CHIBA UNIVERSITY

Self-consistent nuclear structure calculations with Gaussian basis-functions

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Contents :

I. Introduction

Atomic nucleus

$\Longleftrightarrow$

Z **protons** $+$ N **neutrons**
$=$ A **nucleons**

s.p. orbitals (shell structure)

— **Quantum many-body system**

- **isolated**
- **finite**
- **self-bound**

$\rightarrow$ **translational & rotational sym.** — **breaking & restoration**

Nuclear properties

$\rightarrow$

- **interest as quantum many-body physics**
- **nuclear transmutation**
- **key input to astrophysics**
  - ○ **origin of matters** ○ **supernovae** ○ **structure of n-stars**
- **basis to search physics beyond standard model**
  - ○ **ν properties (*e.g.* mass)** ○ **unitarity of CKM matrix**
  - ○ **EDM** ○ **Lorentz inv.**

"Self-consistent MF approx." $\approx$ **"Density Functional Theory (DFT)"**

— **appropriate for global desciption of nuclei**

variational principle $E_0 = \min_{\Psi} E[\Psi]$; $E[\Psi] = \langle\Psi|H|\Psi\rangle$

$\rightarrow$ $E[\Psi] = \langle\Psi|H|\Psi\rangle \approx \langle\Phi|\Lambda^\dagger H\Lambda|\Phi\rangle = \langle\Phi|H_{\rm eff}|\Phi\rangle = E[\{\varrho_{k\ell}\}]$

$|\Psi\rangle \approx \Lambda|\Phi\rangle$ $\big(|\Phi\rangle$: ***e.g.*** **Slater det.**$\big)$, $H_{\rm eff} = \Lambda^\dagger H\Lambda$

note : Λ **need not to be constructed**

$\varrho_{k\ell} = \langle\Phi|a_\ell^\dagger a_k|\Phi\rangle$: **1-body density matrix**

$\rightarrow$ $\delta E[\{\varrho_{k\ell}\}] = 0$ **instead of** $\delta E[\Psi] = 0$

$\rightarrow$ **a set of s.p. equations**

$U = {\rm tr}(\hat{v}\varrho)$ **(: MF pot.)** $\rightarrow$ $\{\varphi\}$ **(: s.p. w.f.)** $\cdots$ **self-consistency**

$\{\varrho\}$

$\big(\{\varrho_{k\ell}\} \rightarrow \{\varrho_{k\ell}, \kappa_{k\ell}, \kappa^*_{k\ell}\}$; $\kappa_{k\ell} = \langle\Phi|a_\ell a_k|\Phi\rangle$ $\cdots$ **HFB or BdG**$\big)$

$E[\{\varrho_{k\ell}\}]$ $\cdots$ $\begin{cases} \text{governs accuracy \& reliability} \\ \text{should be universal for "global description"} \end{cases}$

good $H_{\rm eff}$ **or** $E[\{\varrho_{k\ell}\}]$ $\rightarrow$ **g.s. of (almost) all nuclei**

$$H_{\rm eff} = K + V_N + V_C \left(- H_{\rm c.m.} \right) ;$$

$$K = \sum_i \frac{\boldsymbol{p}_i^2}{2M} , \quad V_N = \sum_{i<j} \hat{v}_{ij} , \quad V_C = \alpha_{\rm em} \sum_{i<j(\in p)} \frac{1}{r_{ij}} , \quad H_{\rm c.m.} = \frac{\boldsymbol{P}^2}{2AM} ;$$

$$\hat{v}_{ij} = \hat{v}_{ij}^{(\rm C)} + \hat{v}_{ij}^{(\rm LS)} + \hat{v}_{ij}^{(\rm TN)} + \hat{v}_{ij}^{(\rm C\rho)} ; \qquad \textbf{(rotational \& translational inv.)}$$

$$\hat{v}_{ij}^{(\rm C)} = \sum_n \left(t_n^{(\rm SE)} P_{\rm SE} + t_n^{(\rm TE)} P_{\rm TE} + t_n^{\rm SO} P_{\rm SO} + t_n^{(\rm TO)} P_{\rm TO} \right) f_n^{(\rm C)}(r_{ij}) ,$$

$$\left(\begin{array}{ll} P_{\rm SE} \equiv \left(\frac{1-P_\sigma}{2} \right) \left(\frac{1+P_\tau}{2} \right), & P_{\rm TE} \equiv \left(\frac{1+P_\sigma}{2} \right) \left(\frac{1-P_\tau}{2} \right) , \\ P_{\rm SO} \equiv \left(\frac{1-P_\sigma}{2} \right) \left(\frac{1-P_\tau}{2} \right), & P_{\rm TO} \equiv \left(\frac{1+P_\sigma}{2} \right) \left(\frac{1+P_\tau}{2} \right) \end{array} \right)$$

$$\hat{v}_{ij}^{(\rm LS)} = \sum_n \left(t_n^{(\rm LSE)} P_{\rm TE} + t_n^{(\rm LSO)} P_{\rm TO} \right) f_n^{(\rm LS)}(r_{ij}) \, \boldsymbol{L}_{ij} \cdot (\boldsymbol{s}_i + \boldsymbol{s}_j) ,$$

$$\hat{v}_{ij}^{(\rm TN)} = \sum_n \left(t_n^{(\rm TNE)} P_{\rm TE} + t_n^{(\rm TNO)} P_{\rm TO} \right) f_n^{(\rm TN)}(r_{ij}) \, r_{ij}^2 S_{ij}$$

$$\hat{v}_{ij}^{(\rm C\rho)} = \left(t_\rho^{(\rm SE)} P_{\rm SE} \, C_1[\rho(\boldsymbol{r}_i)] + t_\rho^{(\rm TE)} P_{\rm TE} \, C_0[\rho(\boldsymbol{r}_i)] \right) \delta(\boldsymbol{r}_{ij}) ;$$

$$\boldsymbol{L}_{ij} \equiv (\boldsymbol{r}_i - \boldsymbol{r}_j) \times \frac{(\boldsymbol{p}_i - \boldsymbol{p}_j)}{2} , \qquad S_{ij} \equiv 3(\boldsymbol{\sigma}_i \cdot \hat{\boldsymbol{r}}_{ij})(\boldsymbol{\sigma}_j \cdot \hat{\boldsymbol{r}}_{ij}) - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$$

$$f_n(r) = e^{-\mu_n r} / \mu_n r \, , \ \textbf{\textit{etc.}}$$

II. Numerical methods for nuclear mean-field calculations

★ **General arguments**

MF cal. $\cdots$ s.p. eq. $\rightarrow$ s.p. w.f. $\rightarrow$ many-body w.f.

Spanning s.p. space

1) coordinate space — mesh in r-space
   1D (spherical sym.), 2D (axial sym.), 3D ;
   homogeneous mesh, adaptive mesh, Lagrange mesh
2) expansion by basis-functions $\rightarrow$ Gaussian
   e.g. h.o. bases $\cdots$ "bias"
   advantage in handling finite-range int.
3) momentum space — mesh in k-space
   not yet well developed, adaptivity for k-rep. int. ?

$\cdots$ influencing quality of solutions

Procedure

A) iteration : s.p. w.f. $\leftrightarrow$ s.p. potential
B) gradient method or imaginary-time evolution

System size $\leftarrow$ short-range attraction (+ Coulomb repulsion)

variety not very wide : $R \sim A^{1/3} \lesssim$ (several) $\cdot\, m_\pi^{-1} \approx$ (several) fm

exception $\cdots$ drip-line nuclei (*e.g.* halo)

Nuclei near drip line — significance of asymptotics at large r

asymptotic form of s.p. w.f. (for neutrons)

$$\left[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + 2MU(r)\right] rR_{n\ell j}(r) = 2M\varepsilon_{n\ell j} \cdot rR_{n\ell j}(r)$$

$$\left(\varphi_{n\ell jm}(\boldsymbol{r}) = R_{n\ell j}(r)\, [Y^{(\ell)}(\hat{\boldsymbol{r}})\chi_\sigma]^{(j)}_m \right)$$

for large r $\cdots$ $U \approx 0$, $1/r^2 \approx 0$

$$\rightarrow \quad R_{n\ell j}(r) \approx \frac{e^{-\eta_{n\ell j} r}}{r}; \quad \eta_{n\ell j} = \sqrt{2M|\varepsilon_{n\ell j}|} \quad (\varepsilon_{n\ell j} < 0)$$

small $|\varepsilon_{n\ell j}| \rightarrow$ long tail

ε-dep. exponential asymptotics !

- h.o. bases $\rightarrow$ impractical
  - cf. transformed h.o. — no ε-dep. for individual orbits
- mesh : homogeneous mesh $\rightarrow$ inefficient ($\rightarrow$ *e.g.* adaptive mesh)
- applicability to finite-range int. ?

sinusoidal asymptotics also relevant in HFB !

★ **Gaussians in nuclear structure calculations**

- **properties of Gaussian**
  - **minimum uncertainty**
  - **good convergence both in coordinate & momentum spaces**
- **s.p. w.f. represented by a single Gaussian (w/o 'self-consistency')**

  cluster model

  cluster ↔ wave packet

  e.g. $|\alpha\text{-particle}\rangle \approx |(0s_{1/2})^4\rangle \approx |(\text{Gaussian})^4\rangle$

  h.o. model

  AMD (antisym. molecular dynamics)
- **superposition of Gaussians — Gaussian as basis-function**

  few-body systems ⋯ GEM

  ↪ **MF cal ?**

★ Gaussian expansion method (GEM)

— developed by Kamimura *et al.* for few-body calculations

E. Hiyama *et al.*, Prog. Part. Nucl. Phys. 51, 223

application to nuclear SCMF (& RPA) calculations

- spherical HF ··· H.N. & M. Sato, N.P.A 699, 511; 714, 696
- spherical HFB ··· H.N., N.P.A 764, 117; 801, 169
- axial HF & HFB ··· H.N., N.P.A 808, 47
- spherical RPA ··· H.N., K. Mizuyama, M. Yamagami & M. Matsuo, N.P.A 828, 283

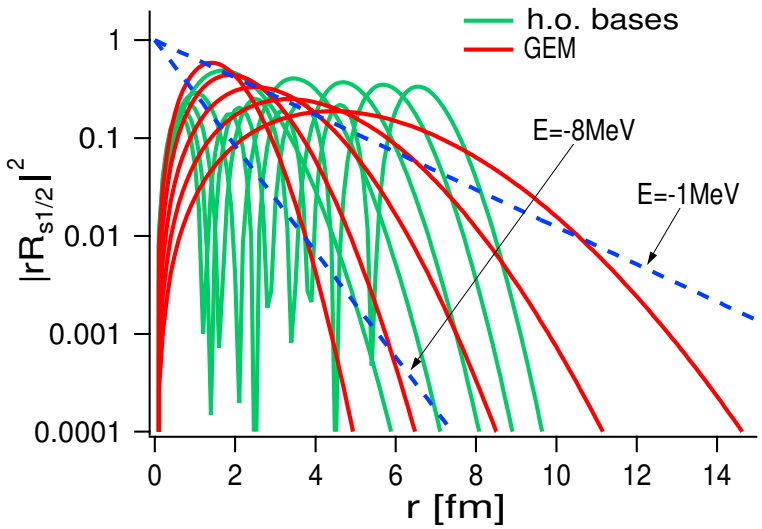
- **basis-functions :**

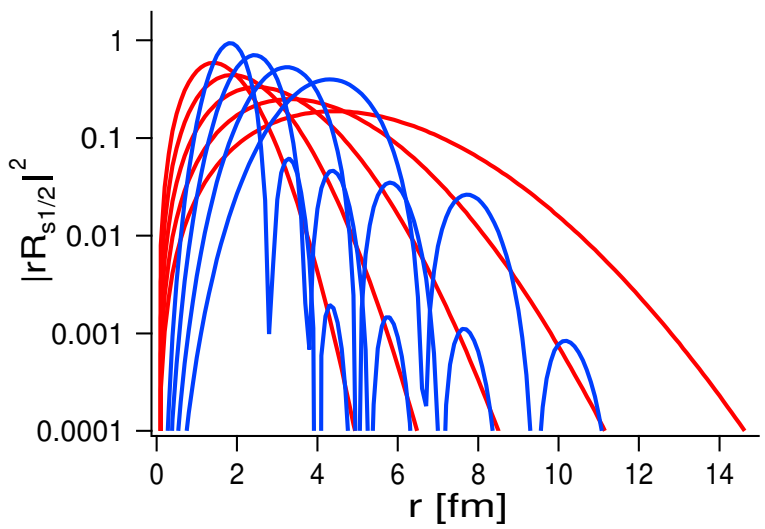
$$\phi_{\nu\ell jm}(\boldsymbol{r}) = R_{\nu\ell j}(r)\,[Y^{(\ell)}(\hat{\boldsymbol{r}})\chi_\sigma]^{(j)}_m\,; \qquad R_{\nu\ell j}(r) = \mathcal{N}_{\nu\ell j}\, r^\ell \exp(-\nu r^2)$$

$\nu \to$ **complex** $\quad \nu = \nu_{\rm r} + i\nu_{\rm i}$ **; with geometric progression**

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

ε-dep. asymptotics ? **oscillating behavior ?**





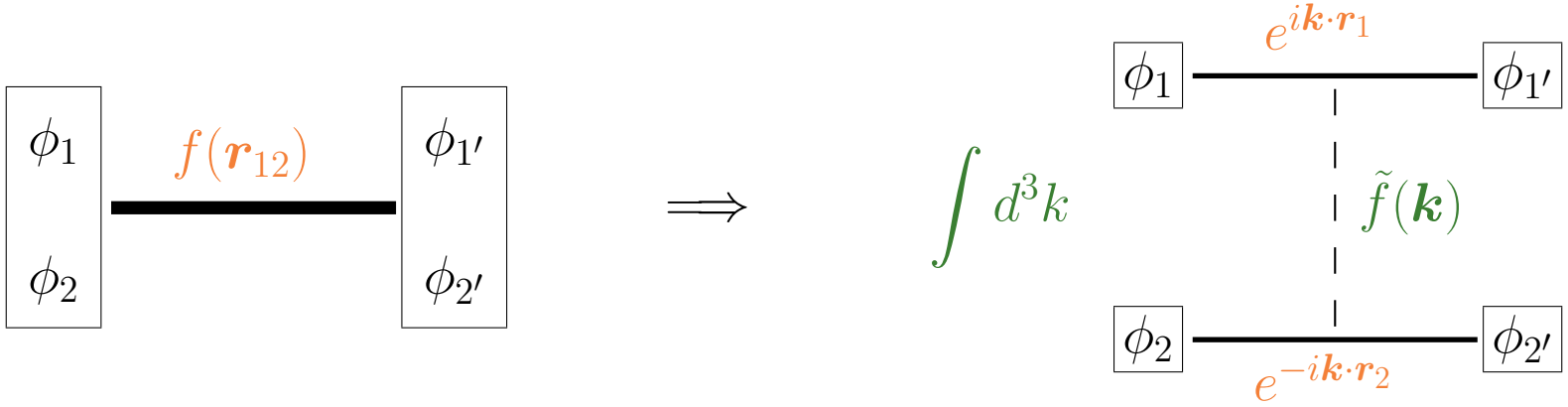
$\leftarrow$ **geometric progression** $\qquad\qquad$ $\leftarrow$ **complex-range**

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

$$\langle \phi_{1'}\,\phi_{2'}|f(\boldsymbol{r}_{12})|\phi_1\,\phi_2\rangle_{\mathrm{A}} = \langle \phi_{1'}\,\phi_{2'}|f(\boldsymbol{r}_{12})|\phi_1\,\phi_2\rangle - \langle \phi_{1'}\,\phi_{2'}|f(\boldsymbol{r}_{12})|\phi_2\,\phi_1\rangle$$

$$\langle \phi_{1'}\,\phi_{2'}|f(\boldsymbol{r}_{12})|\phi_1\,\phi_2\rangle = \frac{1}{(2\pi)^3}\int d^3k\,\langle \phi_{1'}|e^{i\boldsymbol{k}\cdot\boldsymbol{r}_1}|\phi_1\rangle\,\langle \phi_{2'}|e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_2}|\phi_2\rangle\,\tilde{f}(\boldsymbol{k})\,;$$

$$f(\boldsymbol{r}_{12}) = \frac{1}{(2\pi)^3}\int d^3k\,\tilde{f}(\boldsymbol{k})e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)}$$



$$\begin{cases} \langle \phi'|e^{i\boldsymbol{k}\cdot\boldsymbol{r}}|\phi\rangle\text{, angular part} \\ \quad\cdots\ \text{analytic } (\leftarrow \text{Gaussian}) \\ k\text{-integral (1-dim.)} \\ \quad\ \rightarrow \text{numerical integration} \end{cases}$$

⇒ **store matrix elements** ($\sim 6.5\,\mathrm{GB}$ **for** $\ell_{\max} = 7$)

$\cdots$ **crucial for finite-range int.**

Advantages of the method

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

(ii) tractability of various 2-body interactions

(iii) basis parameters insensitive to nuclide

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

(ii) $\rightarrow$ our SCMF (& RPA) code $\cdots$ applicable with Yukawa int.
(up to exchange terms)
— the only one (until now)

(iii) $\rightarrow$ fix the basis-set $\rightarrow$ apply it to all nuclei
$\cdots$ suitable for systematic calculations

for each (ℓ, j) : $\#(\text{bases}) = 12$

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

Notes : 1) bases $\cdots$ non-orthogonal

2) $\hat{v}_{ij}^{({\rm C}\rho)}$ ($\cdots$ cannot be stored) $\rightarrow$ contact form

★ Numerical tests of GEM for MF

(← schematic model & Gogny-D1S int.)

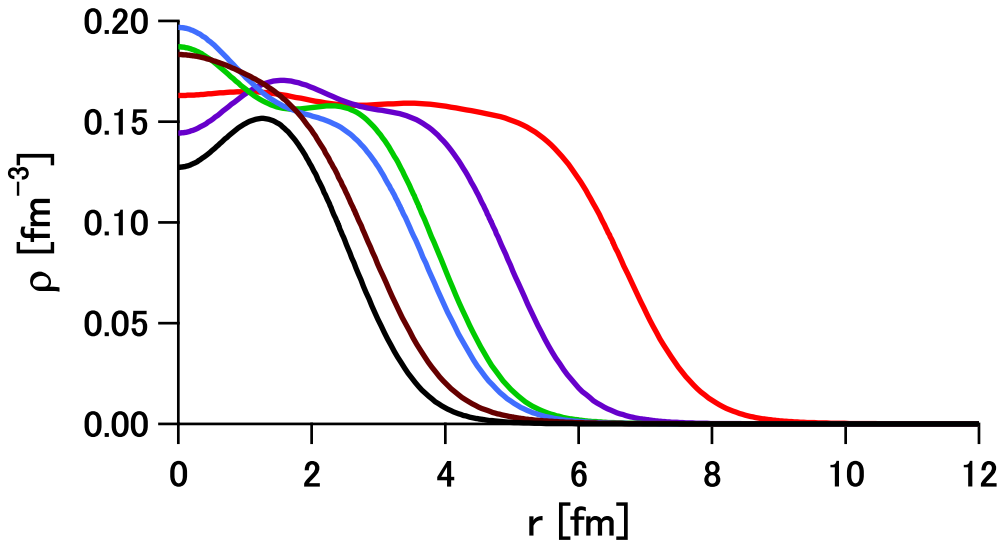
- **spherical nuclei**

Binding energy ($-E$ [MeV]) : GEM *vs.* h.o.

nuclide	h.o.	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

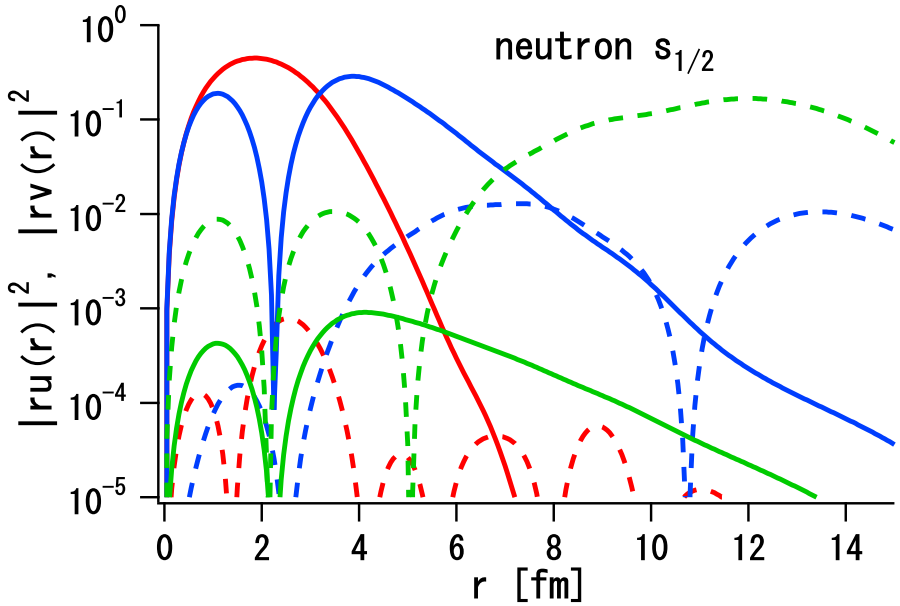
(h.o. : $N_{\rm osc} \leq 15$, $\omega_0 = 41.2\, A^{-1/3}$)

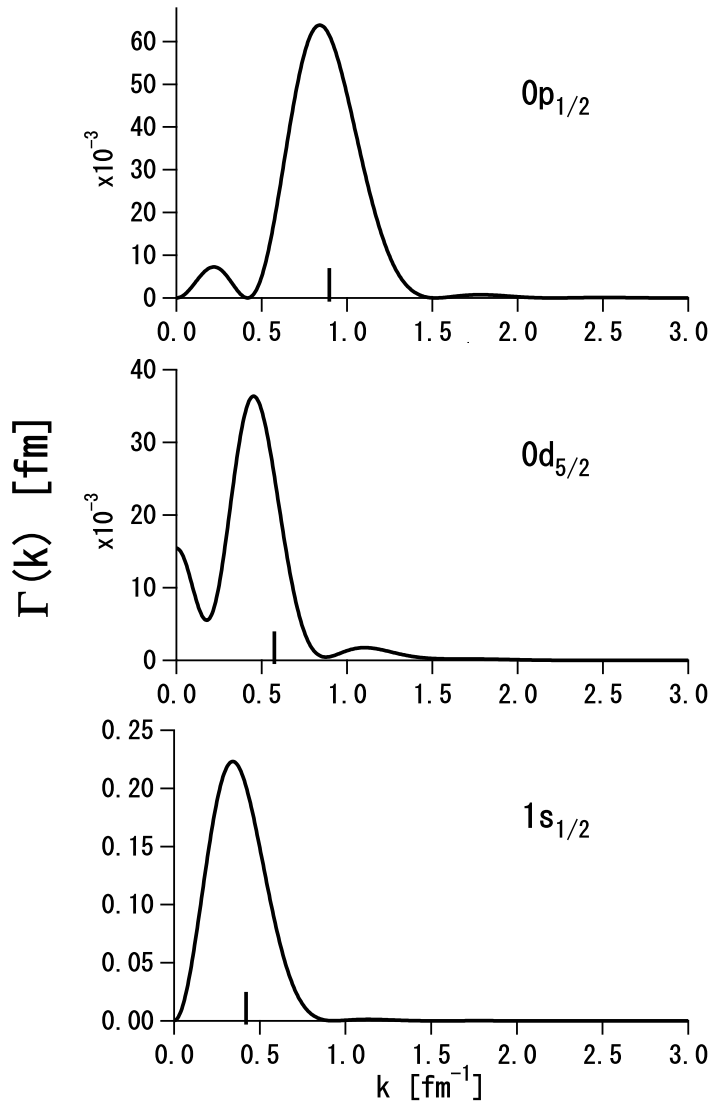
$\rho(r)$ obtained by GEM (from ^{16}O to ^{208}Pb) :



— **wide mass range of nuclei well described by a single basis-set !**

s.p. w.f. in ^{26}O (HFB)



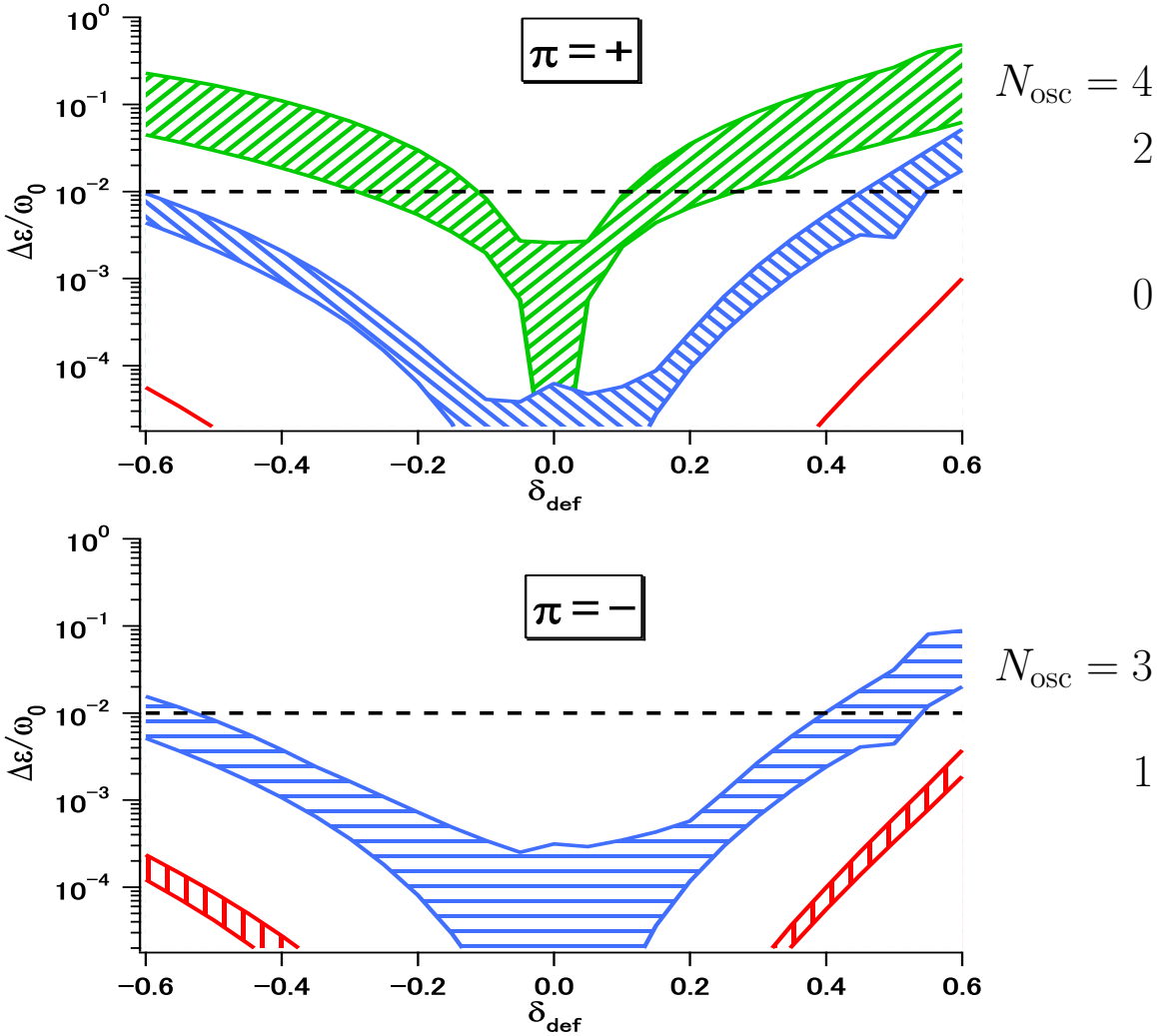


$$\Gamma_{n\ell j}(k) := \frac{1}{\pi}\left|\int_0^\infty r\, u_n^{(\ell j)}(r)\, e^{ikr}\, dr\right|^2$$

— ε-dep. exp. (& sin.) asymptotics described reasonably well

- **deformed nuclei**

error for s.p. energies in deformed h.o.: $\Delta\varepsilon := \varepsilon_{\rm GEM} - \varepsilon_{\rm exact}$



$N_{\rm osc} = 4$

2

0

$N_{\rm osc} = 3$

1

$(\ell_{\rm max} = 7)$

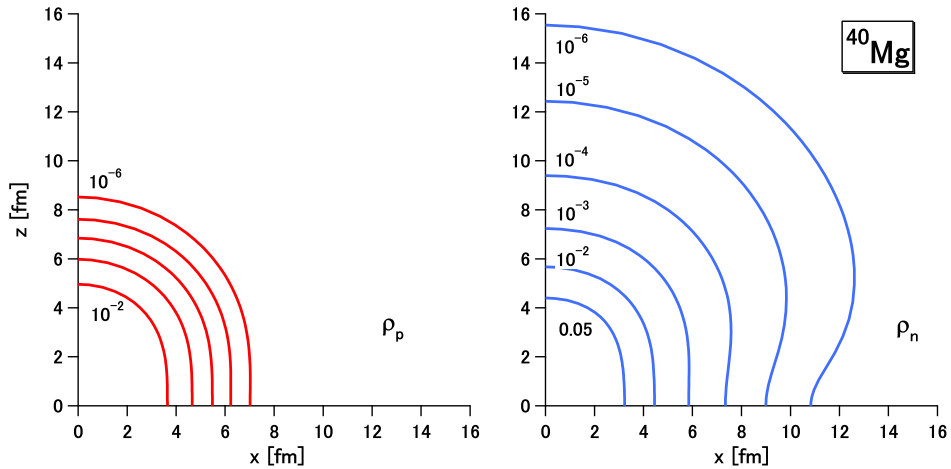
to achieve $\Delta\varepsilon \leq 0.01\omega_0$ — $\ell_{\rm max} \geq N^F_{\rm osc} + 4$ **up to** $|\delta_{\rm def}| \lesssim 0.4$

Binding energy ($-E$ [MeV]) : GEM *vs.* h.o.

nuclide	h.o.	GEM	Exp.
^{30}Mg	239.30	239.48	241.63
^{32}Mg	248.22	248.30	249.69
^{34}Mg	252.82	254.01	256.59

(h.o. : $N_{\rm osc} \leq 10$; PLB 474, 15)

$\rho(r)$ obtained by GEM :



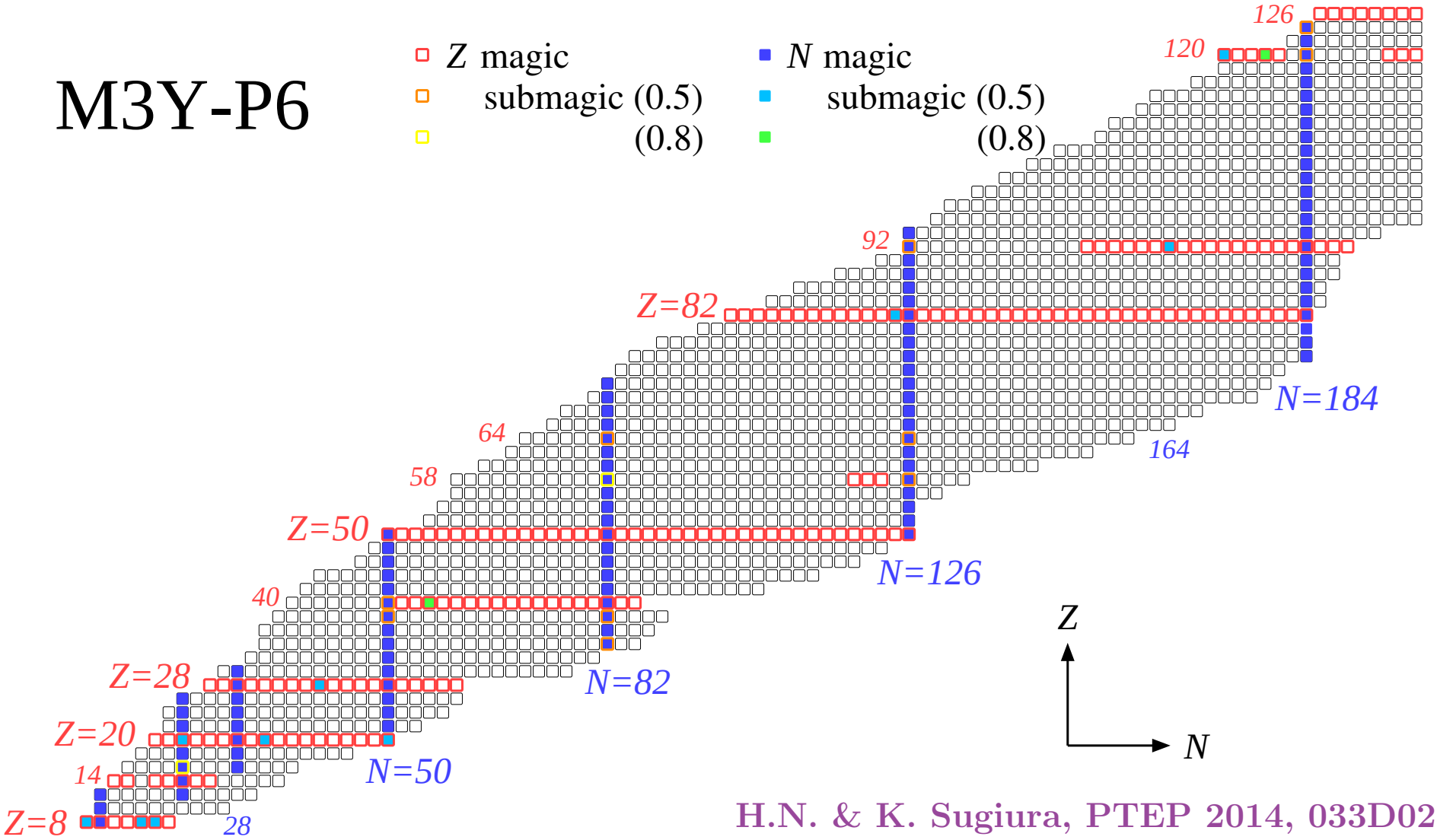
'peanut-shape' halo

— **GEM is advantageous particularly in unstable nuclei,**

with finite-range int.

III. Selected results for nuclear ground-state properties

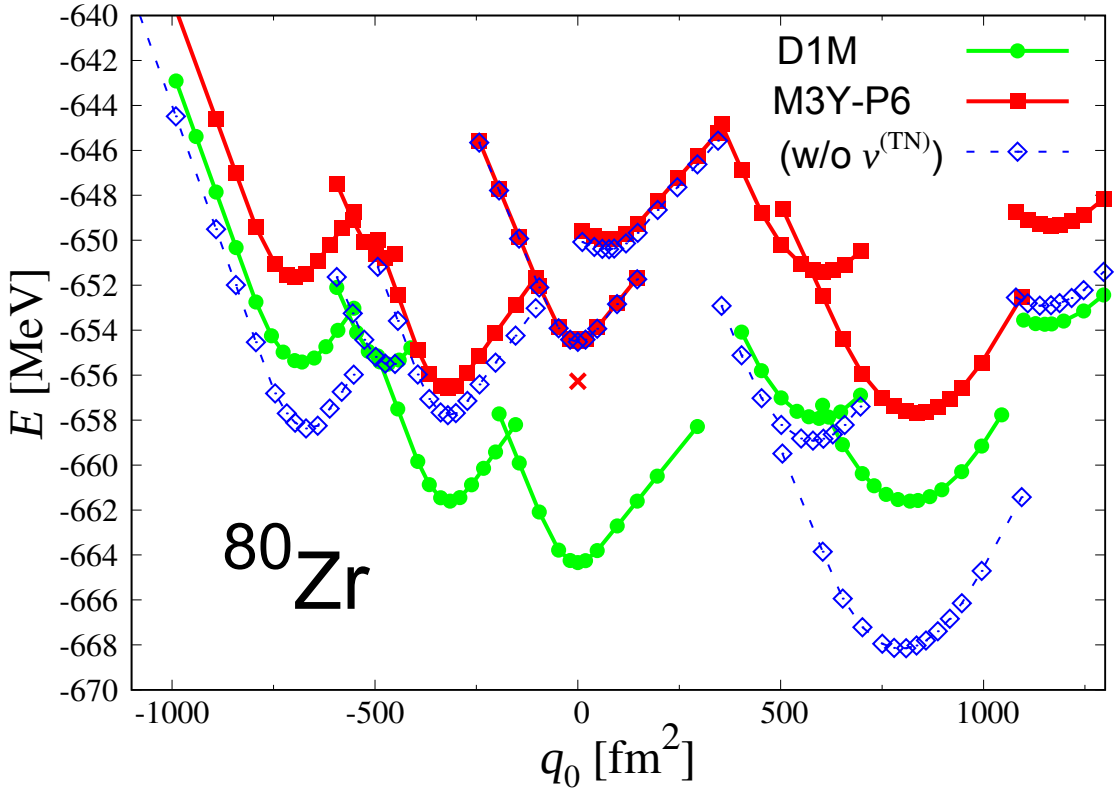
★ **Magic numbers** ← **quenching of pair correlation (sph. HFB)**



H.N. & K. Sugiura, PTEP 2014, 033D02

⇒ **magic # compatible with almost all available data ! + predictions**

★ Nuclear deformation ← spontaneous sym. breaking at the MF level



S. Miyahara & H.N., P.R.C 98, 064318

··· tensor-force effects !

sym. restored in energy eigenstates ↔ superposing degenerate states

= ang. mom. proj.

(cf. K. Abe's talk in Progress reports Session 3)

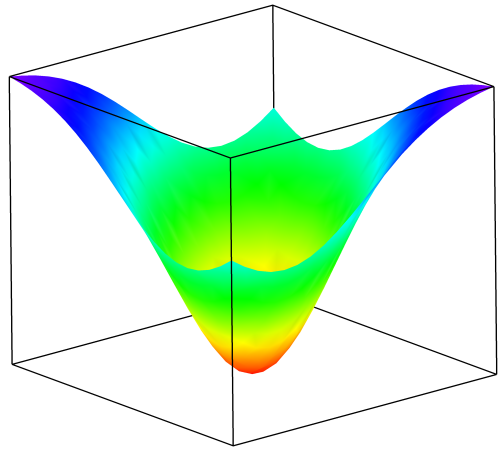
IV. Application of GEM to nuclear RPA calculations

Excitations on top of the MF solutions :

$$E[\varrho] \xrightarrow[\text{constraints}]{} \tilde{E}[\varrho] \approx E[\varrho_0] + \frac{1}{2}\begin{pmatrix}\delta\varrho_{hp} & \delta\varrho_{ph}\end{pmatrix}\begin{pmatrix}A & B\\ B^* & A^*\end{pmatrix}\begin{pmatrix}\delta\varrho_{ph}\\ \delta\varrho_{hp}\end{pmatrix}$$

$$= E[\varrho_0] + \frac{1}{2}\,\delta\mathsf{Z}^\dagger\,\mathrm{diag.}(\omega_\nu)\,\delta\mathsf{Z} \qquad (\{\varrho_0\} \leftarrow \textbf{SCMF})$$

$$\delta Z_\nu := \sum_{i\le\varepsilon_{\mathrm{F}}<m}\left(X^{(\nu)*}_{mi}\delta\varrho_{mi} - Y^{(\nu)*}_{mi}\delta\varrho_{im}\right)$$



RPA eq.

$$\begin{pmatrix}A & B\\ B^* & A^*\end{pmatrix}\begin{pmatrix}X^{(\nu)}\\ Y^{(\nu)}\end{pmatrix} = \omega_\nu\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}X^{(\nu)}\\ Y^{(\nu)}\end{pmatrix}$$

$$\rightarrow \quad Z_\nu(t) = Z_\nu(0)\,e^{-i\omega_\nu t}$$ **(stationary oscillation)**

— **consistency between MF & RPA** **('HF+RPA', 'HFB+QRPA')**

Cases of $A = A^*$, $B = B^*$ (← **time-reversal symmetry**)

$$\begin{cases} AX + BY = X\,\mathrm{diag.}(\omega_\nu) \\ BX + AY = -Y\,\mathrm{diag.}(\omega_\nu) \end{cases} \rightarrow \ (A+B)(A-B)(X-Y) = (X-Y)\,\mathrm{diag.}(\omega_\nu^2)$$

(**Cholesky decomposition** →) $A - B = L\,L^T$

(L : **lower-triangular matrix**)

→ $[L^T(A+B)L]R^{(\nu)} = \omega_\nu^2 R^{(\nu)}$ — **diagonalization of real-sym. matrix**

Cholesky decomp. & (full) matrix diag. → **MPI**

$\cdots$ **important particularly for HFB+QRPA where** $\mathrm{dim.}(A, B) \sim 10^4$

★ **Numerical tests of GEM for RPA**

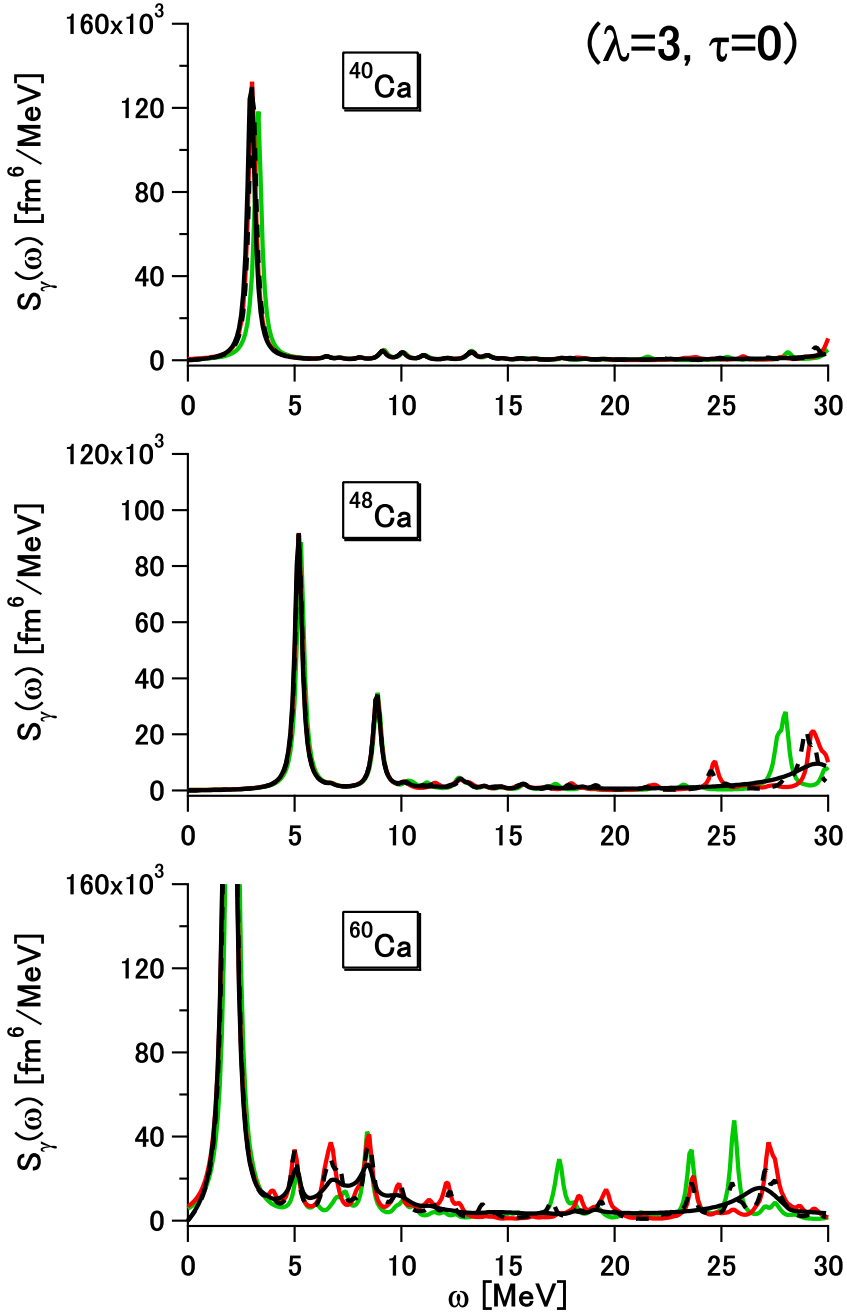
- **comparison with continuum RPA via schematic model**
  - **MF — Woods-Saxon pot.**
  - **residual int. — contact force** **(not consistent)**

$$\hat{v}_{\rm res} = f\left[t_0(1+x_0P_\sigma)\,\delta(\mathbf{r}_1-\mathbf{r}_2) + \frac{1}{6}t_3(1+x_3P_\sigma)\,\rho(\mathbf{r}_1)\,\delta(\mathbf{r}_1-\mathbf{r}_2)\right]$$

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

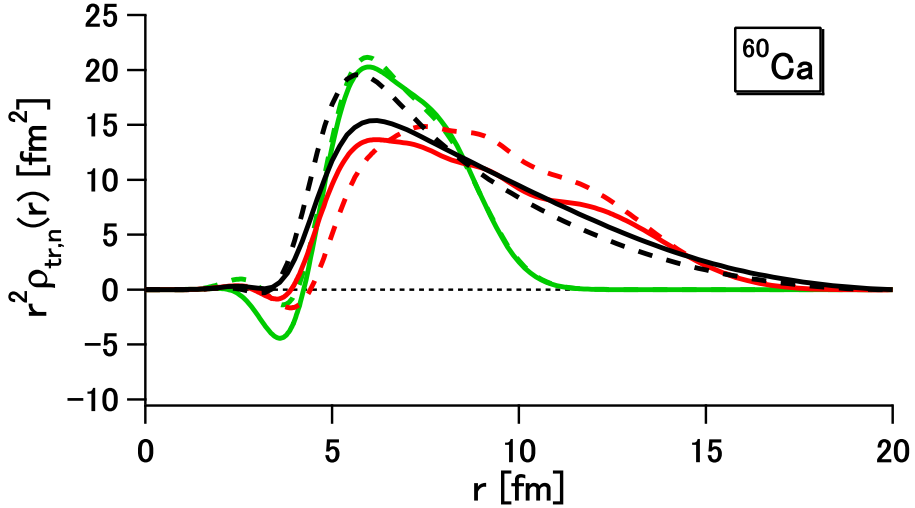
  - **GEM *vs.* quasi-h.o. *vs.* continuum RPA** ($\cdots$ **'exact'**)

strength function



transition density

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



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

Cont.

quasi-h.o.

GEM

- **tests for HF+RPA**

spurious c.m. state

$$\cdots \ \omega_s = 0\,?$$

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

energy-weighted sum rule

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

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

- **performance in HFB+QRPA** M. Takahashi, M. thesis **(using OFP)**

convergence for $\omega_{\rm cut}$ $\cdots$ $E_x(2_1^+)$ **&** $B(E2; 0_1^+ \to 2_1^+)$ **at** ^{116}**Sn**

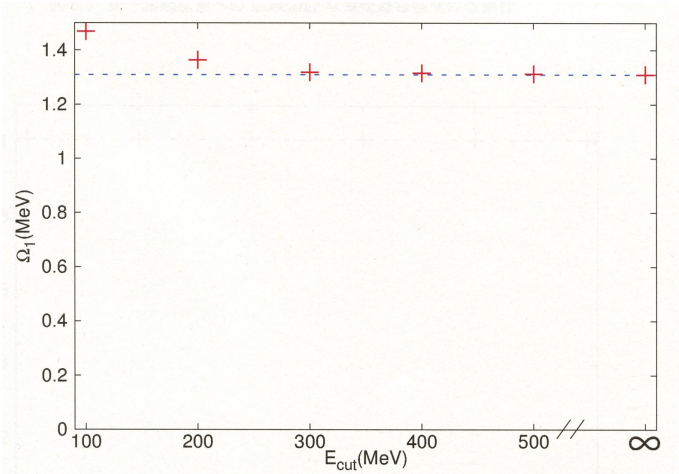


図 5.4: 第一励起状態のエネルギーの収束性

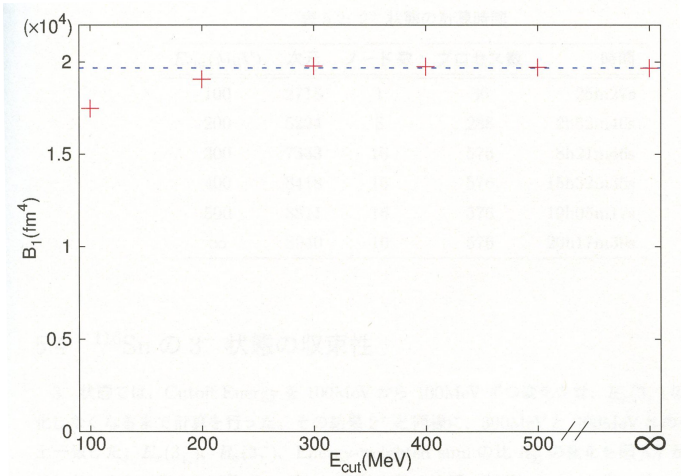


図 5.5: 第一励起状態への isoscalar な電磁遷移強度の収束性

$\to \omega_{\rm cut} = 300\,{\rm MeV}$ ($\omega_{\rm cut}$ **: cut-off energy for unperturbed states)**

MPI performance

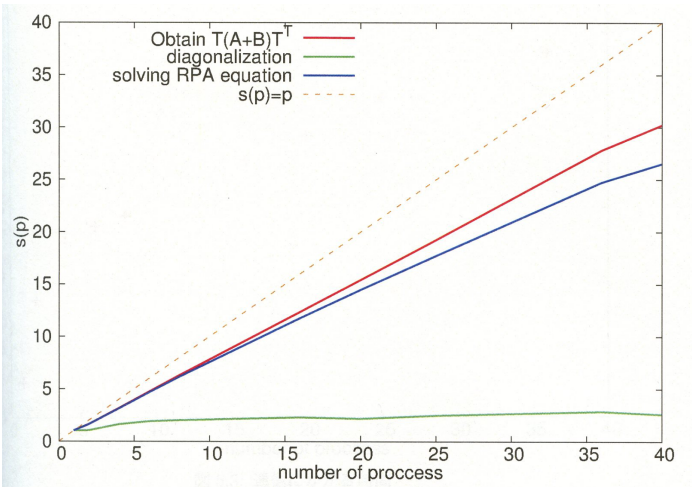
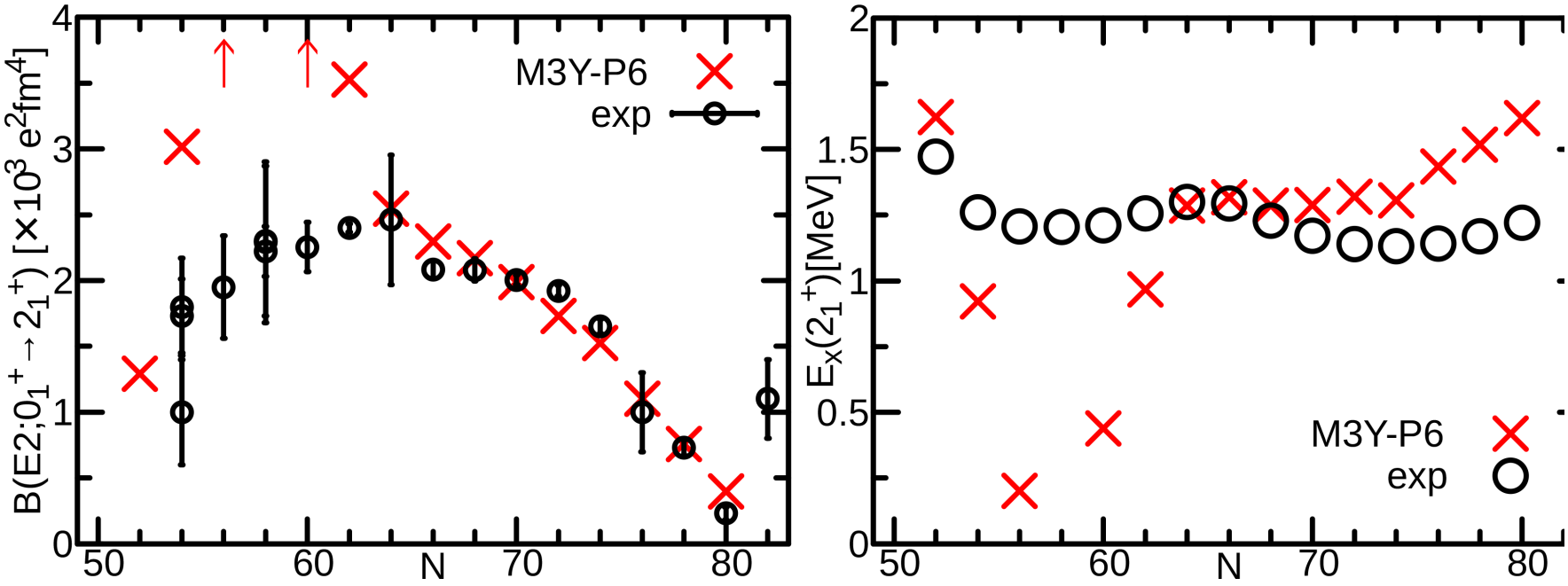


図 5.1: 速度向上率

★ HFB+QRPA results of $B(E2; 0_1^+ \to 2_1^+)$ & $E_x(2_1^+)$ in Sn isotopes

Y. Omura, M. thesis; Y. Omura, H.N., M. Takahashi, in preparation

(using OFP under MCRP-S '20, Project # 10)



- $N \geq 64$ $\cdots$ **well describing exp. w/o adjustable parameters**
- **asymmetric** $B(E2)$ **between** $\pm(N-66)$
  (cf. shell model in 1-major shell)
- $56 \leq N \leq 60$ $\cdots$ **(Q)RPA inappropriate** $\leftarrow$ **instability against** β_2

V. Summary

Self-consistent calculations — valuable to study nuclear structure

∵) isolated, finite self-bound system

Gaussian basis-functions have certain advantages !

'Gaussian expansion method (GEM)'

— Gaussians with complex ranges obeying geometric progression

→ flexibility w.r.t. size & asymptotics (damping, oscillatory),

as well as analyticity & convergence in some parts

↪ useful for nuclear self-consistent cal. (MF, RPA)

Advantages of the method

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

(ii) tractability of various 2-body interactions

(iii) basis parameters insensitive to nuclide

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

Numerical tests & physics results on nuclear low-energy properties

(g.s. & excitations) have been presented.