RPA and QRPA calculations with Gaussian expansion method

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@ DCEN2011 Symposium
(YITP, Sep. 26, 2011)

<u>Contents :</u>

I. Introduction

Exotic structure of unstable nuclei

- presence of halo, skin
- Z,N-dep. of shell structure & magic number
- influence of continuum, resonance
- $\cdots$

$\leftrightarrow$

- asymptotics of wave functions
- effective NN int.
- coupling to continuum
- $\cdots$

$\Rightarrow$ **new methods of numerical calculations desired adaptable to unstable nuclei (as well as stable nuclei)**

MF theory $\rightarrow$ s.p. states $\cdots$

- 1st approx.
- good basis for extensive study in nuclear structure calculations

new methods of MF cal. : PTG basis, WS basis, GEM, GF method, *etc.*

Excitations of unstable nuclei

influence of halo, skin, exotic shell structure, $\cdots$?

$\rightarrow$ reliable MF may be crucial !

$\Rightarrow$ RPA (& QRPA)

- **well connected to MF theory (self-consistency)**
  $\rightarrow$ in principle, no additional parameters !
- **suitable to describe global characters of excitations**
  (in mass table & ω)
- **well adapted to collective excitations**
- **spurious modes well separated (if numerical method is good)**
- **lacks coupling to $2p$-$2h$ d.o.f.** **($\rightarrow$ keep in mind !)**

$$\left(\begin{array}{lcl} \text{MF theory} & \approx & \text{EDF approach} \\ \quad \text{finite-range int.} & \rightarrow & \text{non-local EDF} \\ \text{RPA (\& QRPA)} & \approx & \text{(small amp. limit of) ``TDEDF'' approach} \end{array}\right)$$

II. Test of GEM for MF calculations

"Gaussian expansion method" (GEM)

E. Hiyama *et al.*, Prog. Part. Nucl. Phys. 51, 223 ('03)

Applications of GEM to MF calculations

- **spherical HF** ··· **H.N. & M. Sato, N.P.A 699, 511 ('02); 714, 696 ('03)**
- **spherical HFB** ··· **H.N., N.P.A 764, 117 ('06); 801, 169 ('08)**
- **axial HF & HFB** ··· **H.N., N.P.A 808, 47 ('08)**

Advantages of the method

(i) **ability to describe ε-dep. exponential/oscillatory asymptotics**

(ii) **tractability of various 2-body interactions**

(iii) **basis parameters insensitive to nuclide**

(iv) **exact treatment of Coulomb & c.m. Hamiltonian**

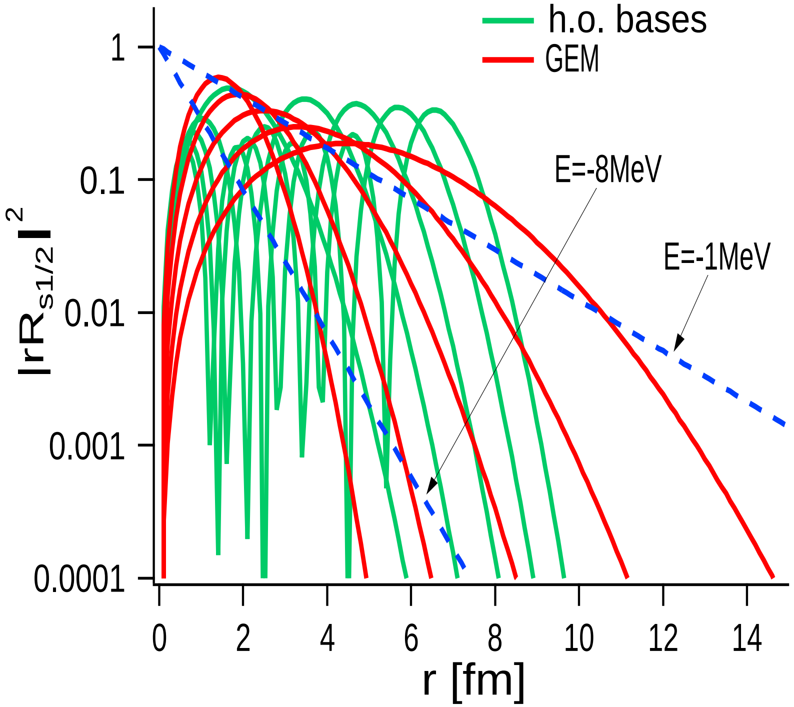
★ Outline of the method

- **basis :** $\phi_{\nu\ell jm}(\boldsymbol{r}) = R_{\nu\ell j}(r)\,[Y^{(\ell)}(\hat{\boldsymbol{r}})\chi_\sigma]^{(j)}_m\,; \qquad R_{\nu\ell j}(r) = \mathcal{N}_{\nu\ell j}\, r^\ell \exp(-\nu r^2)$

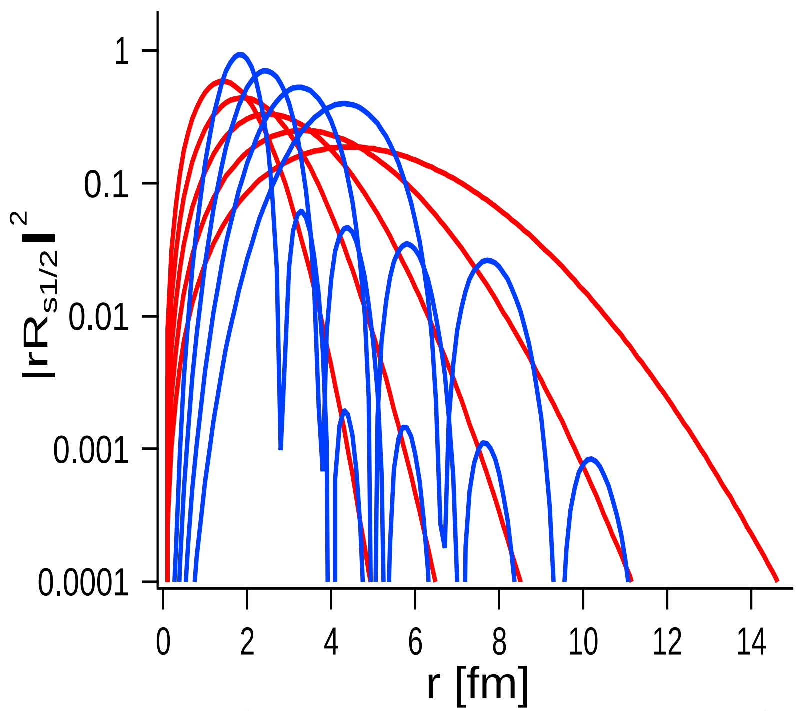
$\nu \to$ **complex** $\quad \nu = \nu_\mathrm{r} + i\nu_\mathrm{i}$

$$\left.\begin{array}{l}\mathrm{Re}[R_{\nu\ell j}(r)]\\ \mathrm{Im}[R_{\nu\ell j}(r)]\end{array}\right\} \propto\; r^\ell \exp(-\nu_\mathrm{r}\, r^2) \left\{\begin{array}{l}\cos(\nu_\mathrm{i}\, r^2)\\ \sin(\nu_\mathrm{i}\, r^2)\end{array}\right.$$

GEM *vs.* HO bases ($s_{1/2}$)



Real- & complex-range GEM bases ($s_{1/2}$, $\nu_\mathrm{i}/\nu_\mathrm{r} = \pi/2$)



$\Rightarrow$ **approximate wave-function asymptotics (ε-dep., exp. & osc.)**

- **2-body int. matrix elements ← Fourier transform.**

  ⇒ various interactions

  - **central, LS, tensor channels**
  - **function form of r — delta, Gauss, Yukawa, *etc.***
  - **c.m., Coulomb (including exchange terms)**

- **solve HF/HFB eq. as generalized eigenvalue problem → iteration**

  (alternatively, gradient method may be applied)

★ Wave-function asymptotics in HFB

for large r

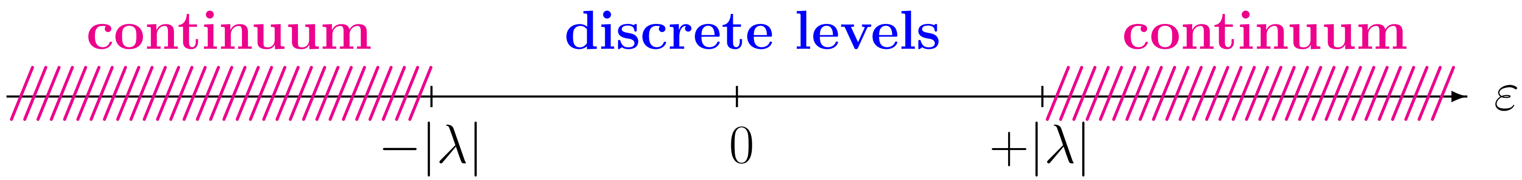
$$U_i(\boldsymbol{r}) \;\approx\; \begin{cases} \cos(p_{i+}r + \theta_{i+})/r \;\; \textbf{for} \;\; \lambda + \varepsilon_i > 0 & \left(\, p_{i+} \equiv \sqrt{2M(\lambda + \varepsilon_i)}\,\right) \\ \exp(-\eta_{i-}r)/r \;\; \textbf{for} \;\; \lambda + \varepsilon_i < 0 & \left(\, \eta_{i-} \equiv \sqrt{2M(-\lambda - \varepsilon_i)}\,\right) \end{cases},$$

$$V_i(\boldsymbol{r}) \;\approx\; \exp(-\eta_{i+}r)/r \;\; \textbf{for} \;\; \lambda - \varepsilon_i < 0 \qquad \left(\, \eta_{i+} = \sqrt{2M(-\lambda + \varepsilon_i)}\,\right)$$

$\lambda(<0)$**: chem. pot.,** $\varepsilon_i(>0)$**: q.p. energy**

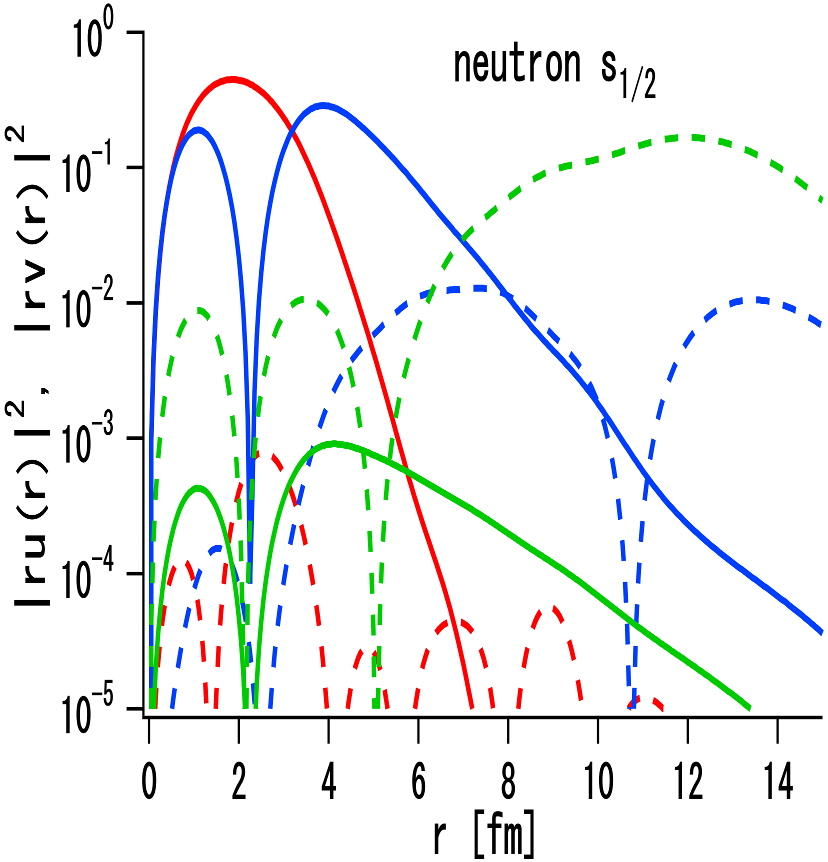
$\cdots$ **exponential & oscillatory asymptotics !**

$\Leftrightarrow$



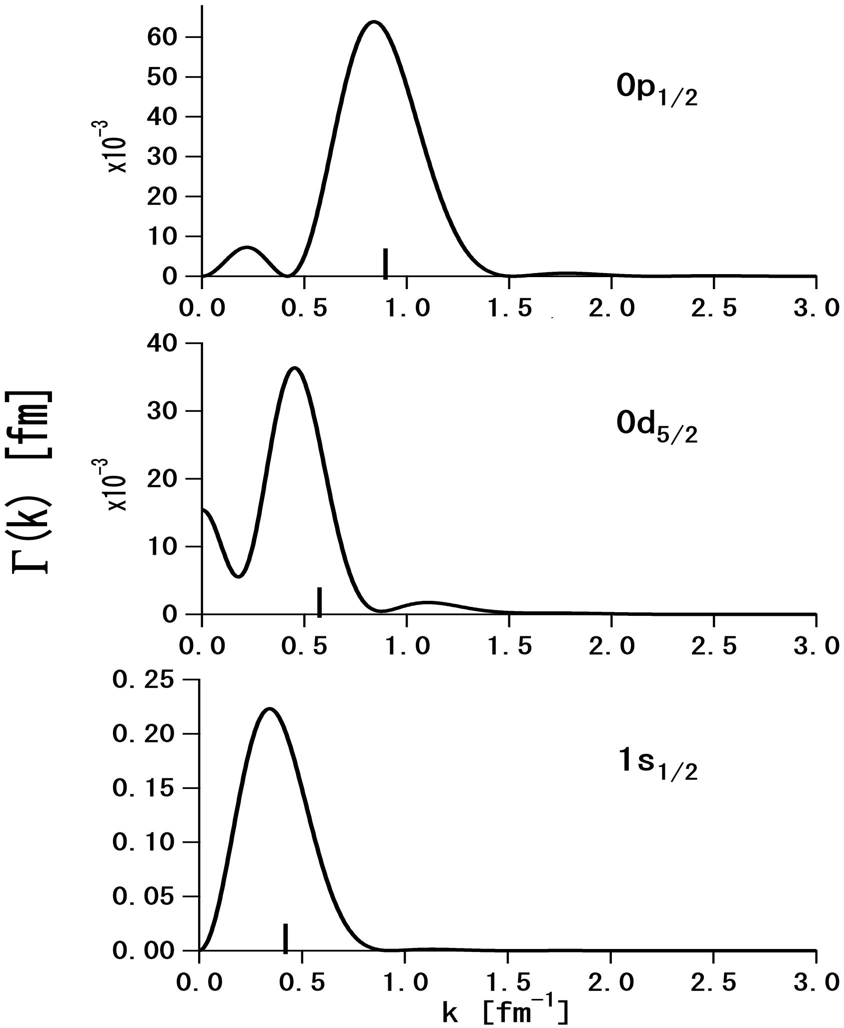
$(\lambda < 0)$

$ns_{1/2}$ **levels in** ^{26}**O** **(Gogny-D1S)**



oscillatory asymptotics?

→ Fourier transform

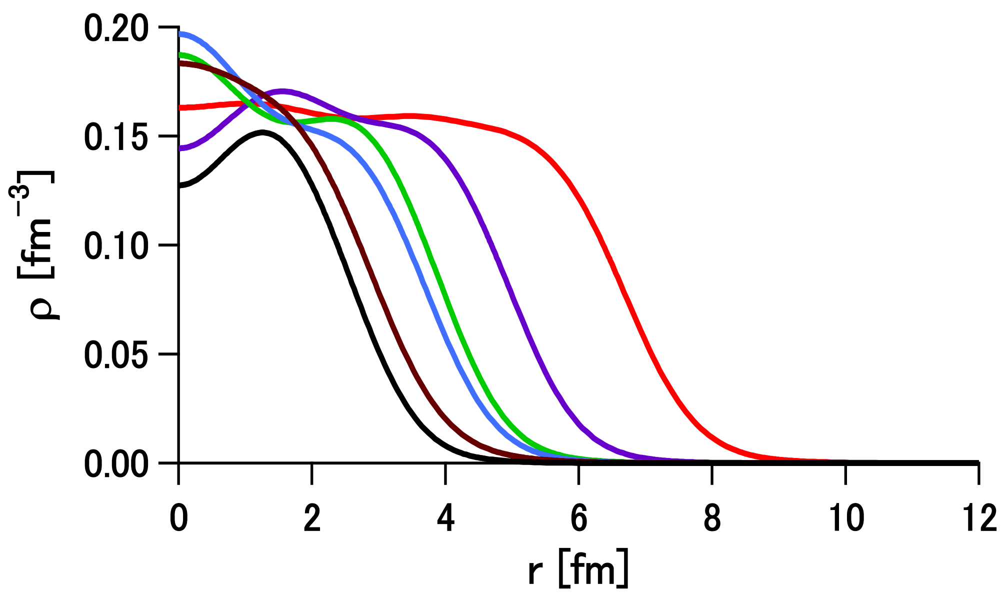


$\cdots$ ε**-dep. exponential & oscillatory asymptotics well described by GEM**

★ **Single basis-set ? — various doubly magic nuclei (HF with Gogny-D1S)**

B.E. (MeV)

Nuclide	HO	GEM
^{16}**O**	129.638	129.520
^{24}**O**	168.573	168.598
^{40}**Ca**	344.470	344.570
^{48}**Ca**	416.567	416.764
^{90}**Zr**	785.126	785.928
^{208}**Pb**	1638.094	1639.047



(^{16}O, ^{24}O, ^{40}Ca, ^{48}Ca, ^{90}Zr & ^{208}Pb)

basis : $R_{\nu\ell j}(r) = \mathcal{N}_{\nu\ell j}\, r^{\ell} \exp(-\nu r^2)\,,\ \nu = \nu_{\rm r} + i\nu_{\rm i}\,:$

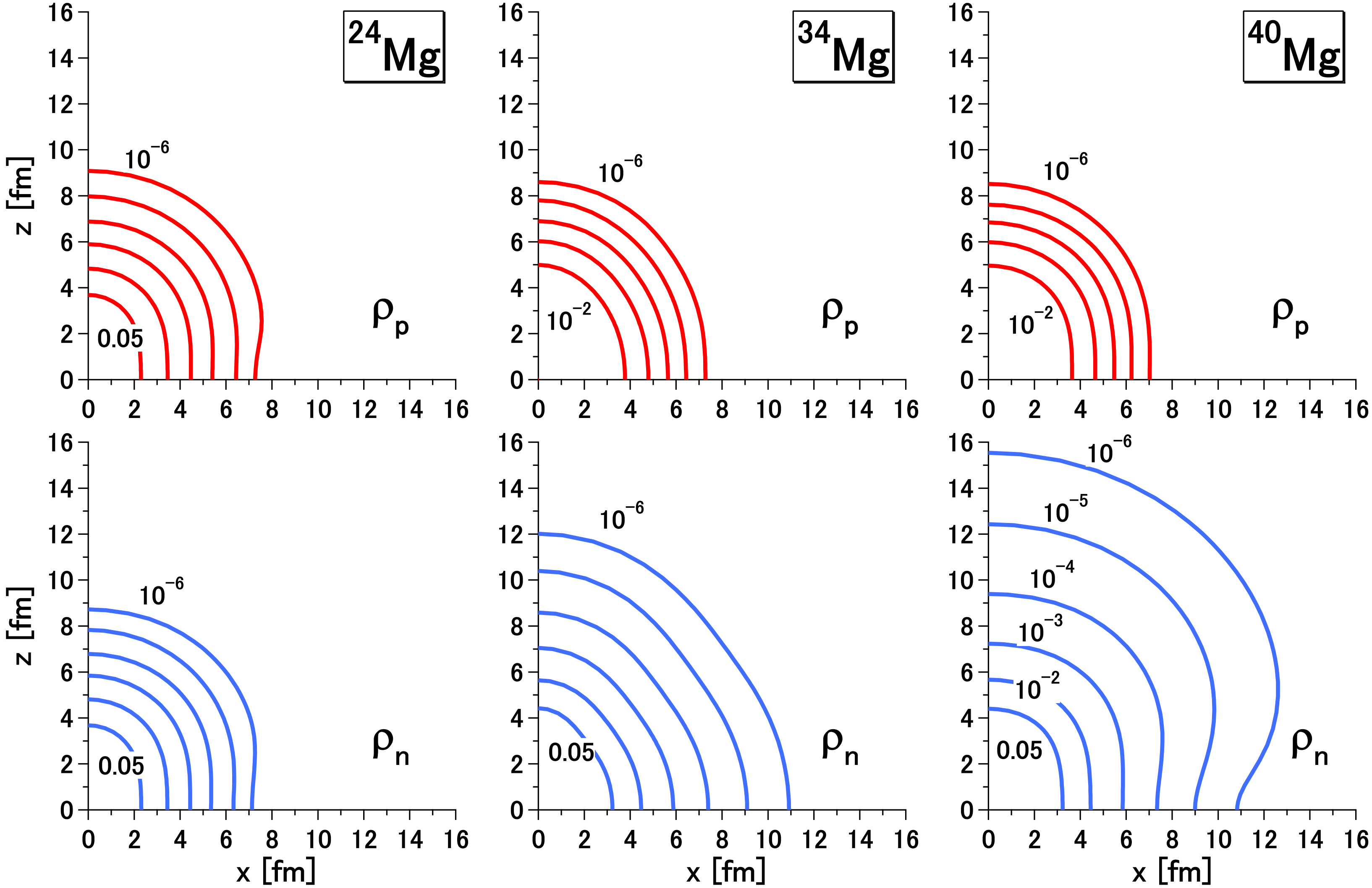
$$\nu_{\rm r} = \nu_0\, b^{-2k}\,,\quad \begin{cases} \nu_{\rm i} = 0 & (k = 0, 1, \cdots, 5) \\ \dfrac{\nu_{\rm i}}{\nu_{\rm r}} = \pm\dfrac{\pi}{2} & (k = 0, 1, 2) \end{cases} \quad ; \qquad \nu_0 = (2.40\,{\rm fm})^{-2}\,,\ \ b = 1.25$$

→ **#(basis)=12, irrespective of** (ℓ, j)

⇒ store int. matrix elements ($\sim 4\,$GB)**, & use them for all calculations !**

★ **Deformation with spherical basis?** → **good for normal deformation**

Contour plot of $\rho_\tau(\boldsymbol{r})$: **(HFB with Gogny-D1S)**



— **"peanut-shape" neutron halo in ^{40}Mg!**

III. Test of GEM for RPA (& QRPA) calculations

★ **Comparison of methods for contact force**

Ref.: H.N. *et al.*, Nucl. Phys. A 828, 283 ('09)

- **MF — Woods-Saxon pot.**
- **residual int. — contact force** Shlomo & Bertsch, N.P.A 243, 507 ('75)

$$\hat{v}_{\mathrm{res}} = f\left[t_0(1 + x_0 P_\sigma)\,\delta(\mathbf{r}_1 - \mathbf{r}_2) + \frac{1}{6}t_3(1 + x_3 P_\sigma)\,\rho(\mathbf{r}_1)\,\delta(\mathbf{r}_1 - \mathbf{r}_2)\right]$$

$$f \leftarrow \omega_s = 0 \ \text{(spurious c.m. state)}$$

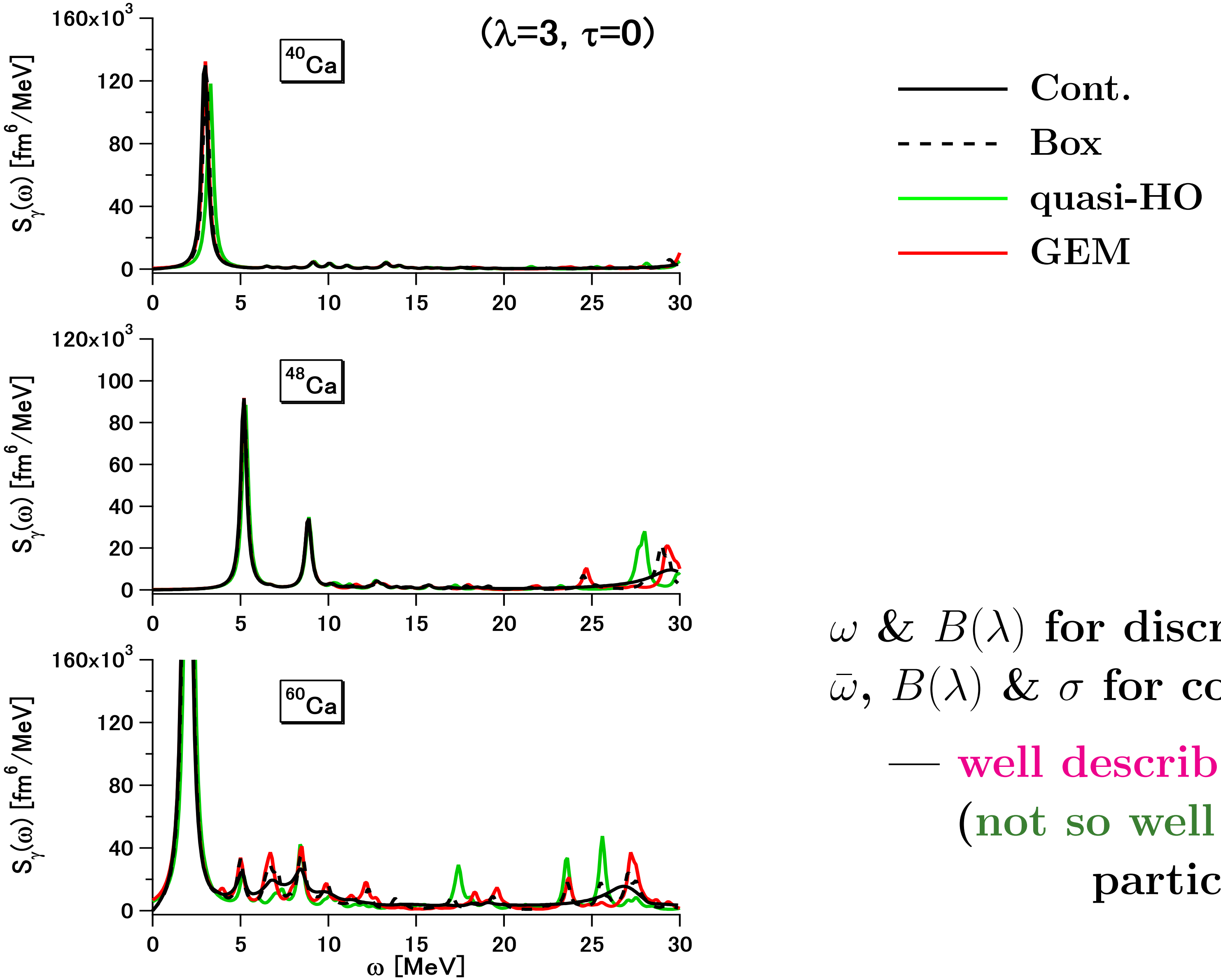
- **sample nuclei —** ^{40,48,60}**Ca**

Methods to be compared

1. **GEM** (basis-set adopted in HF & HFB cal.)
2. **quasi-HO basis** ($N_{\mathrm{osc}} \lesssim 11$)
3. **r-space with box boundary** ($h = 0.2\,\mathrm{fm}$, $r_{\max} = 20\,\mathrm{fm}$, $\Delta\varepsilon_{\mathrm{cut}} \geq 50\,\mathrm{MeV}$)
4. **continuum RPA** ($h = 0.2\,\mathrm{fm}$) ⋯ '**exact**'

1, 2 (, 3). ⋯ MF cal. → solve RPA eq.

• **Strength function :** $\mathcal{O}^{(\lambda,\tau=0)} = \sum_i r_i^\lambda Y^{(\lambda)}(\hat{\mathbf{r}}_i)$

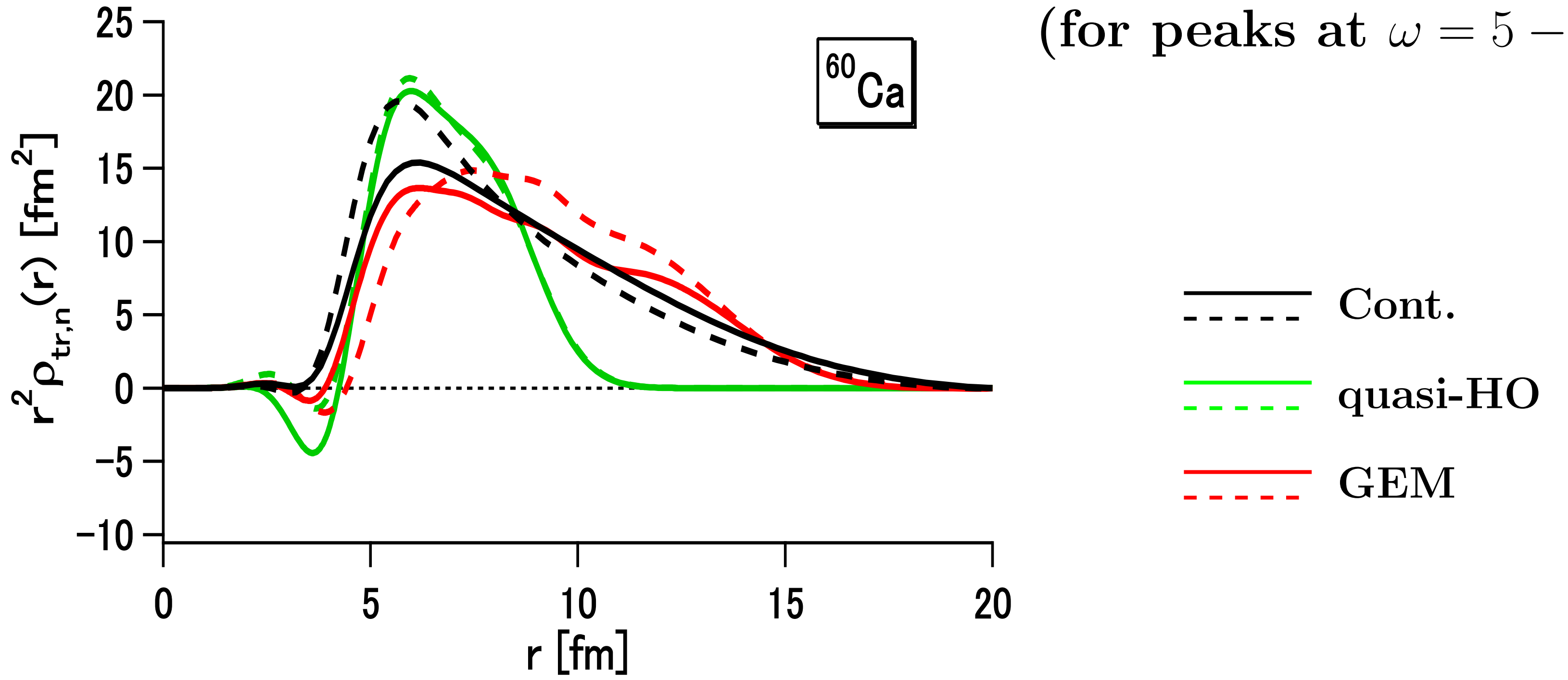


ω & $B(\lambda)$ **for discrete states**
$\bar{\omega}$, $B(\lambda)$ & σ **for continuum**

— **well described by GEM**
(**not so well by quasi-HO**,
particularly for ^{60}**Ca**)

• **Transition density :**

(for peaks at $\omega = 5 - 7\,\mathrm{MeV}$**)**



∘ **The GEM results are in fair agreement with the 'exact' ones**

∘ **The quasi-HO results have significant discrepancy for low-energy excitation near the drip line**

$\leftrightarrow$ **difficulty in describing** $r \gtrsim 10\,\mathrm{fm}$ **components**

★ **HF + RPA** **(by GEM with Gogny-D1S)**

$$\hat{H} = \hat{K} + \hat{V}_N + \hat{V}_C - \hat{H}_{\text{c.m.}}$$

$$\hat{K} = \sum_i \frac{\boldsymbol{p}_i^2}{2M}$$

$\hat{V}_N$ **: effective NN int. (finite-range !)**

$\hat{V}_C$ **: Coulomb int. (including exchange terms exactly)**

$\hat{H}_{\text{c.m.}}$ **: c.m. Hamiltonian (1- + 2-body terms)**

- **Spurious c.m. state — $\omega_s = 0$?**

nuclide	ω_s^2
^{40}**Ca**	-5.80×10^{-6}
^{48}**Ca**	-8.61×10^{-6}
^{60}**Ca**	-2.67×10^{-6}

$\cdots$ **well separated from physical mode**

(also confirmed by $B(E1)$)

- **EWSR**

$$\sum_\alpha \omega_\alpha \left|\langle\alpha|\mathcal{O}^{(\lambda,\tau=0)}|0\rangle\right|^2 = \frac{1}{2}\langle 0|[\mathcal{O}^{(\lambda,\tau=0)\dagger},[H,\mathcal{O}^{(\lambda,\tau=0)}]]|0\rangle$$

$$= \frac{\lambda(2\lambda+1)^2}{4\pi}\frac{1}{2M}\Big[\Big(1-\frac{1}{A}\Big)\langle 0|\sum_i r_i^{2\lambda-2}|0\rangle - \frac{4\pi}{2\lambda-1}\frac{1}{A}\langle 0|\sum_{i\neq j} r_i^{\lambda-1}Y^{(\lambda-1)}(\hat{\mathbf{r}}_i)\cdot r_j^{\lambda-1}Y^{(\lambda-1)}(\hat{\mathbf{r}}_j)|0\rangle\Big]$$

(**last term ← 2-body terms of** $H_{\rm c.m.}$)

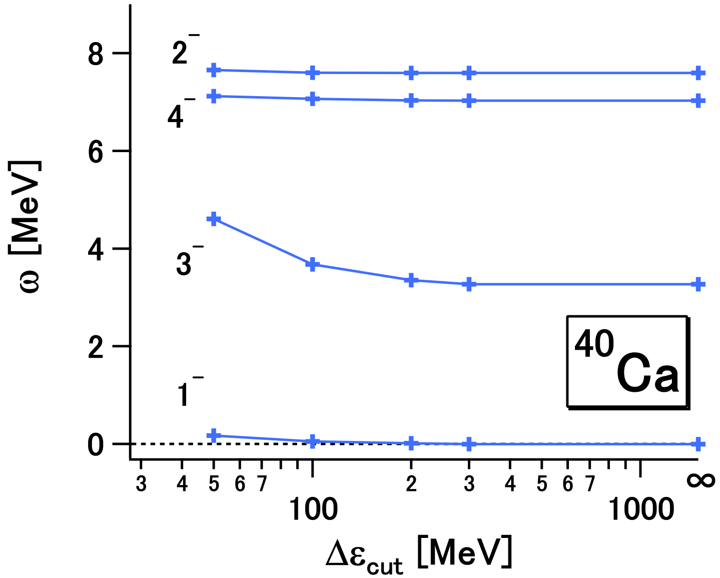
$$\rightarrow \quad \mathcal{R}^{(\lambda,\tau)} = \sum_\alpha \omega_\alpha \left|\langle\alpha|\mathcal{O}^{(\lambda,\tau)}|0\rangle\right|^2 \Big/ \frac{1}{2}\langle 0|[\mathcal{O}^{(\lambda,\tau)\dagger},[H,\mathcal{O}^{(\lambda,\tau)}]]|0\rangle = 1\,\textbf{?}$$

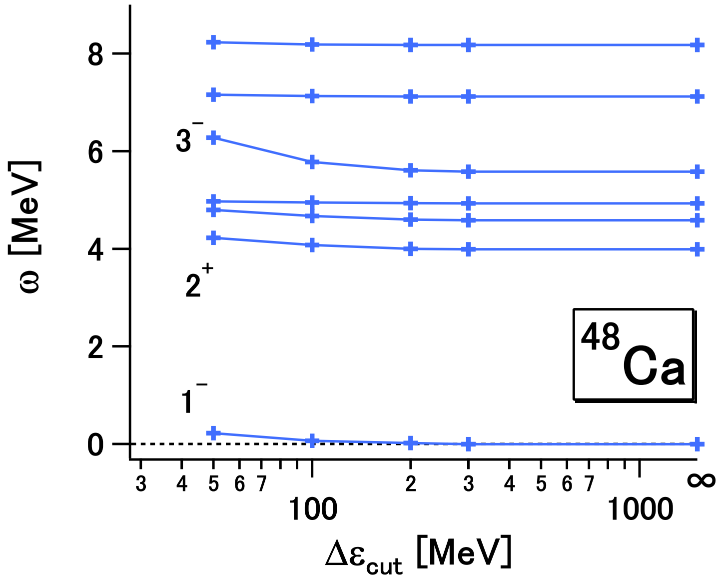
nuclide	$\mathcal{R}^{(\lambda=2,\tau=0)}$	$\mathcal{R}^{(\lambda=3,\tau=0)}$
^{40}**Ca**	1.005	1.031
^{48}**Ca**	1.006	1.033
^{60}**Ca**	1.003	1.010

★ **HFB + QRPA** (by GEM with Gogny-D1S)

$\Delta\varepsilon_{\rm cut}$: cut-off energy for unperturbed 2 q.p. states → convergence ?

HF + RPA (for reference)





HFB + QRPA

$\omega_s^2\,(\mathrm{MeV}^2)$:

$\Delta\varepsilon_{\rm cut}$ (MeV)	^{44}**Ca** 1^-	^{110}**Sn** 0^+
100	—	2.4×10^{-1}
200	-4.9×10^{-4}	5.5×10^{-2}
300	-1.8×10^{-5}	4.4×10^{-2}
500	—	5.3×10^{-3}
1000	—	-4.8×10^{-6}

IV. Several topics

★ **Application with *semi-realistic* interaction**

'M3Y-Pn' ← **M3Y int. + phenomenological modification (mainly, saturation & ℓs splitting)**

Ref. : H.N., P.R.C 68, 014316 ('03)

'M3Y-P5' & 'P5′' — **full inclusion of $v_{\rm OPEP}^{\rm (C)}$ (central part of OPEP) & $v^{\rm (TN)}$ (G-matrix-based tensor force)**

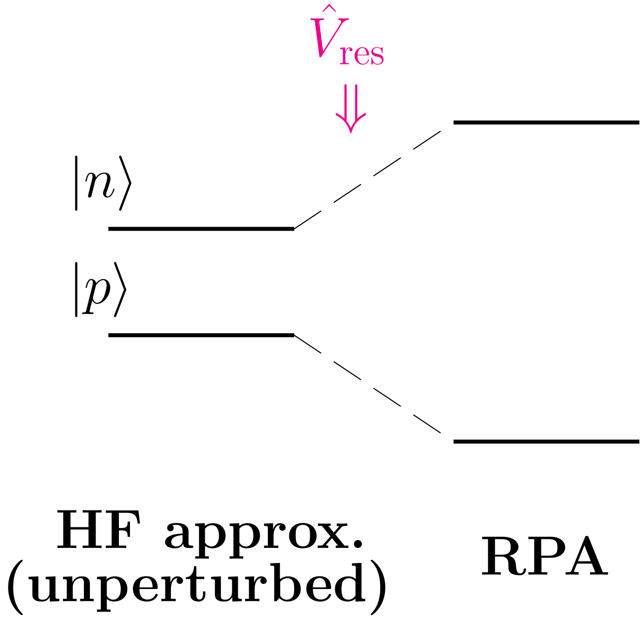
Ref. : H.N., P.R.C 78, 054301 ('08); 82, 029902(E) ('10)
P.R.C 81, 027301 ('10); 82, 029903(E) ('10)

- **Effects of $v_{\rm OPEP}^{\rm (C)}$ & $v^{\rm (TN)}$ on shell structure** → **see Refs.**

Ref. : H.N., P.R.C 81, 051302(R) ('10)
E.P.J.A 42, 565 ('09)
in AIP Proc. 1377 (to be published)

- **Tensor-force effects on $M1$ transition in ^{208}Pb   (HF + RPA)**

  $1p$-$1h$ **excitation** — p**:** $(0h_{11/2})^{-1}(0h_{9/2})$ **,** n**:** $(0i_{13/2})^{-1}(0i_{11/2})$



$$|\text{“}\mathbf{IV}\text{”}\rangle = -c_2|p\rangle + c_1|n\rangle = -c_2'|\mathbf{IS}\rangle + c_1'|\mathbf{IV}\rangle$$

$$(c_1 > c_2 > 0)$$

$$|\text{“}\mathbf{IS}\text{”}\rangle = c_1|p\rangle + c_2|n\rangle = c_1'|\mathbf{IS}\rangle + c_2'|\mathbf{IV}\rangle$$

$(c_1.c_2)$ **or** $(c_1', c_2') \leftrightarrow \hat{V}_{\rm res}$

IV dominance $\rightarrow$ $B(M1; 0_1^+ \rightarrow 1^+(\text{“}\mathbf{IS}\text{”}))$ **sensitive to** $\hat{V}_{\rm res}$

			M3Y-P5		Exp.
			$\hat{v} - \hat{v}^{(\mathrm{TN})}$	$\hat{v}$	
"IS"	E_x	(MeV)	6.87	5.85	5.85
	$B(M1)\uparrow$	(μ_N^2)	4.7	2.4	2.0
"IV"	E_x	(MeV)	9.2 – 10.9	9.2 – 10.9	7.1 – 8.7
	$(\bar{E}_x)$		(9.9)	(9.6)	
	$\sum B(M1)\uparrow$	(μ_N^2)	16.3	19.4	16.3 **or** 18.2

($\hat{T}^{(M1)}$ ··· **including corrections from $2p$-$2h$ & MEC**)

··· **role of tensor force reconfirmed**

Ref. : T. Shizuma *et al.*, P.R.C 78, 061303(R) ('08)

(**effects of 2-body correlations ?** — { **IS** ··· **weak**; **IV** ··· **strong** })

★ **Low-energy excitations of "doubly-magic" nuclei**

- **^{78}Ni**

erosion of $Z = 28$ magicity due to $v^{(\mathrm{TN})}$?

Ref. : T. Otsuka *et al.*, P.R.L. 95, 232502 ('05)

MF cal. with semi-realistic int. (incl. $v^{(\mathrm{TN})}$) → magicity preserved

⇒ will be resolved by near-future experiments !

a key exp. — $E_x(2_1^+)$ → HF + RPA prediction

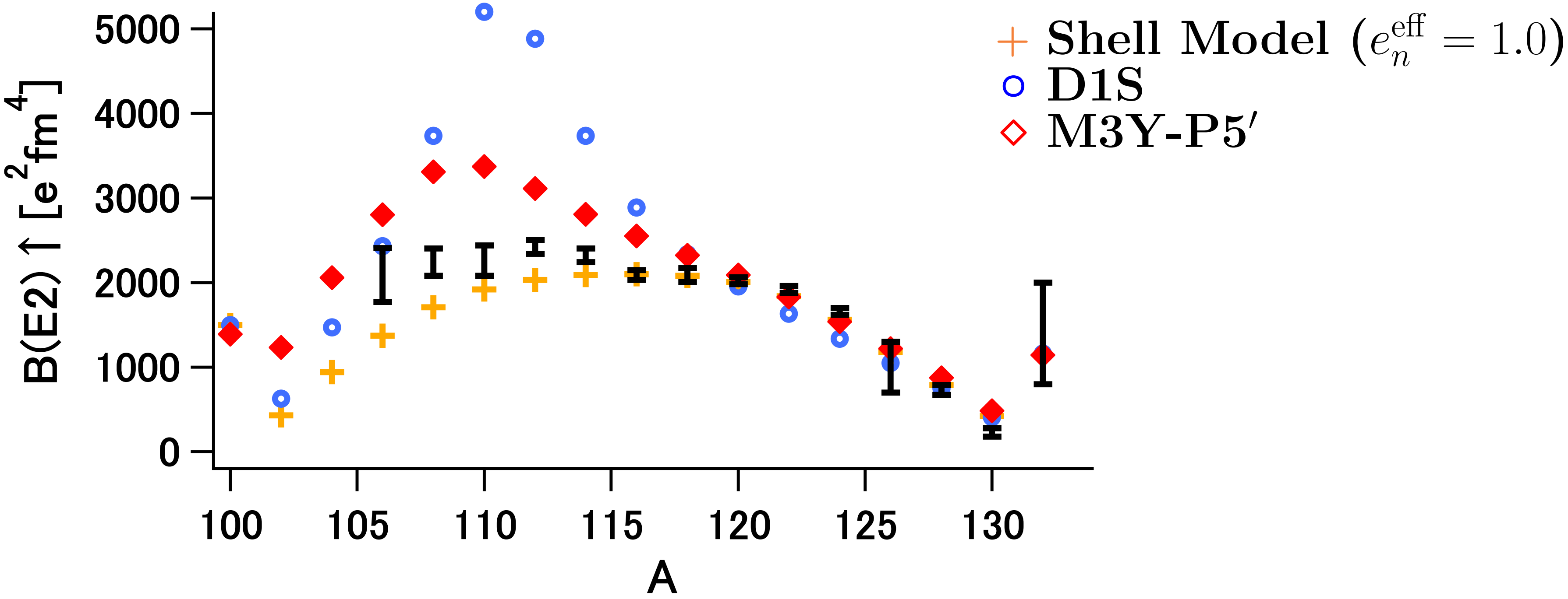
(with $Z = 28$ magicity)

→ reference of experiments

		D1S	**D1M**	**M3Y-P5′**
$E_x(2_1^+)$	(MeV)	3.15	3.00	3.25
$B(E2; 2_1^+ \to 0_1^+)$	($e^2\mathrm{fm}^4$)	84.4	83.4	84.4

Ref. : H.N., P.R.C 81, 051302(R) ('10)

★ $B(E2)$ **in Sn isotopes** (— preliminary !)



$B(E2; 0_1^+ \to 2_1^+)$ **in** $N \geq 70$

- ○ **well adjusted to exp. by** $e_n^{\text{eff}} = 1.0\,e$ **in shell model**

Ref. : A. Banu *et al.*, P.R.C 72, 061305(R) ('05)

- ○ well reproduced in HFB + QRPA with no adjustable parameters

$B(E2;0_1^+ \to 2_1^+)$ **in** $N \sim 60$

A) underestimate in shell model (with $e_n^{\rm eff} = 1.0\,e$**)**

B) overestimate in HFB + QRPA with M3Y-P5′

C) severe overestimate in HFB + QRPA with D1S

(& SLy4 ? Ref. : J. Terasaki *et al.*, P.R.C 78, 044311 ('08))

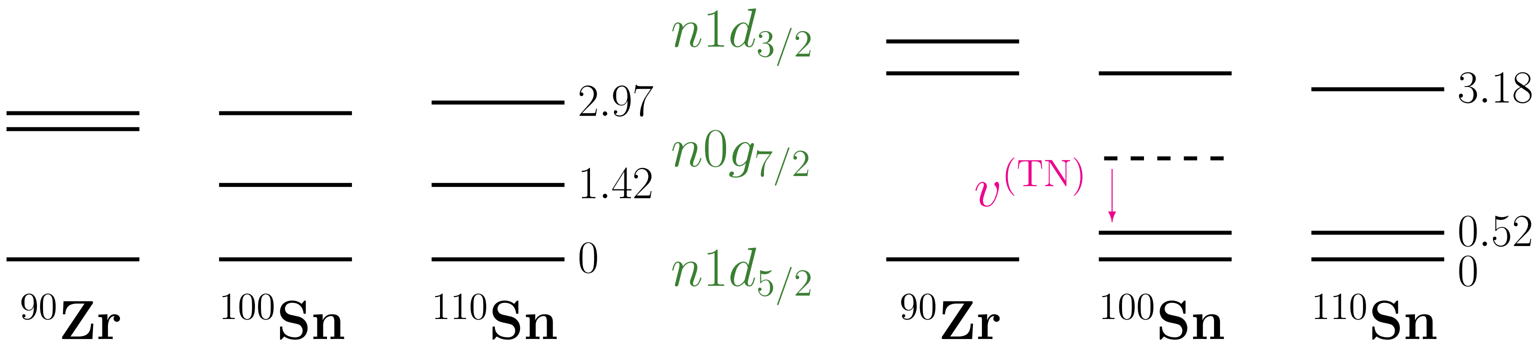
⇒ A) *vs.* B) & B) *vs.* C)

- **B) QRPA with M3Y-P5′ *vs.* C) QRPA with D1S**

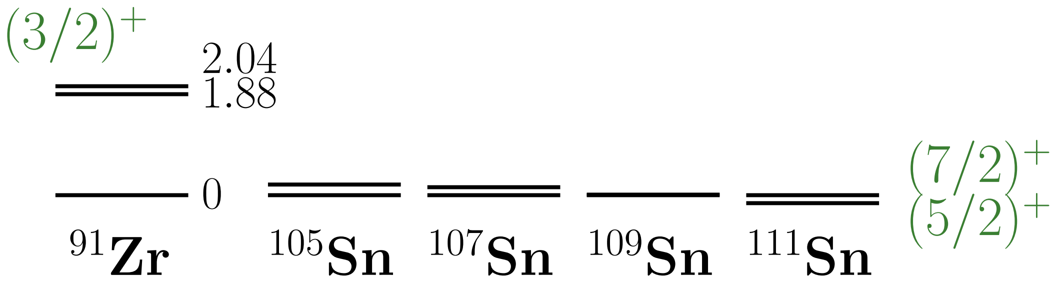
— **problem of D1S at $N \sim 60$**

close to deformation because of strong $n0g_{7/2} \rightarrow n1d_{3/2}$ excitation

← **shell structure!**



D1S **M3Y-P5′**



Exp.

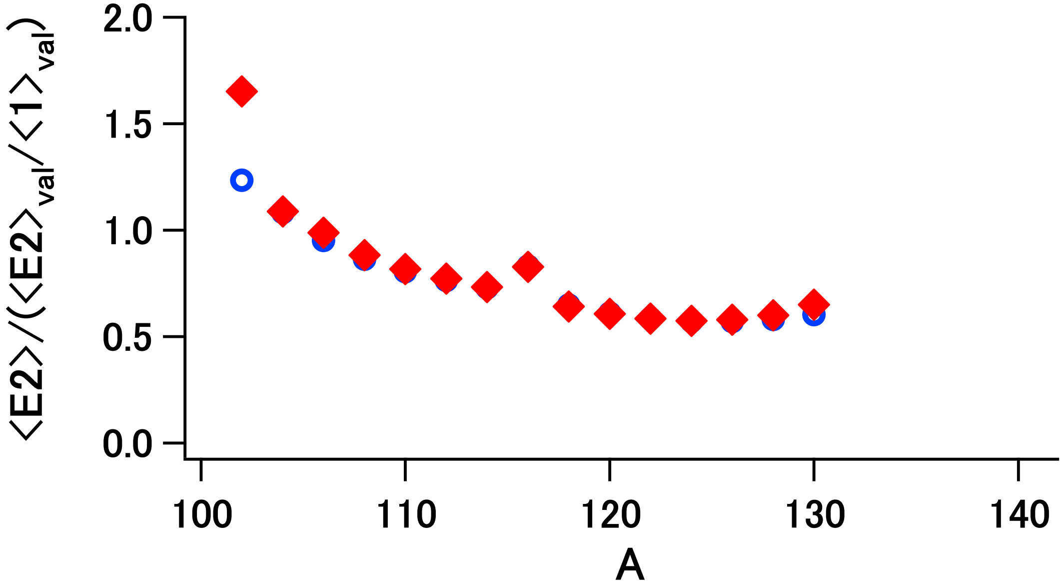
- **A) Shell model *vs.* B) QRPA with M3Y-P5′**

  shell model (on top of ^{100}Sn core) — only neutrons in valence shell

  coupling to GQR (core pol.) $\rightarrow e_n^{\rm eff} \rightarrow E2$ **strength**

  constant $e_n^{\rm eff}$ hypothesis — true ?

$$e_n^{\rm eff} \approx \frac{\langle T_p^{(E2)}\rangle}{\langle T_n^{(E2)}\rangle_{\rm valence}/(\textbf{norm within valence})} \quad \leftarrow \textbf{HFB + QRPA}$$



$\rightarrow$ ***A*-dep. of $e_n^{\rm eff}$?** (**but overshooting**)

to be considered

- **q.p. states $\rightarrow$ canonical bases (in defining valence orbits)**

  Ref.: J. Dobaczewski *et al.*, P.R.C 53, 2809 ('96)

- **backward amp. — on/off**

IV. Summary

- **Gaussian expansion method (GEM) has successfully been applied to MF & RPA calculations.**

  <u>**Advantages :**</u>

  (i) **ability to describe ε-dep. exponential/oscillatory asymptotics**
  (ii) **tractability of various 2-body interactions**
  (iii) **basis parameters insensitive to nuclide**
  (iv) **exact treatment of Coulomb & c.m. Hamiltonian**

- **Several results have been shown :**
  - **Tensor-force effects on $M1$ transition in ^{208}Pb**
  - **Low-energy excitation of "doubly-magic" nuclei (*e.g.* 2_1^+ in ^{78}Ni)**
  - **$B(E2)$ in Sn isotopes (tensor-force effect, A-dep. effective charge ?)**

Contributors :

HF :	**M. Sato**	**(*Chiba U.* until 2004)**
RPA :	**K. Mizuyama**	**(*Milan*)**
	M. Yamagami	**(*Aizu*)**
	M. Matsuo	**(*Niigata*)**
^{208}**Pb** $M1$ **:**	**T. Shizuma**	**(*JAEA*)**
	⋮	

Sn $E2$ **:** **Special thanks to K. Matsuyanagi**
(for giving key information)