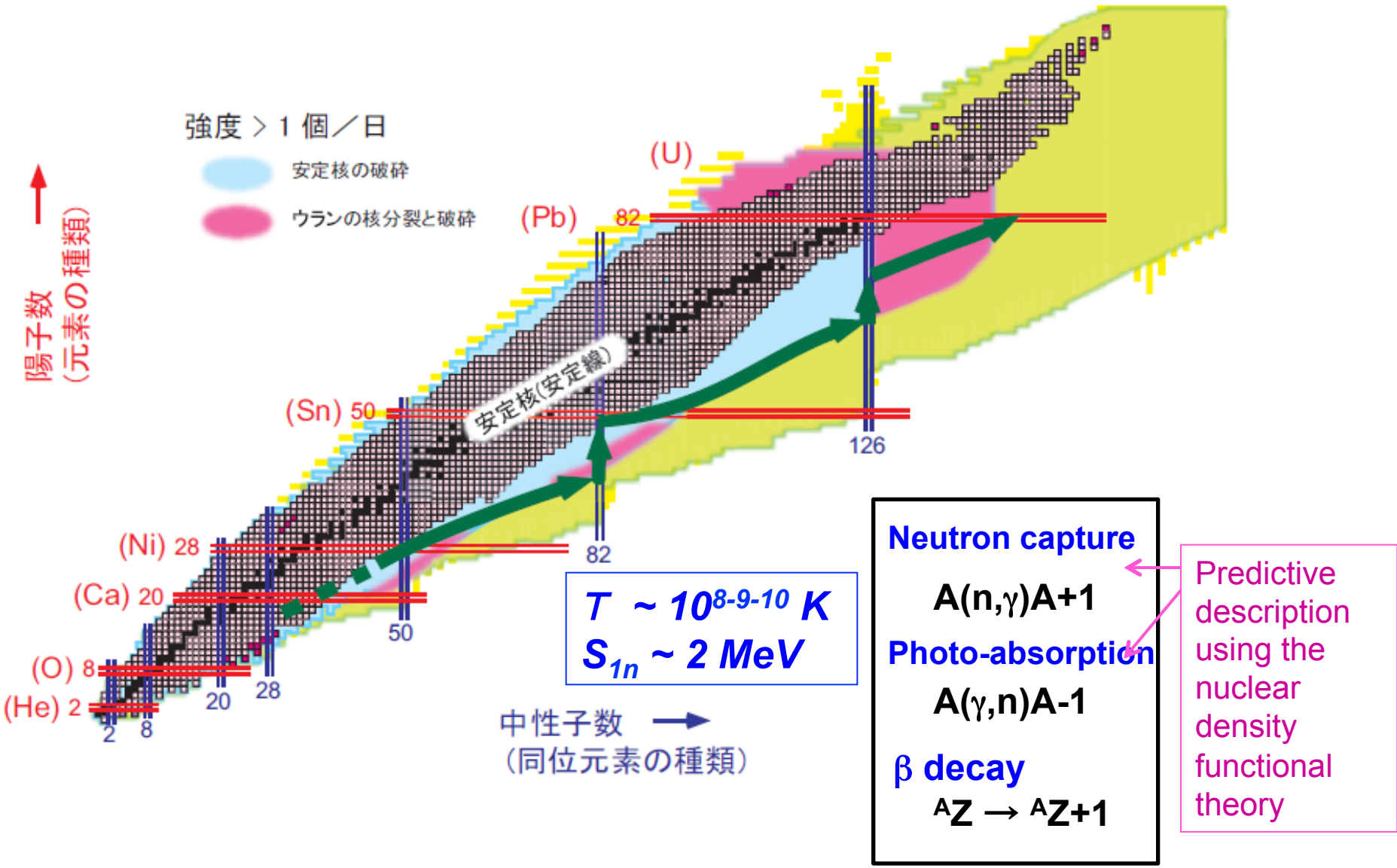


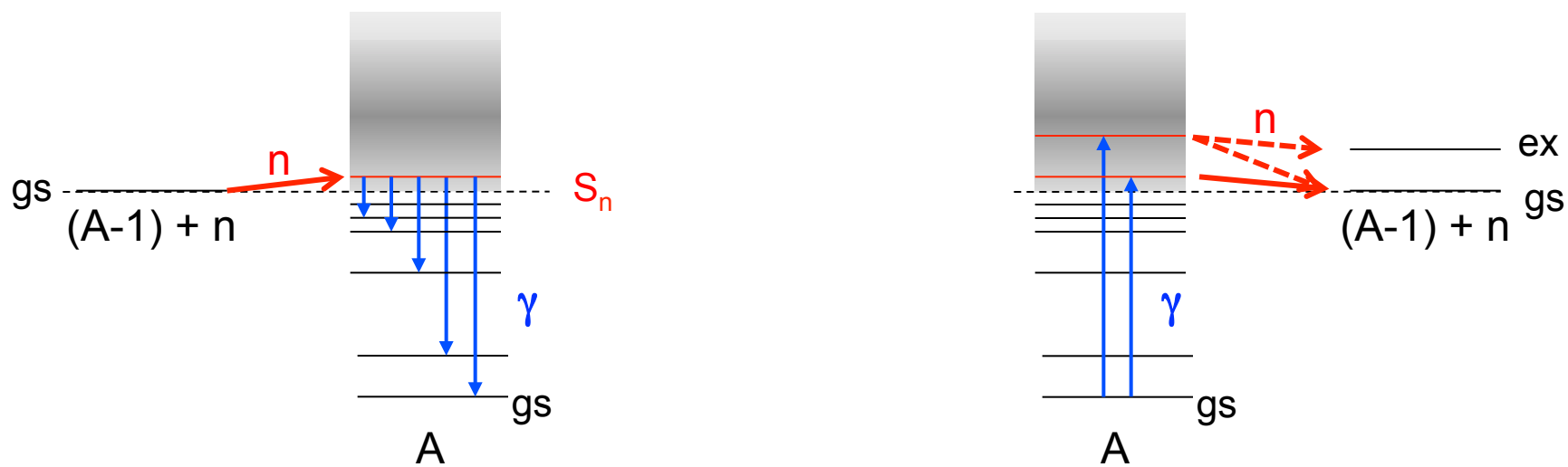
密度汎関数理論でr過程中性子捕獲反応 を記述する

M. Matsuo (Niigata U.)

r-process nucleosynthesis



(n, γ) 反応 / (γ, n) 反応

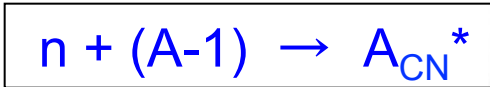


中性子捕獲の統計模型：大部分の理論計算

安定核近傍、S過程

→ ドリップラインから離れた中性子過剰核

1. 複合核状態の形成

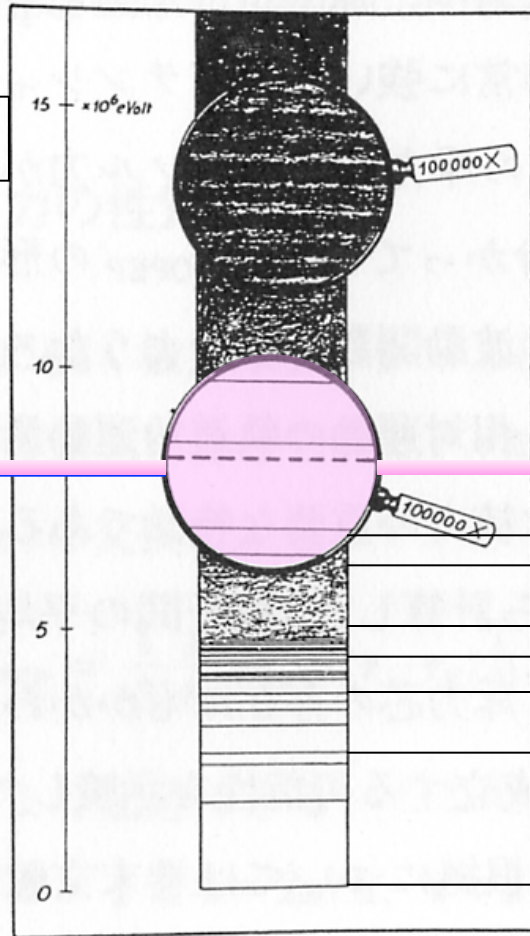


$$E_n \sim kT < \sim 100 \text{keV}$$

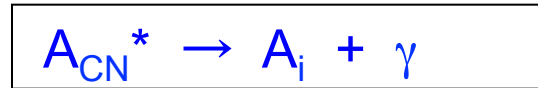
$$S_n \sim 8 \text{MeV}$$

中性子吸収(透過係数)

$T_n \leftarrow$ optical model



2. 複合核状態からの統計的ガンマ崩壊

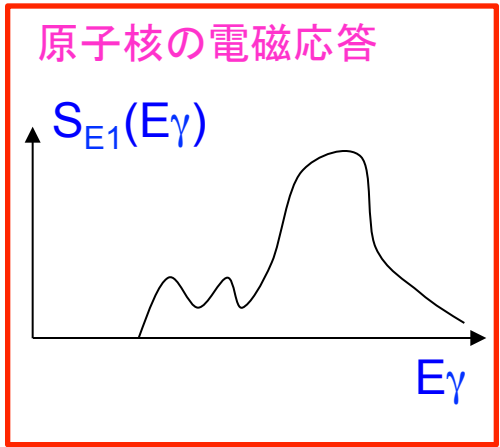


E1, M1 decay

準位密度

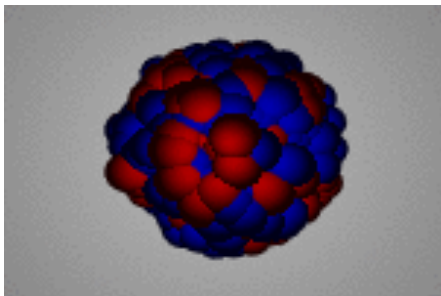
電磁遷移強度関数

$$\leftarrow S_{E1}(E\gamma)$$



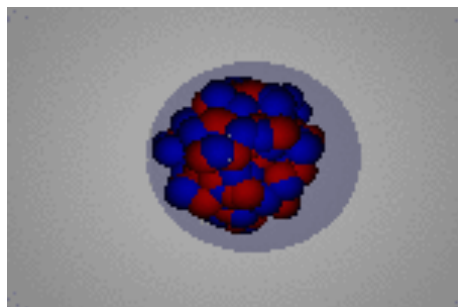
原子核の電気双極子応答

巨大双極子共鳴GDR

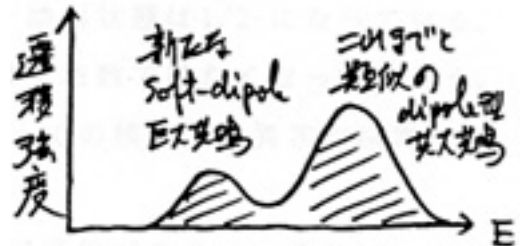
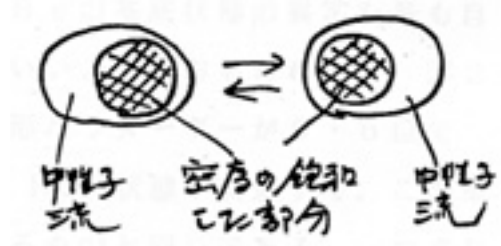
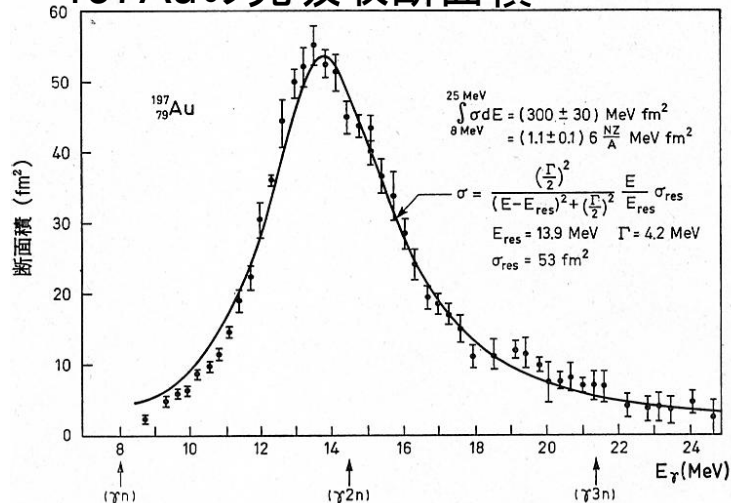


中性子過剰核では？

ピグミー共鳴



197Auの光吸収断面積

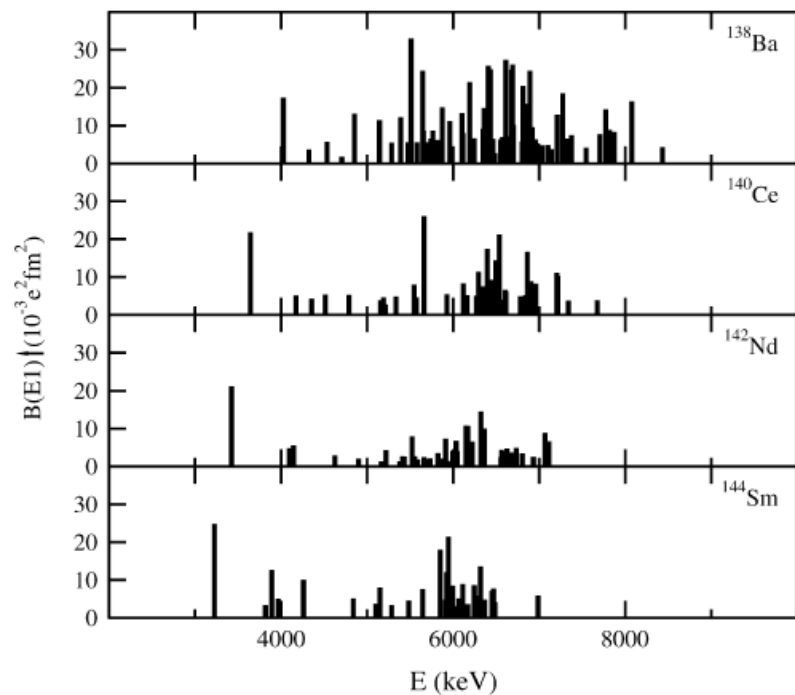


E1 応答実験の発展：安定核

Pygmy dipole resonance

Darmstadt (γ, γ') on stable N=82 isotones

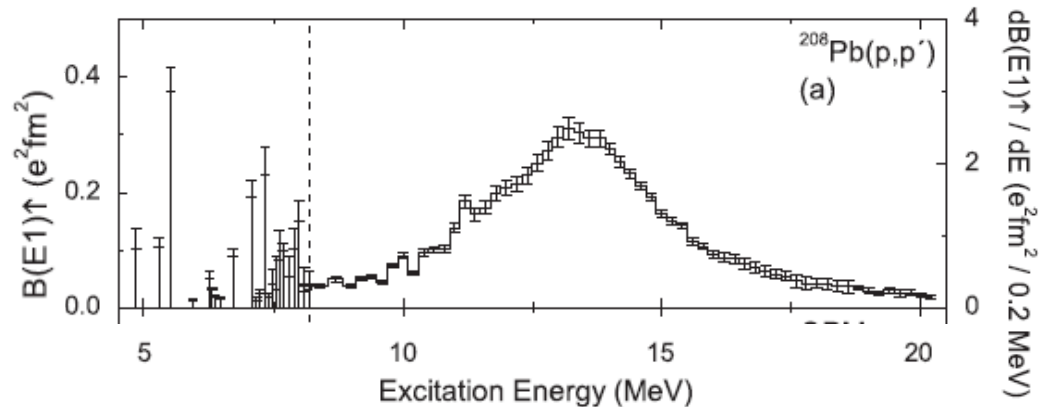
Volz et al. NPA779,1 (2006)



Whole E1 response : pygmy + GDR

RCNP (p, p') on ^{208}Pb

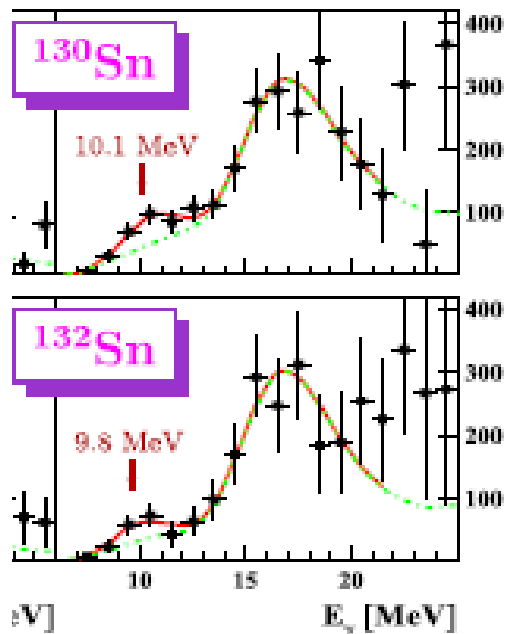
Tamii et al. PRL107, 062502 (2011)



E1 応答実験の発展：不安定核、中性子過剰核

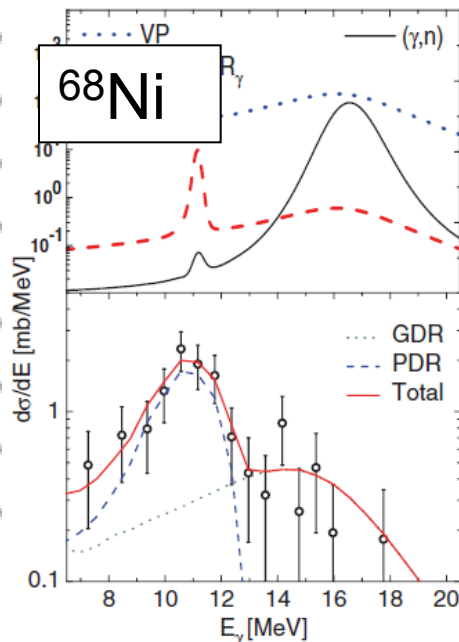
Pygmy dipole resonance
not necessarily small S_{1n}
(Heavy mass nuclei)

$S_{1n}=7.3$ MeV



Adrich et al. PRL (2006)

$S_{1n}=7.8$ MeV

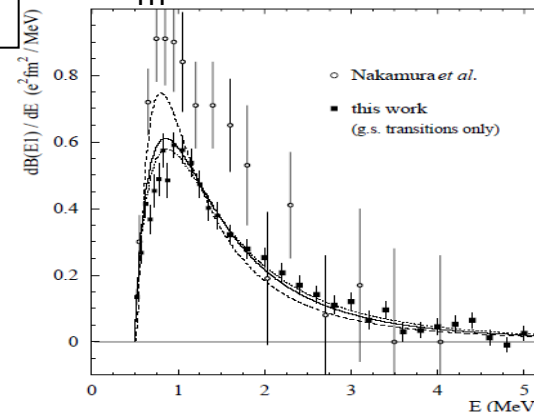


Wieland et al. PRL (2009)

Threshold strength
very small S_{1n}
(light mass nuclei)

^{11}Be

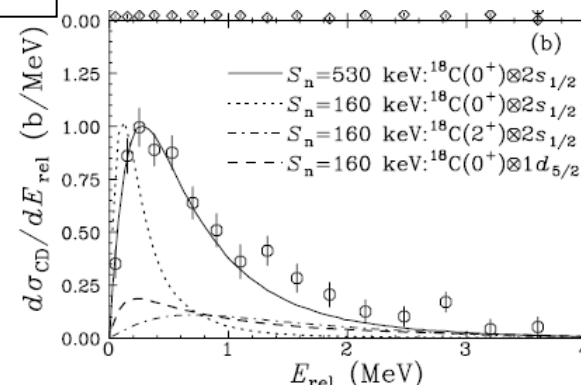
$S_{1n}=0.5$ MeV



Palit et al. PRC(2003)

^{19}C

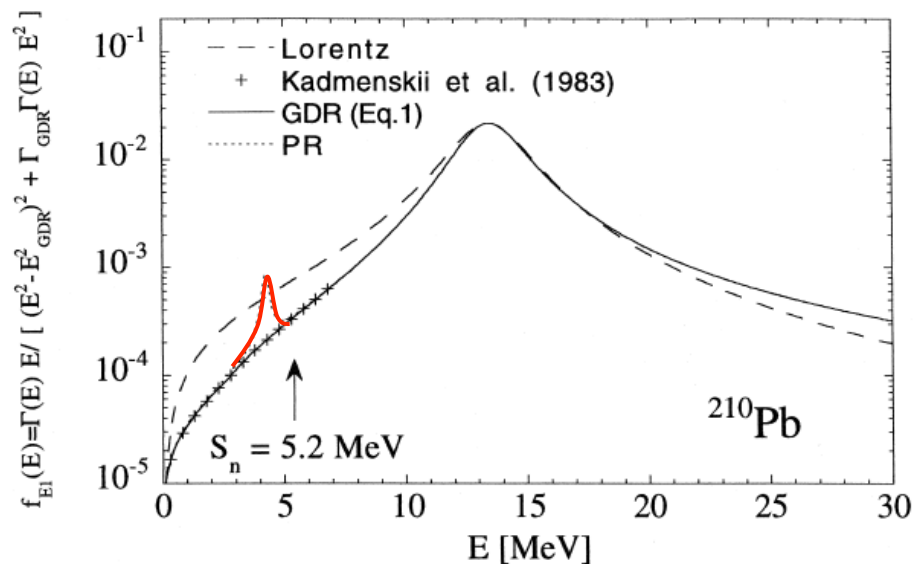
$S_{1n}\sim 0.6$ MeV



Nakamura et al. PRL (1999)

Gorielyによる初期研究

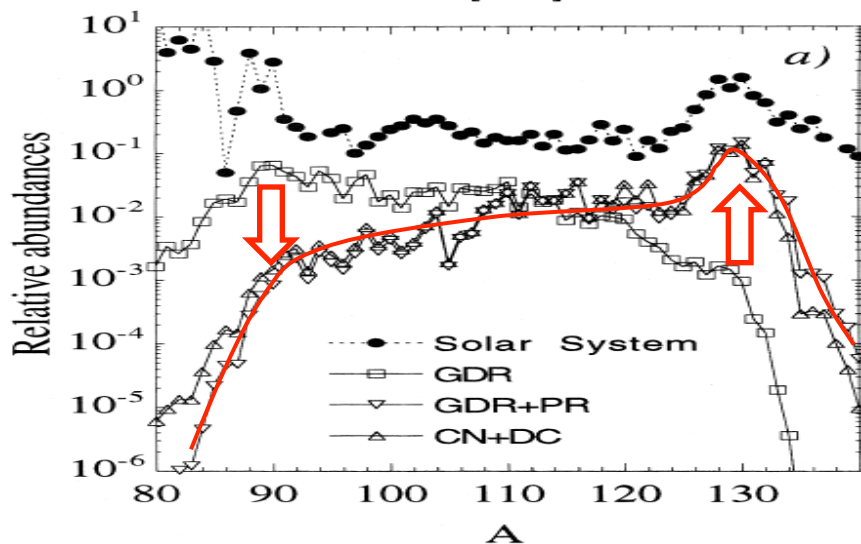
S. Goriely PLB436, 10 (1998)



Adopted E1 strength function (schematic)

Existence of **pygmy resonance** below S_n

in Hauser-Feshbach statistical (n, γ) model



Resultant r-process abundance

Accelerated neutron-capture

conditions

low T , low ρ_n
no n - γ equilibrium

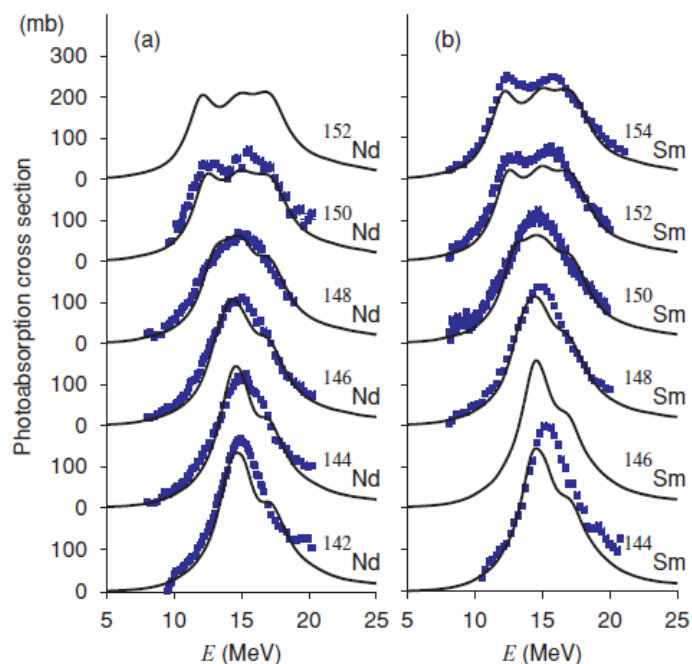
密度汎関数理論による原子核応答の記述

軽い核を除けば、“原子核密度汎関数モデル＋乱雑位相近似(線形応答)”、
DFT+QRPA (閉殻の場合は DFT+RPA)

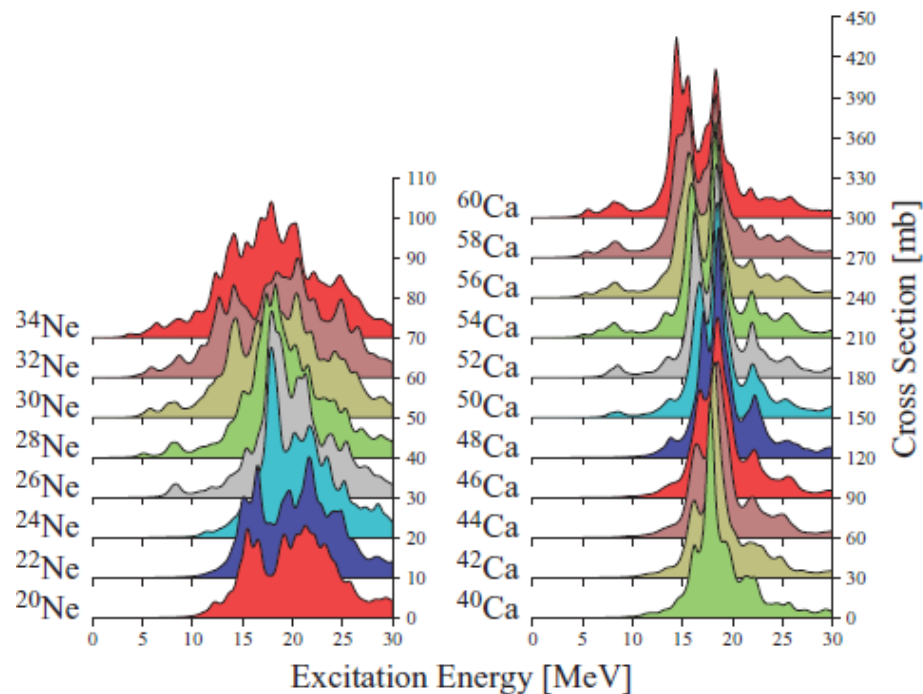
またはその拡張、による記述が有望と多くの人が考えている。

最近の発展を示す例2つを挙げる

Yoshida & Nakatsukasa, PRC83, 021304 (2011)



Inakura, Nakatsukasa & Yabana, PRC84, 021302 (2011)



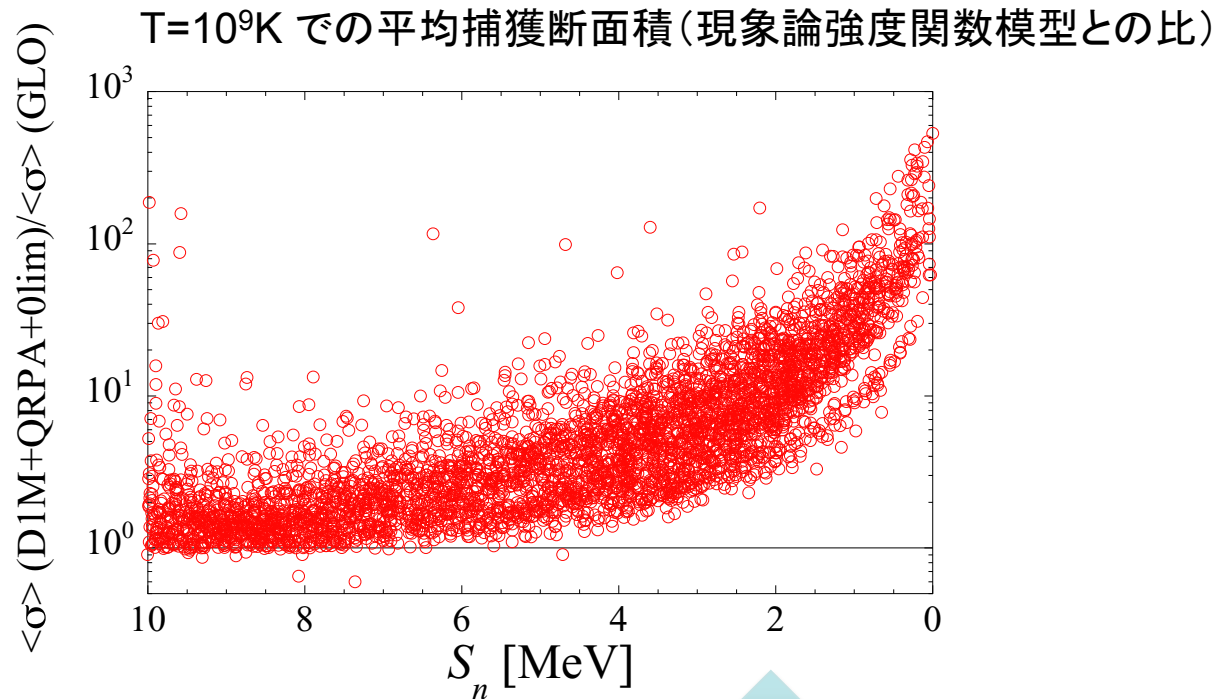
see eg. a review : Nakatsukasa, Matsuyanagi, Matsuo, Yabana, Rev. Mod. Phys. 88 (2016)

中性子捕獲統計模型＋密度汎関数理論

- Griely とその共同研究者、など多数

Eg. S.Goriely, E.Khan, M.Shamin, NPA739(2004)331
E. Litvinova, et al. NPA823 (2009) 26

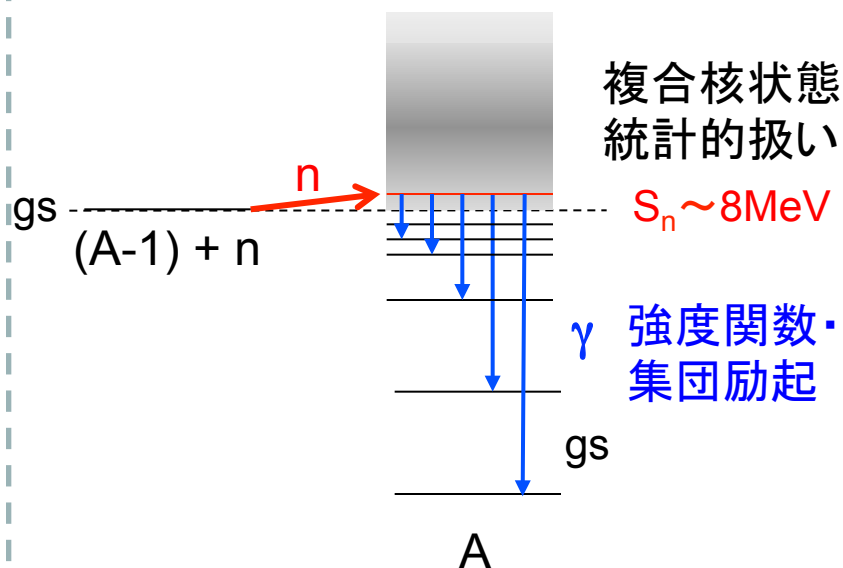
S.Goriely, S. Hilaire, S. Peru, K. Sieja, PRC98, 014327 (2018)



統計模型 vs. 直接捕獲過程

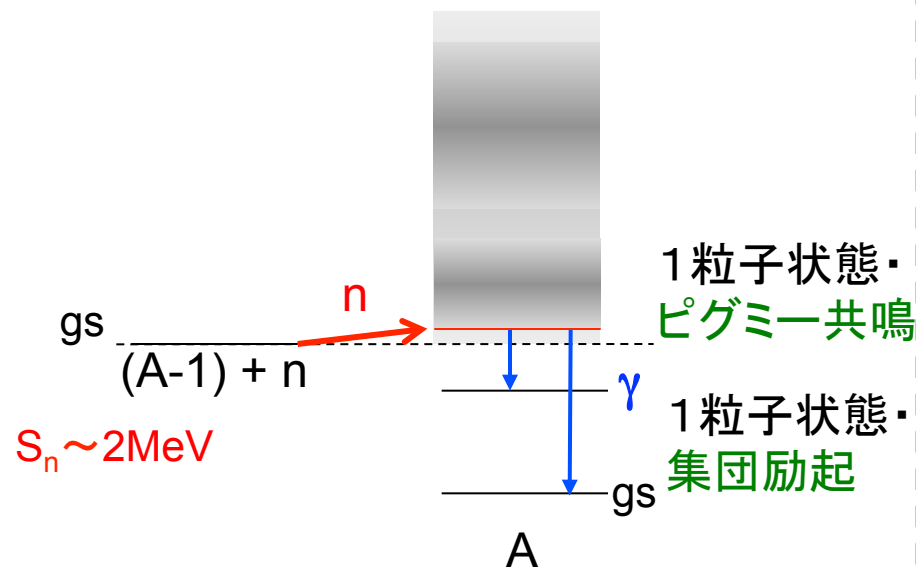
安定核近傍、S過程

ドリップラインから離れた中性子過剰核, R過程



中性子捕獲統計模型

ドリップライン近傍の中性子過剰核, R過程



直接中性子捕獲過程

← 反応の全プロセス、関与する
状態を明示的に記述する必要

従来、1粒子ポテンシャル模型で扱う

Single-particle model of direct n-capture

$$\frac{dB(E1)}{dE} \propto \left| \langle \phi_f | M(E1) | \phi_i(E) \rangle \right|^2$$

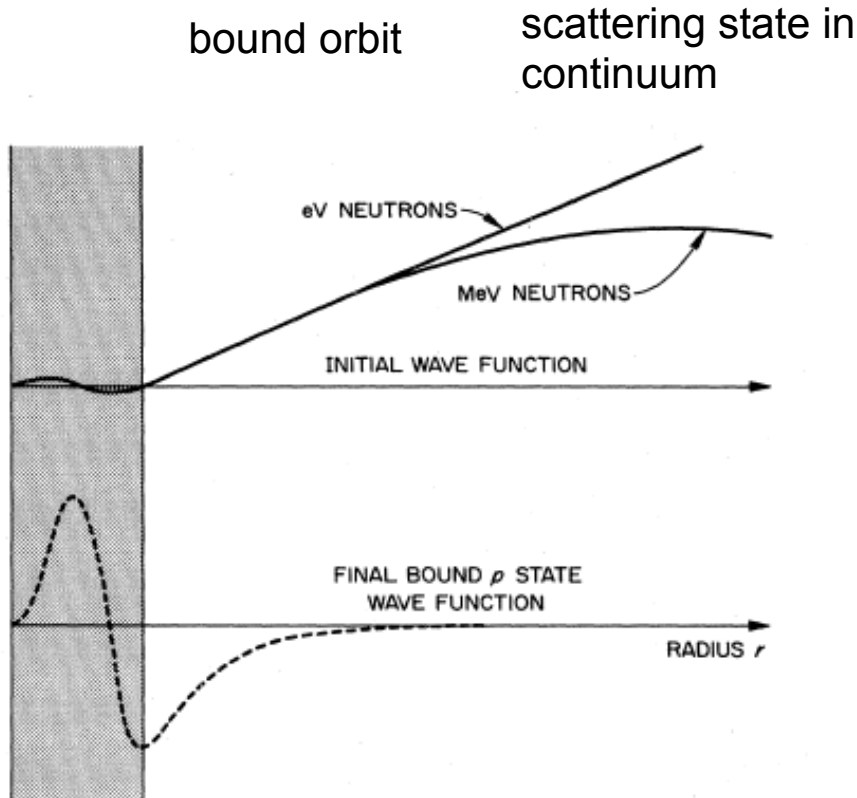
Analytic expression

using the asymptotic wave forms

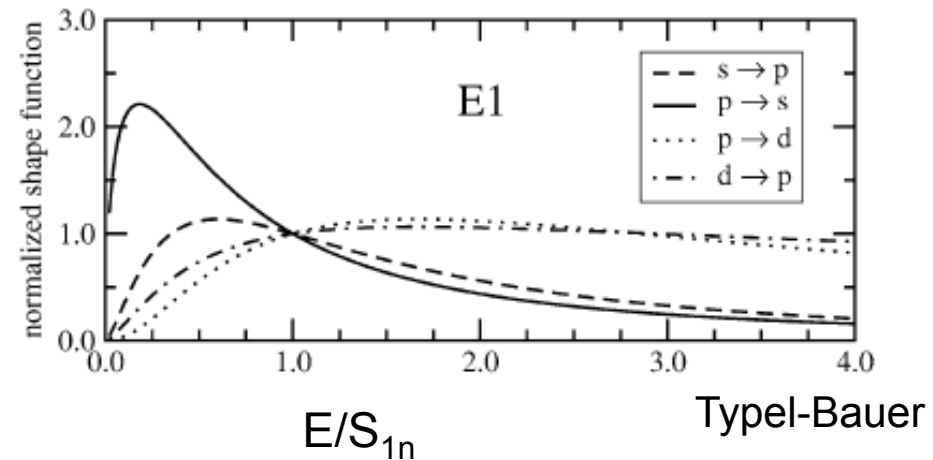
S. Raman et al. PRC32 (1985) 18

S. Typel and G. Bauer NPA759 (2005) 247

M.A.Nagarajan, S.Lenzi, A.Vitturi EPJA24 (2005) 63

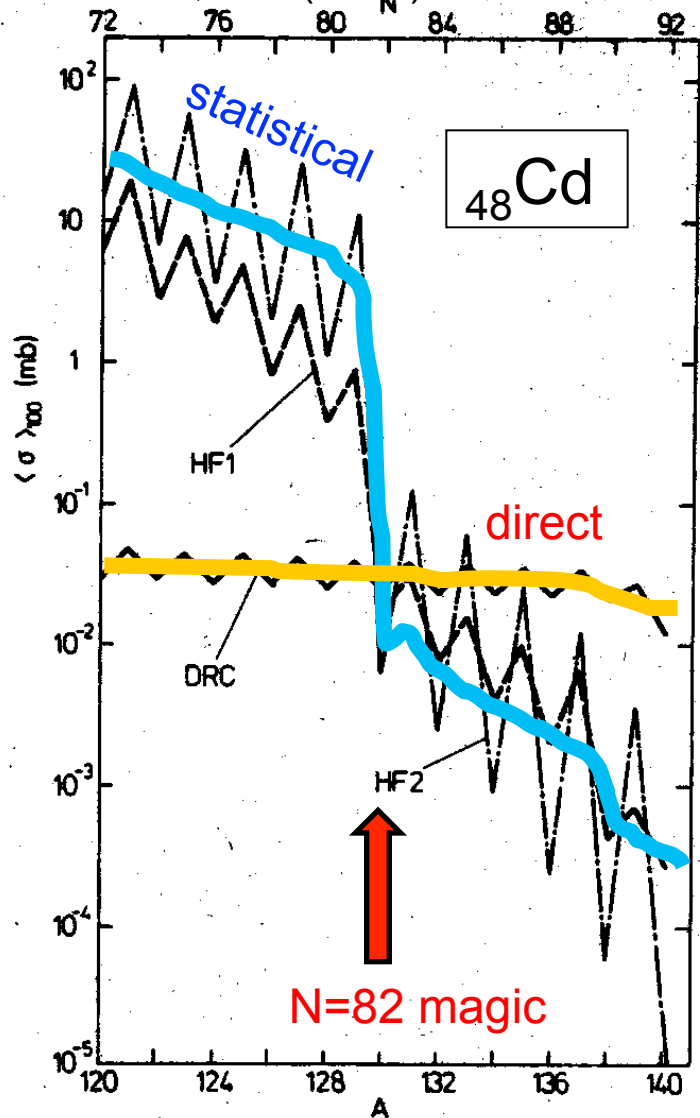


S. Raman et al.

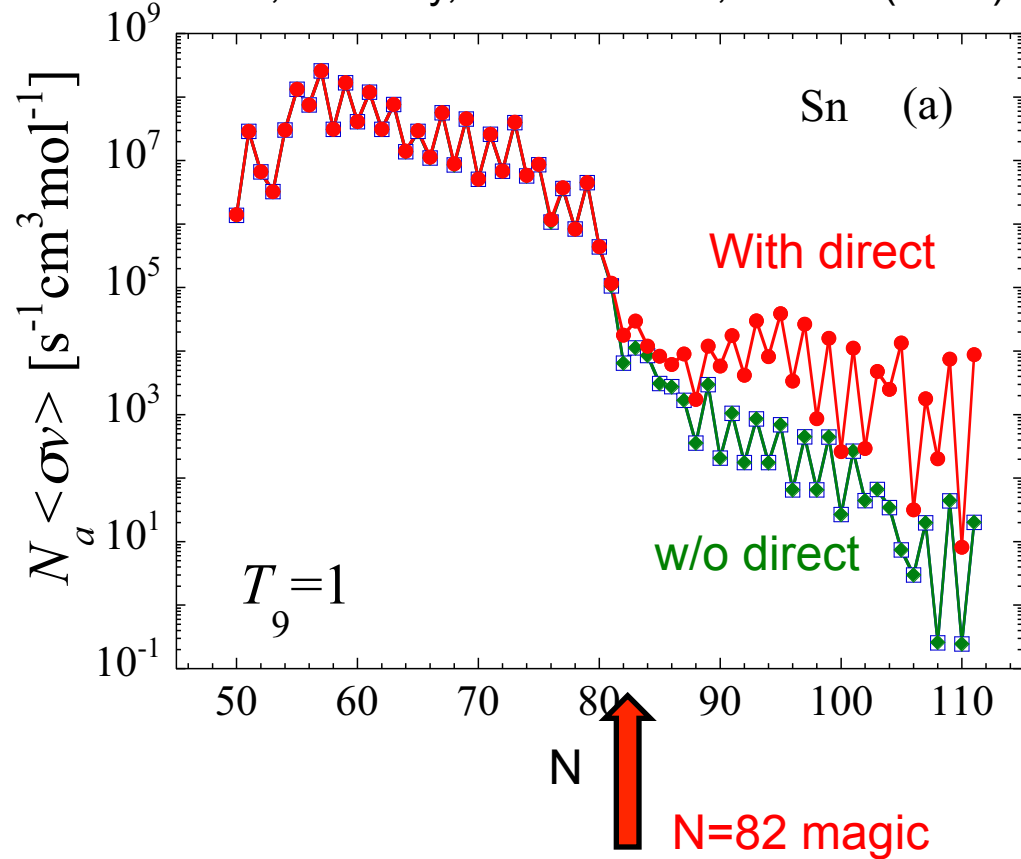


ドリップラインに近づくると直接捕獲過程が支配的

G.J. Mathews et al. Astrophysical
J. 270, 740 (1983)



Y. Su, S.Griery, et al PRC90 , 024604(2018)



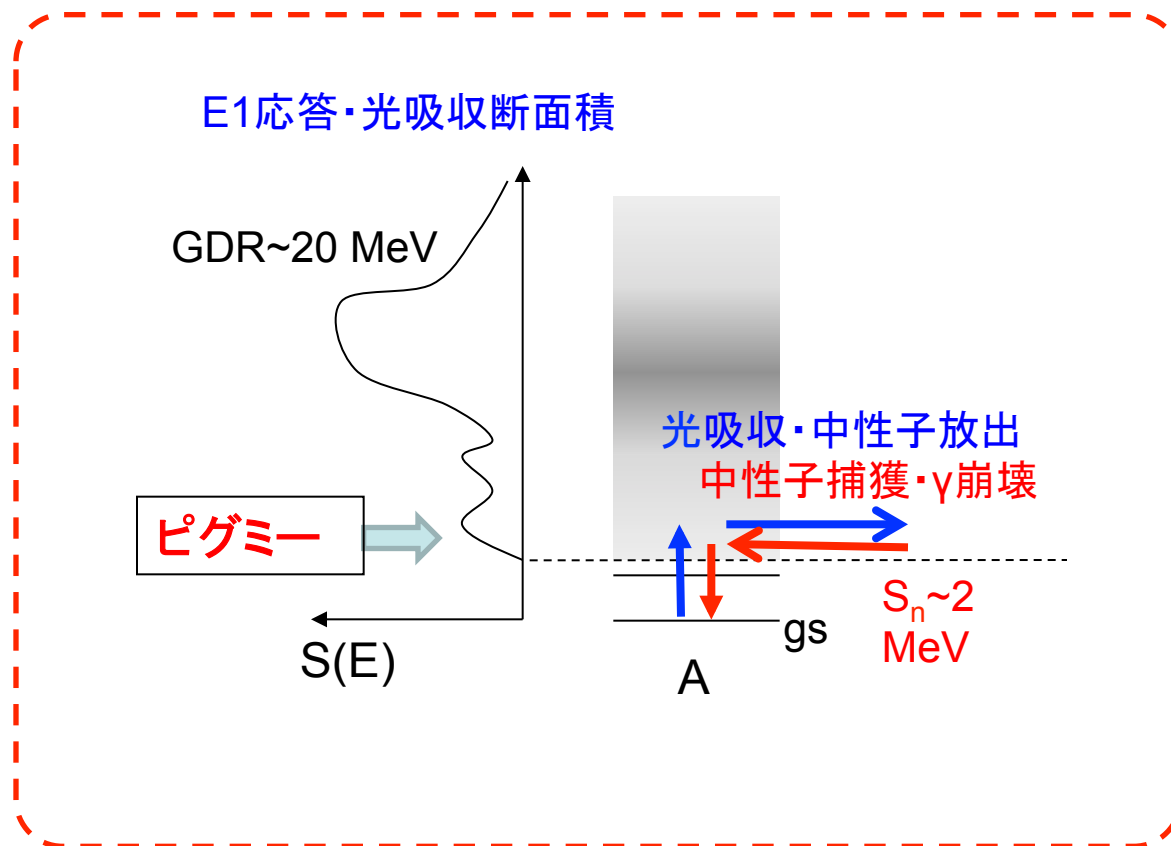
Also S.Chiba et al, PRC77 , 015809(2008)

ただし、これらの直接捕獲はポテンシャル模型

私たちのアプローチ

光吸収断面積に集団運動エンハンス(ピグミー共鳴など)

→ 逆過程の直接中性子捕獲もエンハンスするだろう



← 密度汎関数理論で記述する

密度汎関数理論とは

1. 密度汎関数理論（電子多体系）

1998 Nobel prize in chemistry
to W. Kohn

Hohenberg-Kohn 定理 PR 136, 8844 (1964)

基底状態の多体波動関数 $|\psi\rangle$ 、基底状態エネルギー E_{gs} は
1体密度 $\rho(x) = \langle \Psi | \psi^+(x)\psi(x) | \Psi \rangle$ の汎関数である。

エネルギー汎関数 $E[\rho] = \langle \Psi[\rho] | H | \Psi[\rho] \rangle$ を知ることができ
れば、密度 ρ に関する変分により「厳密な」基底状態エネルギーが
求まる。

Kohn-Sham 理論 PR 140, A1133 (1965)

Hohenberg-Kohn変分原理
密度汎関数の変分
 $E[\rho] = \langle \Psi[\rho] | H | \Psi[\rho] \rangle$
厳密な多体波動関数 $|\psi\rangle$
厳密な基底状態エネルギー

等価

独立粒子型の多体波動関数 $|\Phi\rangle = \det\{\phi_i(x_k)\}$
 $\rho(x) = \langle \Phi | \psi^+(x)\psi(x) | \Phi \rangle = \sum_i |\phi_i(x)|^2$
 $E[\rho] = \langle \Phi | \sum_k \frac{\hbar^2 \Delta_k}{2m} | \Phi \rangle + E_{\text{corr}}[\rho]$

変分原理: 独立粒子型波動関数 $|\Phi\rangle$ についての汎関数変分



自己無撞着場を通じて非線形結合する連立1粒子問題

$$-\frac{\hbar^2 \Delta}{2m} \phi_i(x) + \Gamma_{\text{corr}}[\rho] \phi_i(x) = e_i \phi_i(x) \quad (i = 1, \dots, N)$$

(Hartree-Fock理論と同じ計算手法)

電子多体系

原子分子・ナノ系・凝縮系
に対する第一原理計算のひとつ

時間依存密度汎関数理論

3. 時間依存 Kohn-Sham 理論 → ダイナミクス・励起・応答

核子系: Skyrme TDHF計算1970's~

厳密な多体波動関数 $|\psi(t)\rangle$

$$\delta \int dt \langle \Psi[\rho(t)] | i \frac{\partial}{\partial t} - H | \Psi[\rho(t)] \rangle = 0$$



等価

時間依存有効場を通して非線形結合する連立1粒子問題

$$i \frac{\partial}{\partial t} \phi_i(xt) = -\frac{\Delta}{2m} \phi_i(xt) + \Gamma_{\text{corr}}[\rho(t)] \phi_i(xt) \quad (i = 1, \dots, N)$$

Runge-Gross定理 PRL 52, 997 (1984) Van Leeuwen定理 PRL 82, 3863 (1999)

4. 粒子相関・超流動性の明示的な記述

(時間依存) Kohn-Sham-Bogoliubov理論 (電子・原子系)
時間依存Hartree-Fock-Bogoliubov理論 (核子系)

2000前後から大きく発展

時間依存有効場、時間依存ペア場を通して非線形結合する無限連立準粒子

$$i \frac{\partial}{\partial t} \begin{bmatrix} \phi_i^1(xt) \\ \phi_i^2(xt) \end{bmatrix} = \begin{bmatrix} -\frac{\Delta}{2m} + \Gamma_{\text{corr}}[\rho] - \lambda & \Delta_{\text{pair}}[K] \\ \Delta_{\text{pair}}[K] & \frac{\Delta}{2m} - \Gamma_{\text{corr}}[\rho] + \lambda \end{bmatrix} \begin{bmatrix} \phi_i^1(xt) \\ \phi_i^2(xt) \end{bmatrix} \quad (i = 1, \dots, \infty)$$

中性子星

原子核質量大
域計算

BCS理論・Leggett理論
BCS-BECクロスオーバー
ダイニュートロン相関の記述

核物質・中性子物質

グリーン関数法・Bethe-Salpeter方程式
弱束縛核子・核反応の記述

線形応答理論・QRPA理論
原子核の応答・集団励起の記述

ハロー核・スキン核

核分裂

大振幅形状運

Time-dependent density-functional description of nuclear dynamics

Takashi Nakatsukasa

*Center for Computational Sciences, University of Tsukuba, Tsukuba 305-8577, Japan
and RIKEN Nishina Center, 2-1 Hirosawa, Wako 351-0198, Japan*

Kenichi Matsuyanagi

*RIKEN Nishina Center, 2-1 Hirosawa, Wako 351-0198, Japan
and Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan*

Masayuki Matsuo

Department of Physics, Faculty of Science, Niigata University, Niigata 950-2181, Japan

Kazuhiro Yabana

Center for Computational Sciences, University of Tsukuba, Tsukuba 305-8577, Japan

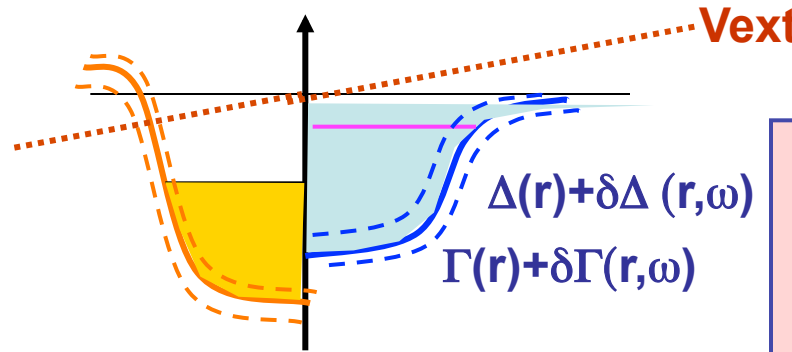
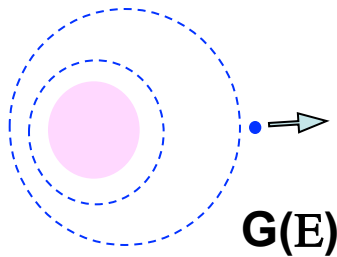
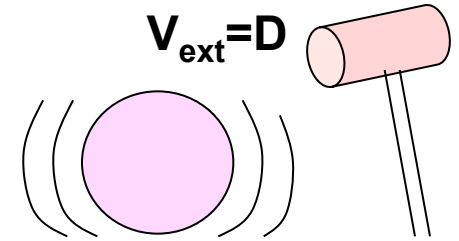
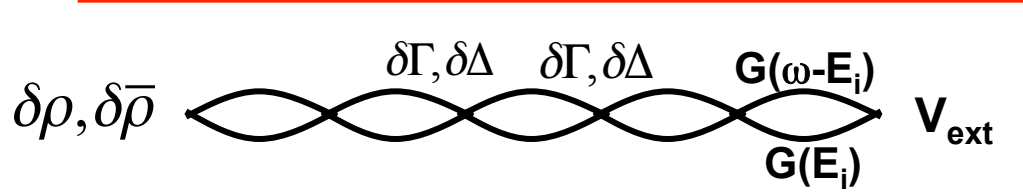
(published 9 November 2016)

QRPA理論: TDDFT理論に基づく線形応答

Matsuo, NPA696,2001
 Mizuyama, et al PRC79,2009
 Serizawa, et al PTP121,2009

Density & pair density oscillation

$$\begin{pmatrix} \delta\rho(\omega) \\ \delta\tilde{\rho}(\omega) \\ \delta\tilde{\rho}^*(\omega) \end{pmatrix} = \int dE G(E) G(\omega - E) \begin{pmatrix} \delta\Gamma(\omega) + V_{ext} \\ \delta\Delta(\omega) \\ \delta\Delta^*(\omega) \end{pmatrix}$$



External field

$$e^{-i\omega t} V_{ext}(r)$$

Propagation of quasi-particle wave in the continuum

$$\begin{pmatrix} \delta\varphi_i^{(1)}(r, E) \\ \delta\varphi_i^{(2)}(r, E) \end{pmatrix} = G(E) \begin{pmatrix} \delta\Gamma + V & \delta\Delta \\ \delta\Delta & -\delta\Gamma - V \end{pmatrix} \begin{pmatrix} \varphi_i^{(1)}(r) \\ \varphi_i^{(2)}(r) \end{pmatrix}$$

Induced fields (polarization)

$$\delta\Gamma(r, \omega) = \frac{\partial^2 E[\rho]}{\partial \rho^2} \delta\rho(r, \omega)$$

$$\delta\Delta(r, \omega) = \frac{\partial^2 E_{pair}[\tilde{\rho}]}{\partial \tilde{\rho}^2} \delta\tilde{\rho}(r, \omega)$$

Selfconsistent field

$$V_{scf}(\omega) = \begin{pmatrix} V_{ext} + \delta\Gamma(\omega) \\ \delta\Delta(\omega) \\ \delta\Delta^*(\omega) \end{pmatrix}$$

中性子放出部分断面積への分解: Zangwill-Soven

Cf. A.Zangwill, P.Soven, PRA 21(1980)1561

T.Nakatsukasa, K.Yabana JCP 114(2001)2550

M.Matsuo PRC91 (2015)034604

correlated response External field

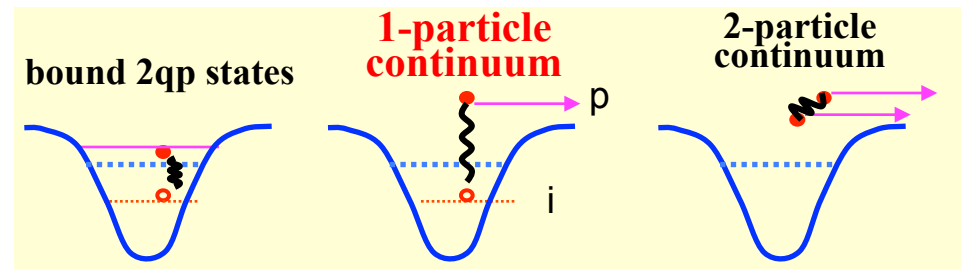
$$S(\omega) = -\frac{1}{\pi} \text{Im} \iint dr dr' V_{ext}^+(r) R_{\text{RPA}}(r, r', \omega) V_{ext}(r') = \sum_k \left| \langle \Omega_k | V_{ext} | 0 \rangle \right|^2 \delta(\omega - \Omega_k)$$

$$= -\frac{1}{\pi} \text{Im} \iint dr dr' \underbrace{V_{scf}^+(r, \omega)}_{\text{Selfconsistent field}} \underbrace{R_0(r, r', \omega)}_{\text{uncorrelated response}} \underbrace{V_{scf}(r, \omega)}_{\text{incl. correlation}} = \sum_{i>j} \left| \langle ij | V_{scf}(\omega) | 0 \rangle \right|^2 \delta(\omega - E_{ij})$$

Selfconsistent field
incl. correlation

uncorrelated
response

- Decomposition w.r.t. uncorrl. 2qp states
- Matrix elements of selfconsistent field



$$S(\omega) = \text{Im} \left[\text{Diagram 1} \right]$$

$$= \text{Im} \left[\text{Diagram 2} \right] = \left| \gamma \text{Diagram 3} \right|^2$$

Diagram 1: A chain of two-particle states connected by an external field V_{ext} .

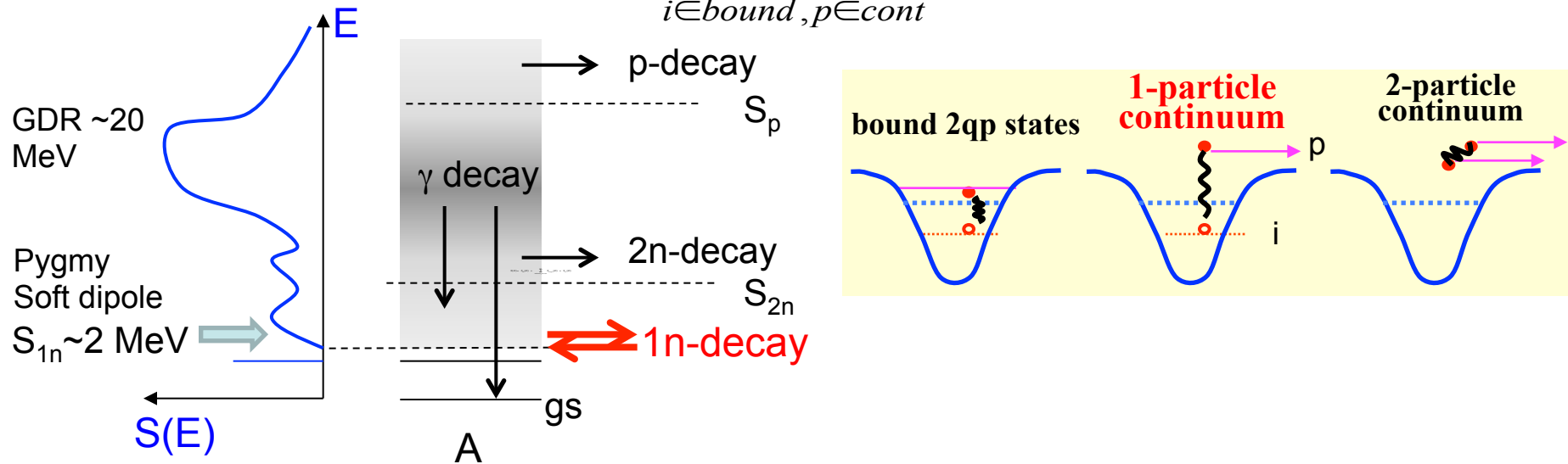
Diagram 2: A two-particle state with a selfconsistent field V_{scf} and labels i and j .

Diagram 3: A chain of two-particle states with a coupling γ and labels i and j .

中性子放出部分断面積と中性子捕獲断面積

E1 strength function (Photo-absorption cross section)

$$S(E) = S_{bb}(E) + \sum_{i \in \text{bound}, p \in \text{cont}} S_{1c(ip)}(E) + S_{2c}(E)$$



- **Partial** photo-absorption x sect. for **direct 1n decay** $\gamma + A \rightarrow A^* \rightarrow (A-1) + n$

$$\sigma(\gamma + A \rightarrow (A-1)_i + n_p) = \frac{16\pi^3 e^2}{9\hbar c} E_\gamma S_{1c(ip)}(E_\gamma)$$

- Inverse **direct neutron capture** x sect. $n + (A-1) \rightarrow A^* \rightarrow A + \gamma$

$$\sigma((A-1)_i + n_p \rightarrow \gamma + A) = S_{J_A}^{J_{A-1}} \frac{k_\gamma^2}{k_n^2} \sigma(\gamma + A \rightarrow (A-1)_i + n_p)$$

NB. neutron energy $E_n \sim kT \sim 10\text{-}100\text{-}1000 \text{ keV}$

Demonstration

1. Sn isotopes beyond A=132: expected r-process nuclei

^{134}Sn ,

^{136}Sn ,

^{138}Sn ,

^{140}Sn ,

^{142}Sn ,

^{144}Sn ,

^{146}Sn ,

^{148}Sn

$$S_{1n} = 2-4 \text{ MeV}$$

expected r-process nuclei

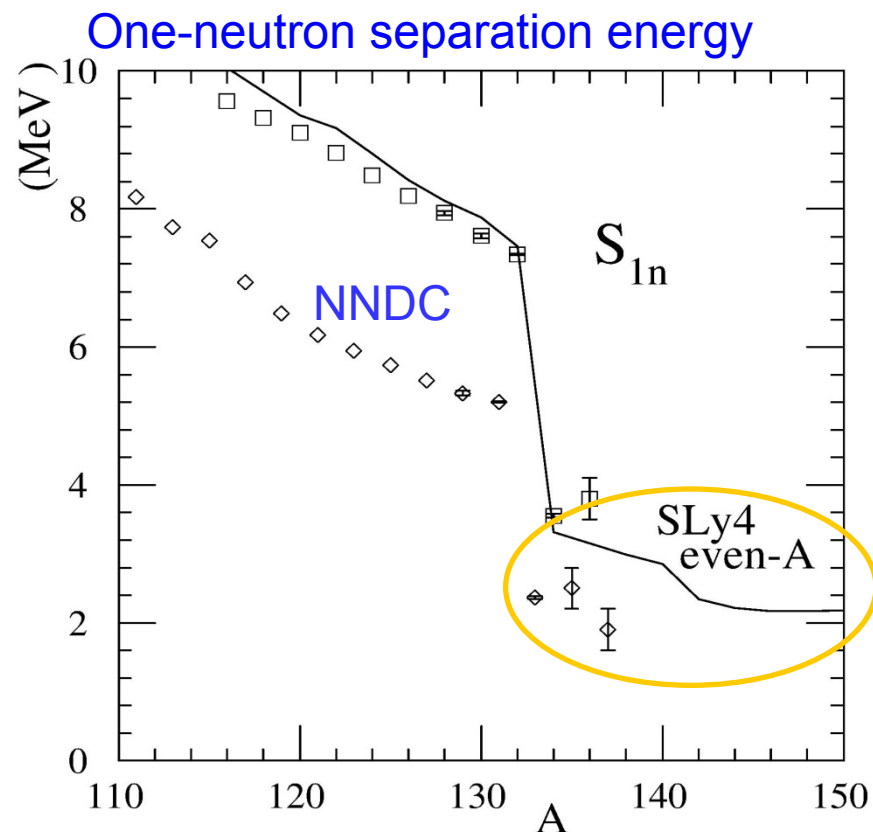
2. HFB with Skyrme functional & DDDI

SLy4, DDDI pairing (mix)

$E_{\text{cut}}=60 \text{ MeV}$, $R_{\text{max}}=20 \text{ fm}$

3. Continuum QRPA in coordinate space

Landau-Migdal approx.



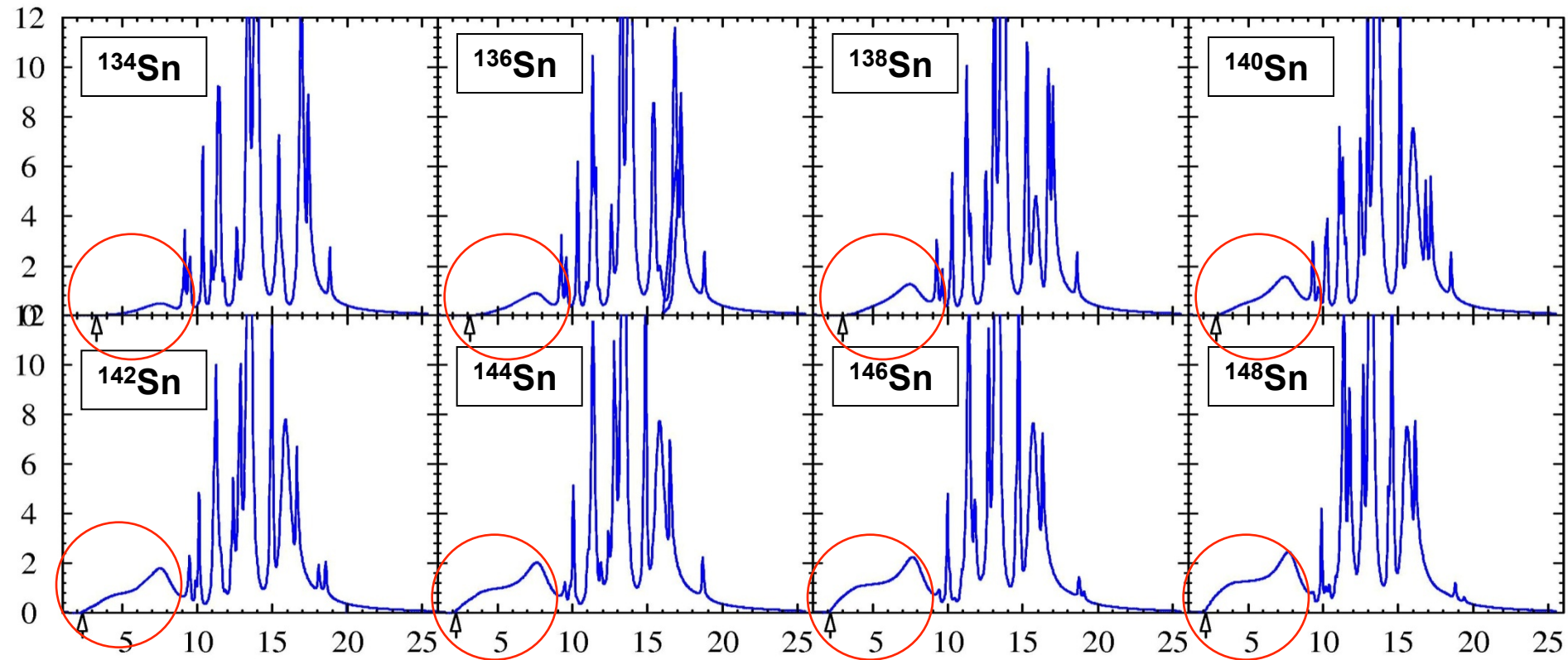
Spherical code:

Serizawa-Matsuo, Prog.Theor.Phys. 121 (2009) 97

Skyrme HFB + Continuum QRPA

Parameter set: *SLy4* *DDDI-mix*
Landau-Migdal approx.

width=0.1MeV



Arrows: neutron separation energy $S_n \sim 2-3$ MeV

Dipole strength in ^{142}Sn

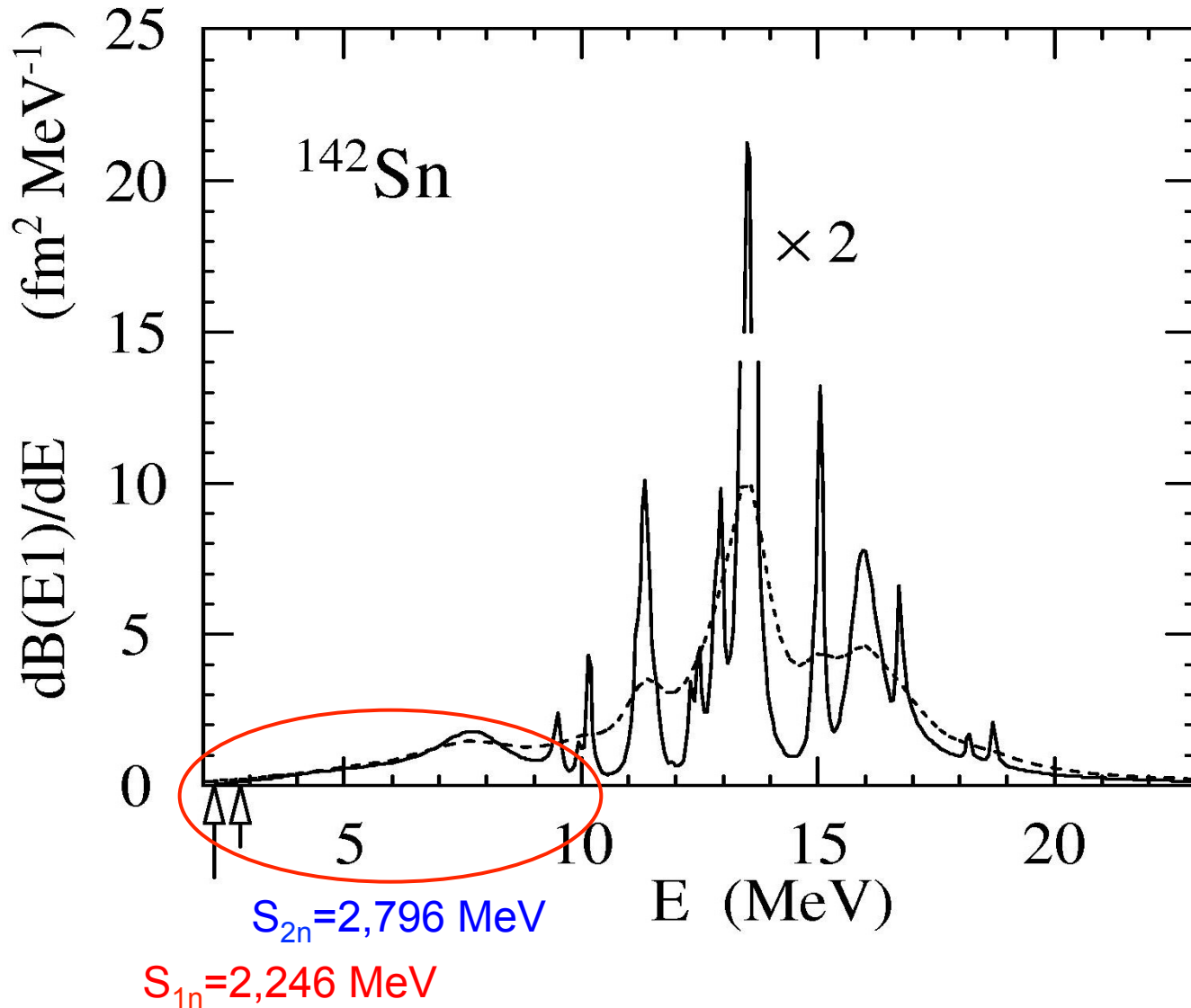
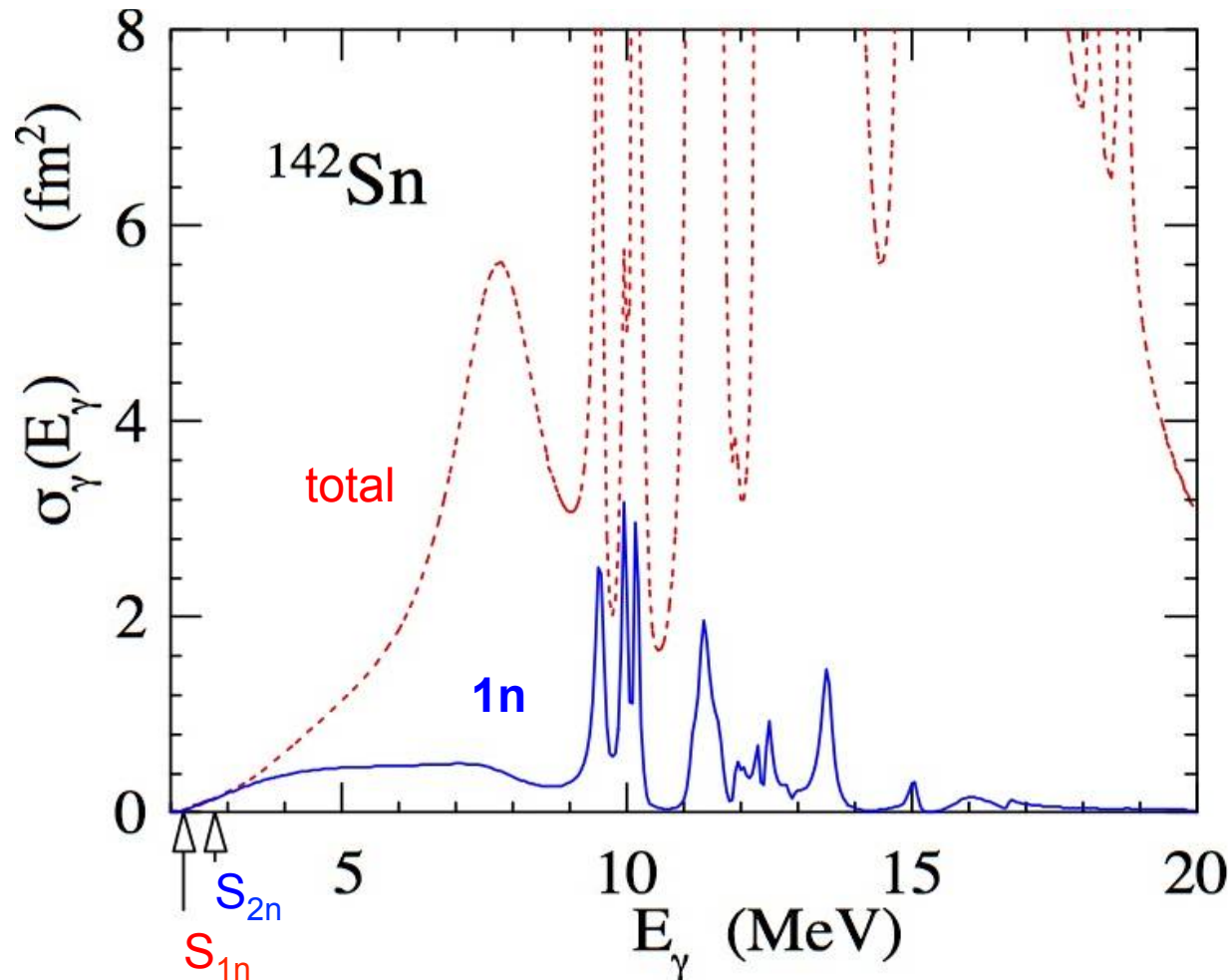
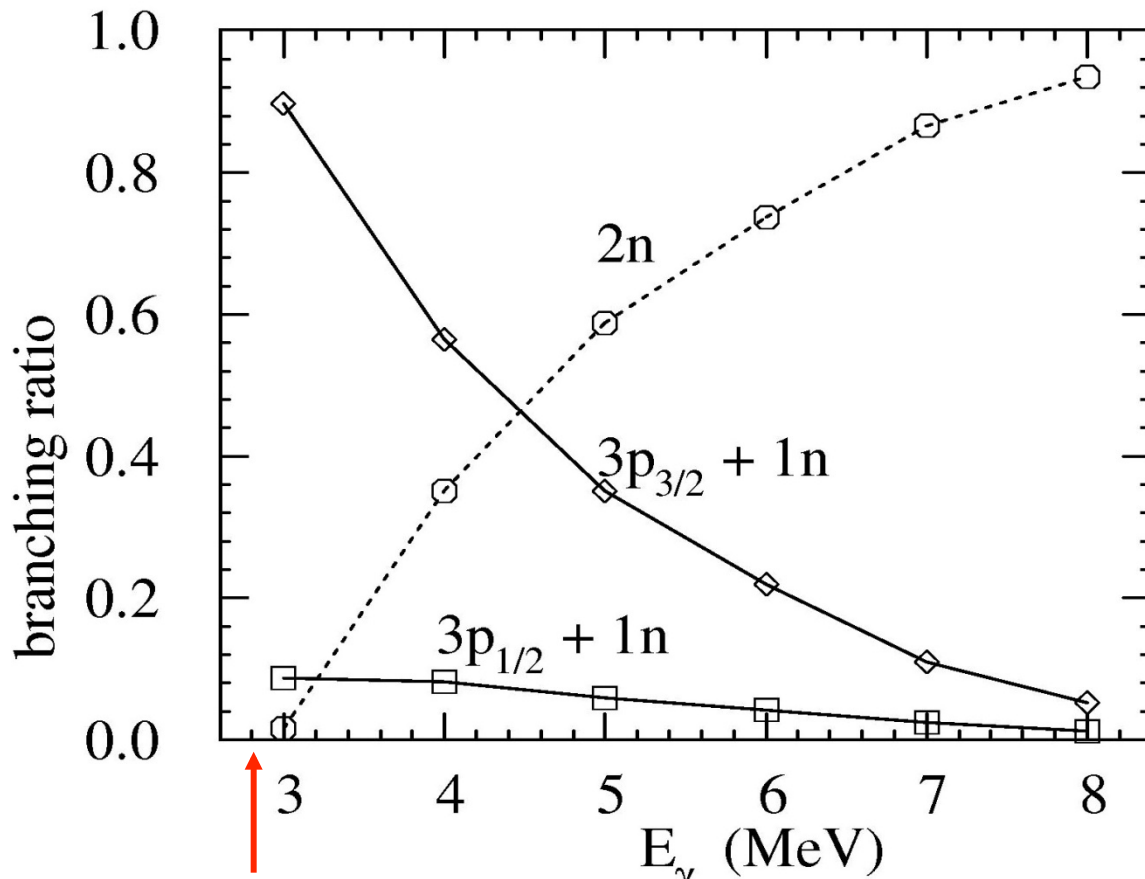


Photo-absorption cross section Total vs Partial (for 1n-decay)



- 1n-decay probability survives even above S_{2n} ,
- Branching ratio of 1n-decay decreases only gradually with increasing energy
- The complex energy-dependence reflects the configuration mixing & correlations in the dipole states. .

Decay branching ratio of photo-excited dipole states

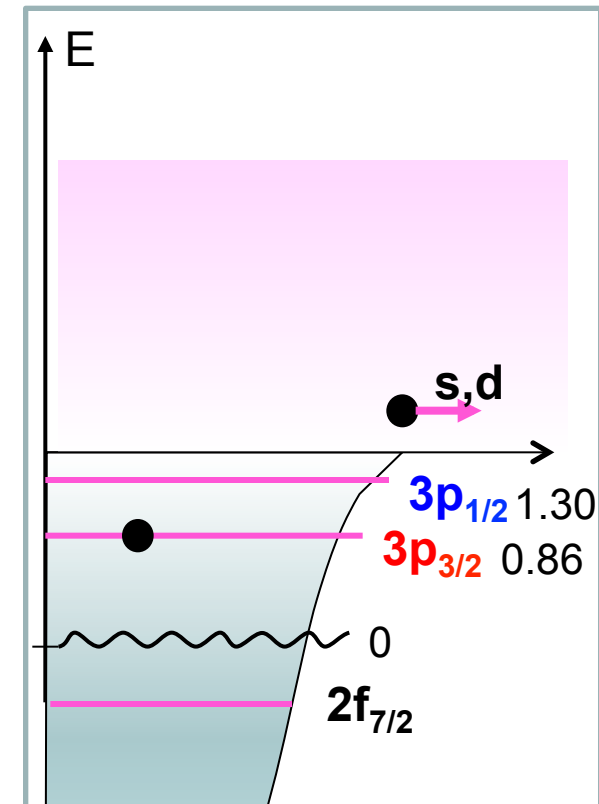
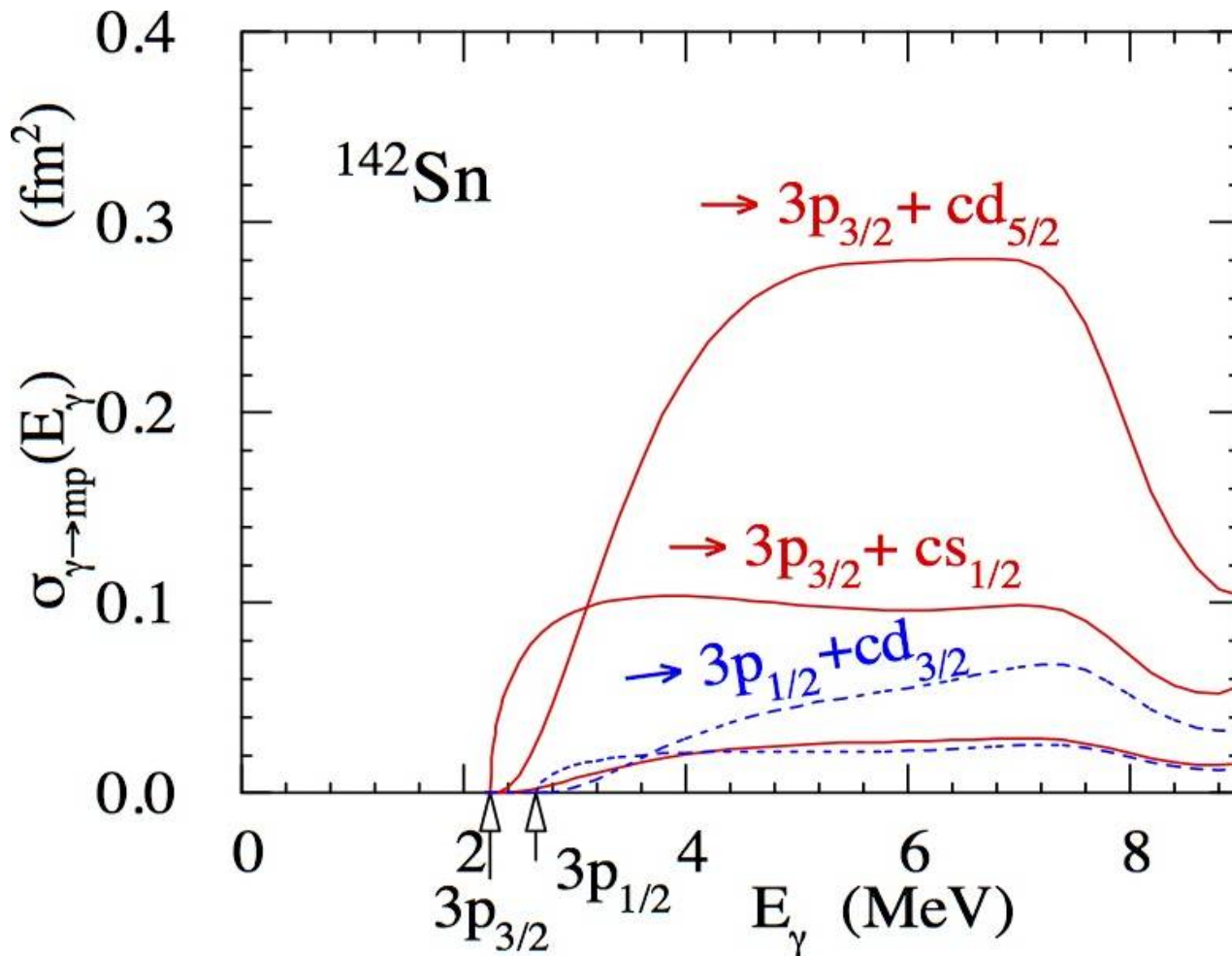


$S_{2n} = 2,796$ MeV

● Branching ratio of 2n-decay increases only gradually with increasing energy

● Two states of ^{141}Sn are populated after 1n-decay

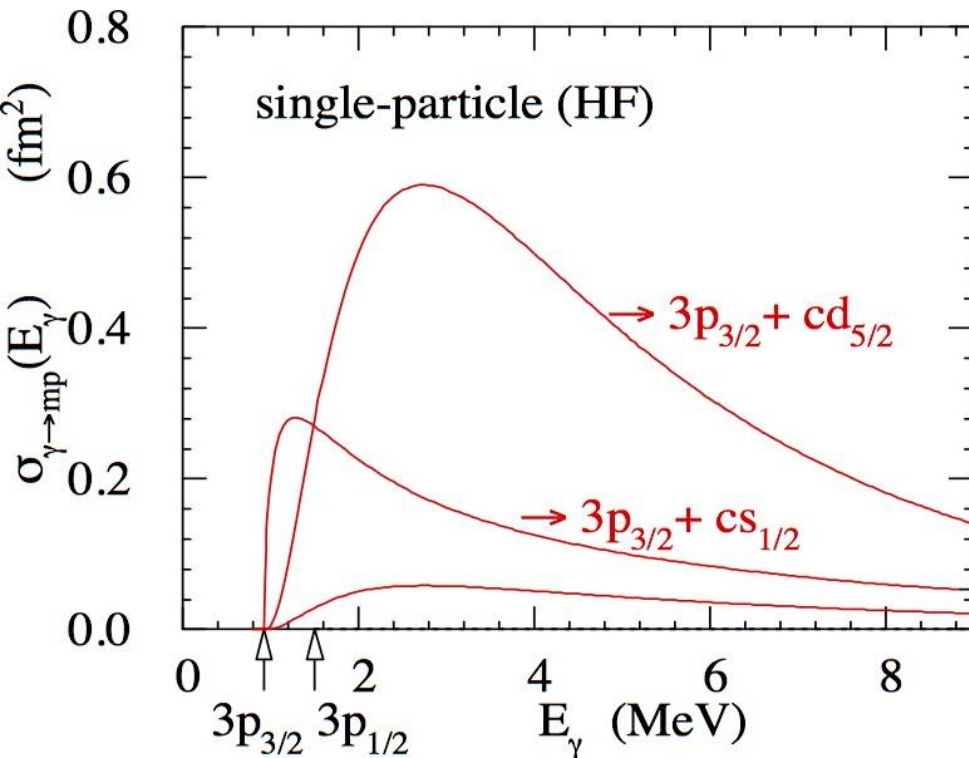
Partial photo-absorption σ for specific 1n-decay channel



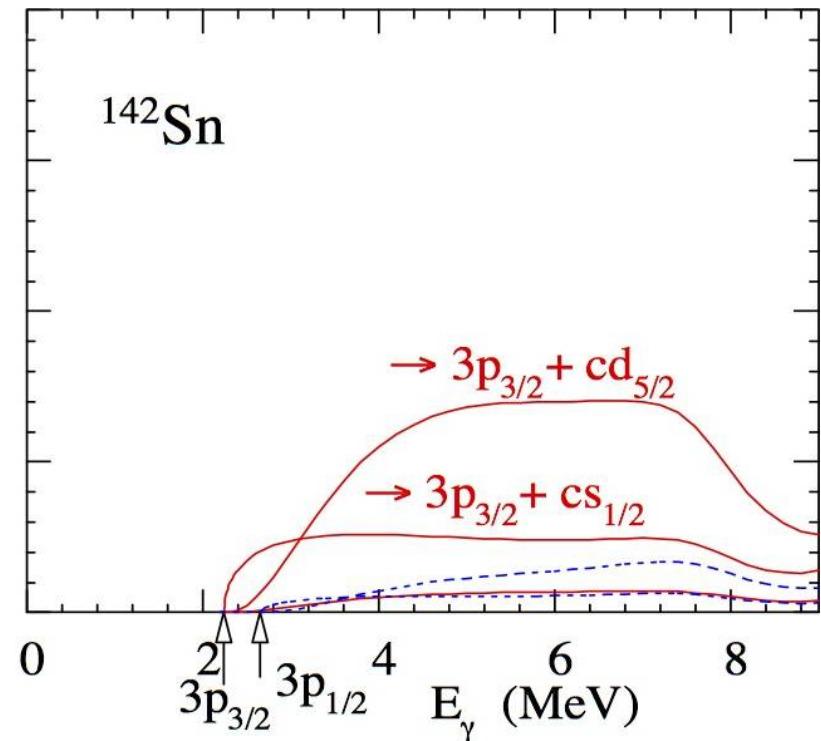
Comparison with single-particle transitions

Hartree-Fock + single-particle transition *Hartree-Fock-Bogoliubov + QRPA*

- Simple structure governed by energies and angular momenta of orbits



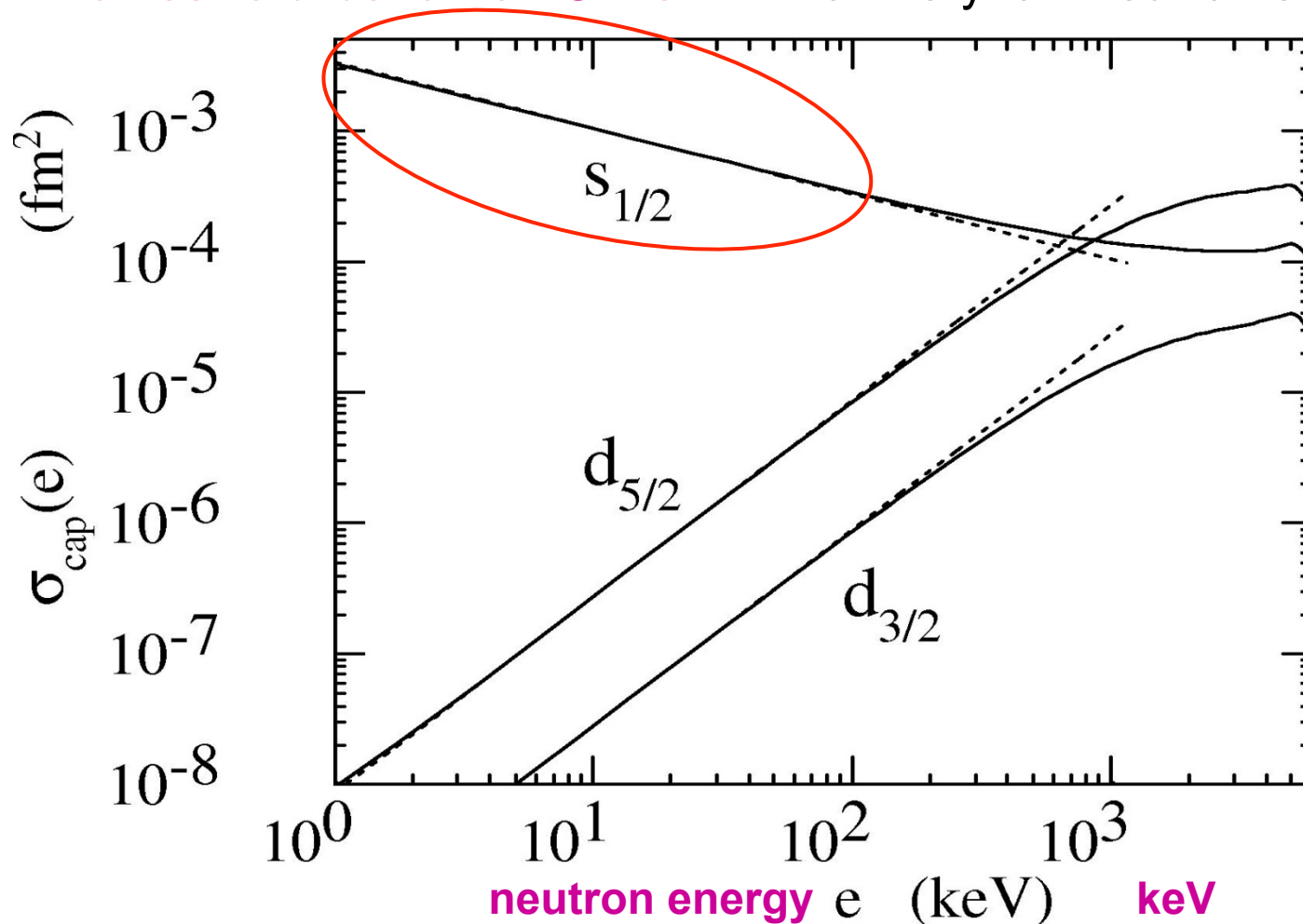
- Threshold energy is higher due to the additional binding caused by the pairing
- Populate also $3p_{1/2}$ state of the daughter
- Energy-dependence is complex



Direct neutron capture cross section



- calculation with wide dynamic range: neutron energy = 1 keV - 6 MeV
- s-wave capture dominates at low energy
- threshold behavior $\sigma \sim e^{-1/2}$ for very low neutron energy < 100 keV



直接過程の包括的記述に向けて

1. 励起状態への遷移 → next talk 齊藤照之
2. 偶奇核、奇奇核 → 先ずは、quasiparticle 近似から
準粒子共鳴の寄与？



結論

- r過程における中性子捕獲反応において、複合核過程(統計模型)だけではなく直接中性子捕獲として記述する必要がある。
- 複合核過程(統計模型)に加え、直接中性子捕獲も密度汎関数理論による核子多体計算が可能になりつつある。

continuum QRPA + Zangwill Soven method

- 包括的な記述を可能にする拡張(励起状態間遷移)も進行中
next talk
- 中性子過剰核の (γ, n) 反応・クーロン分解反応で実験的にも検証可能か