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Collaboration

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LANL
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CEA
Thomas Duguet

RIKEN
Takashi Nakatsukasa

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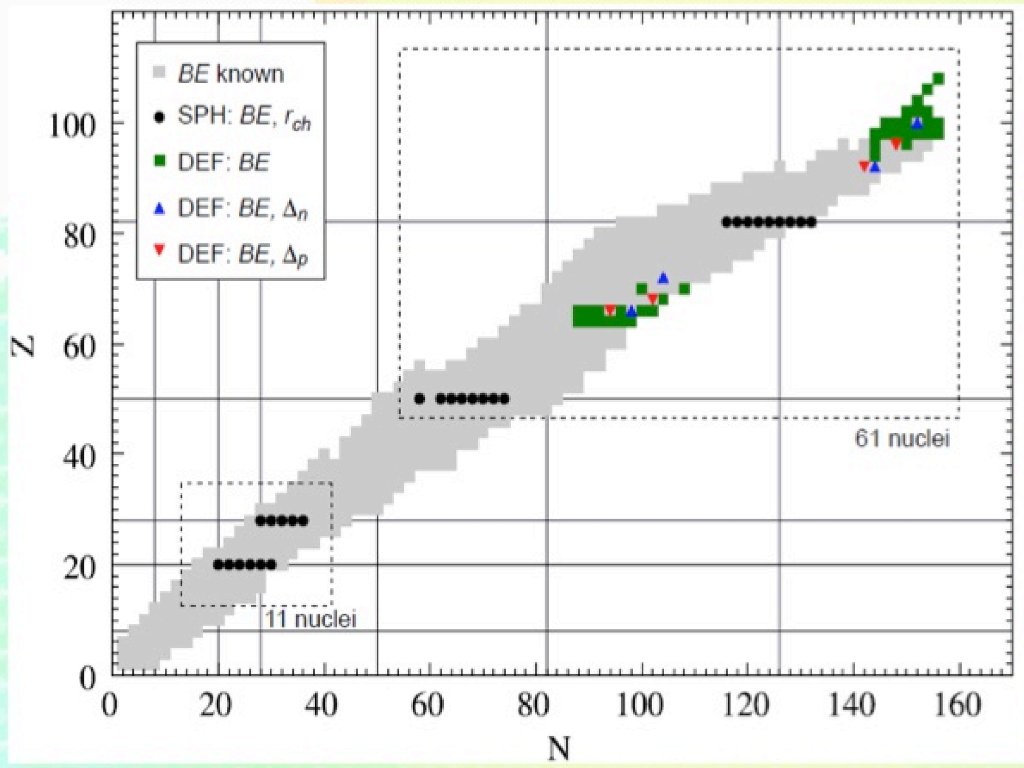
SciDAC Scientific Discovery through Advanced Computing

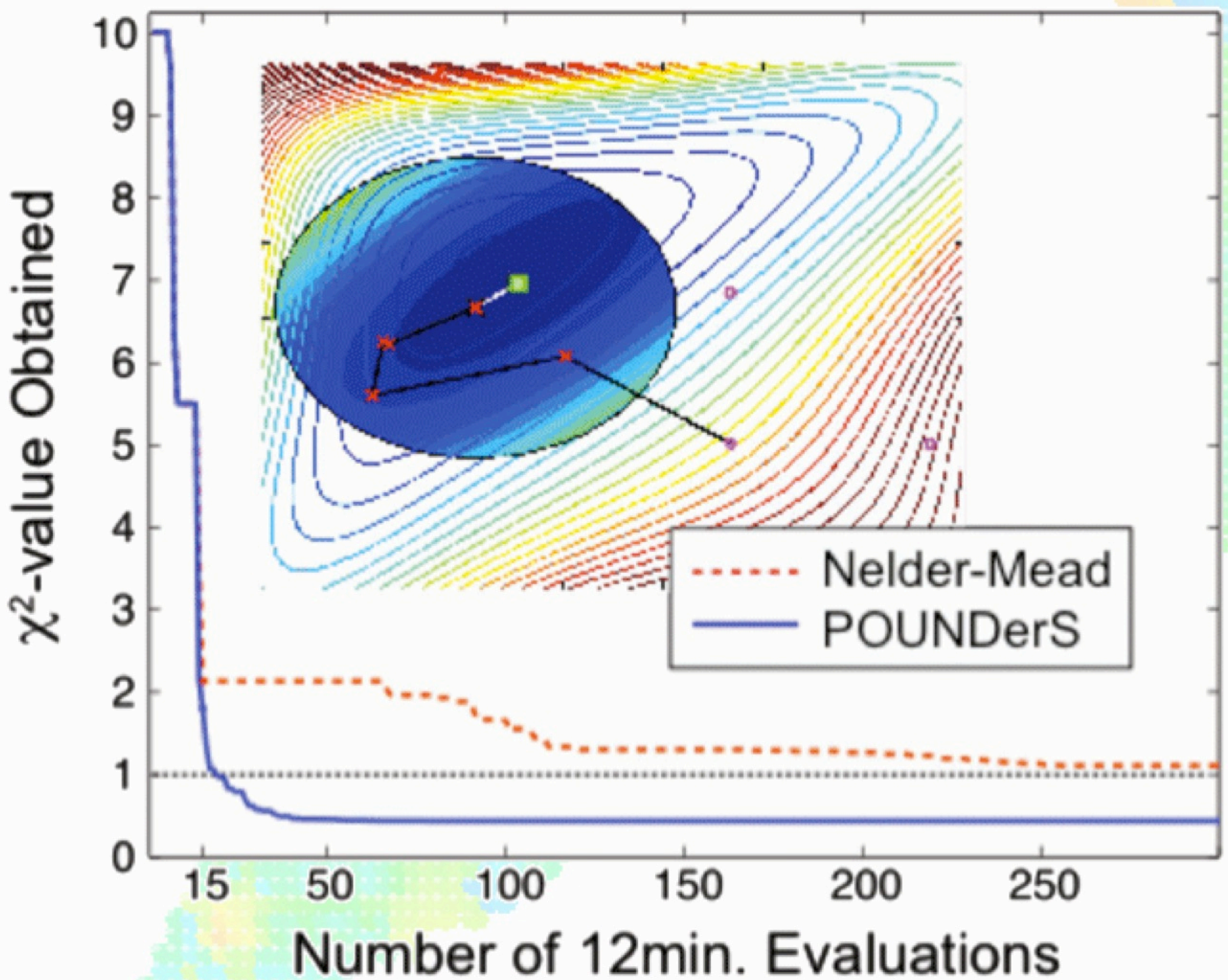
M.Kortelainen, T.Lesinski, J.Moré, W.Nazarewicz, J.Sarich, N.Schunck, M.V.Stoitsov, and S.Wild, Phys. Rev. C **82, 024313 (2010)**

- 12 parameters fit
- Emphasis on heavy nuclei (A>100)

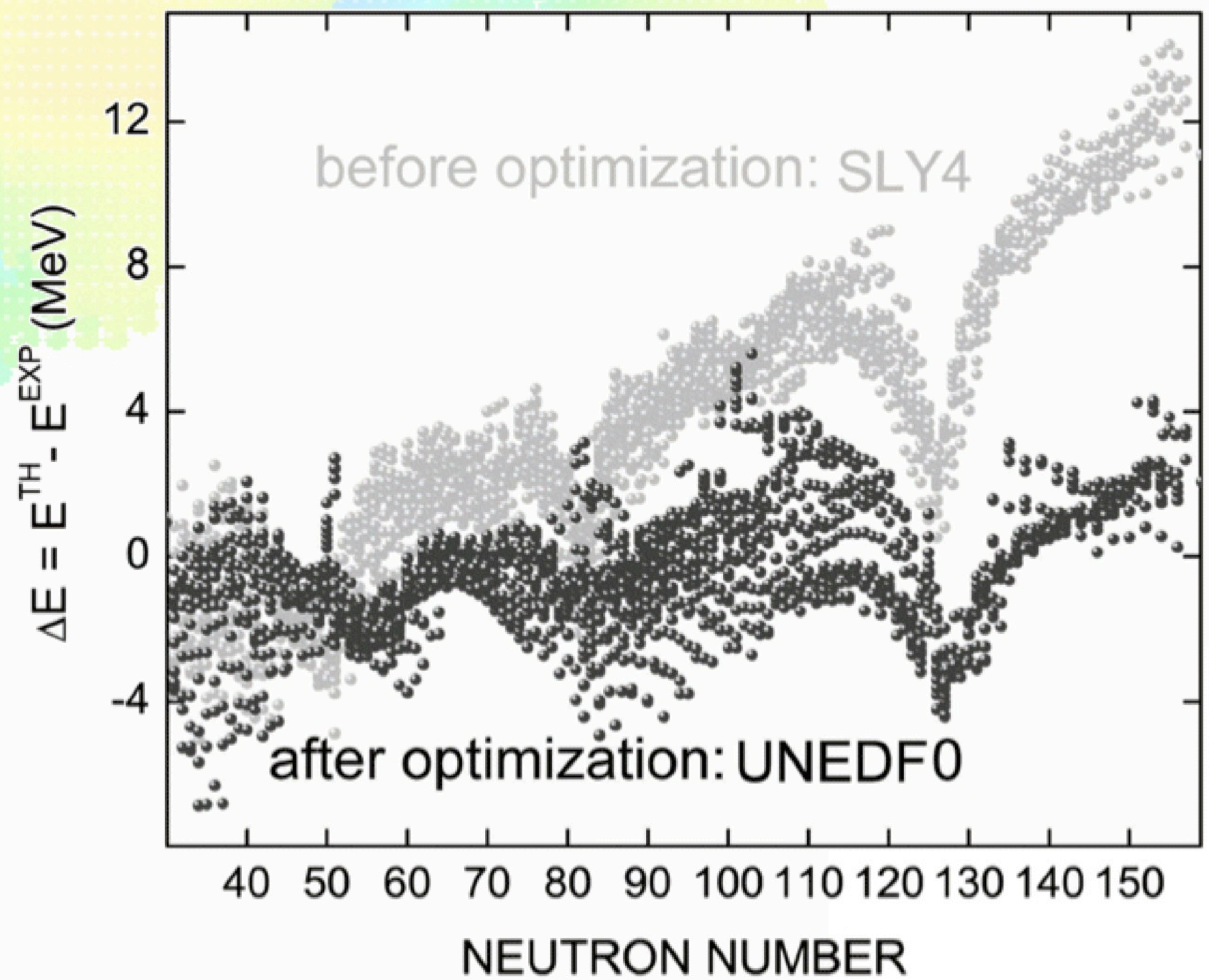
108 data points:
- 28 spherical masses
- 28 r.m.s. radii
- 44 deformed masses
- 8 OEM points



Optimization of the energy functional



Calculating nuclear properties



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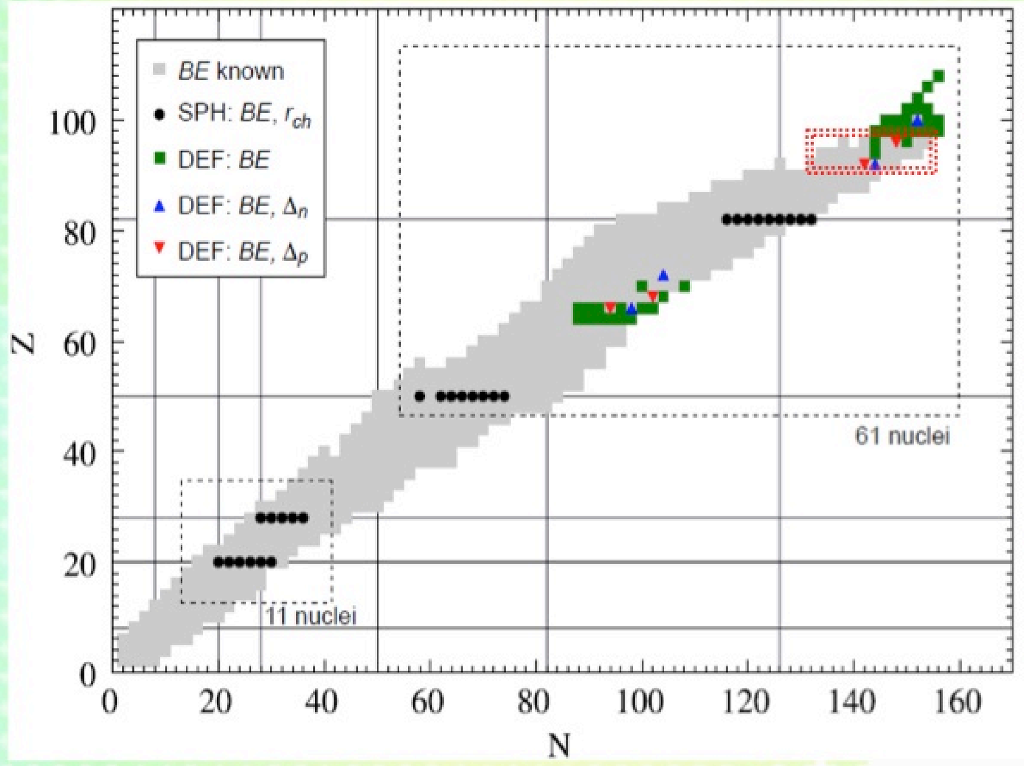
New data points added

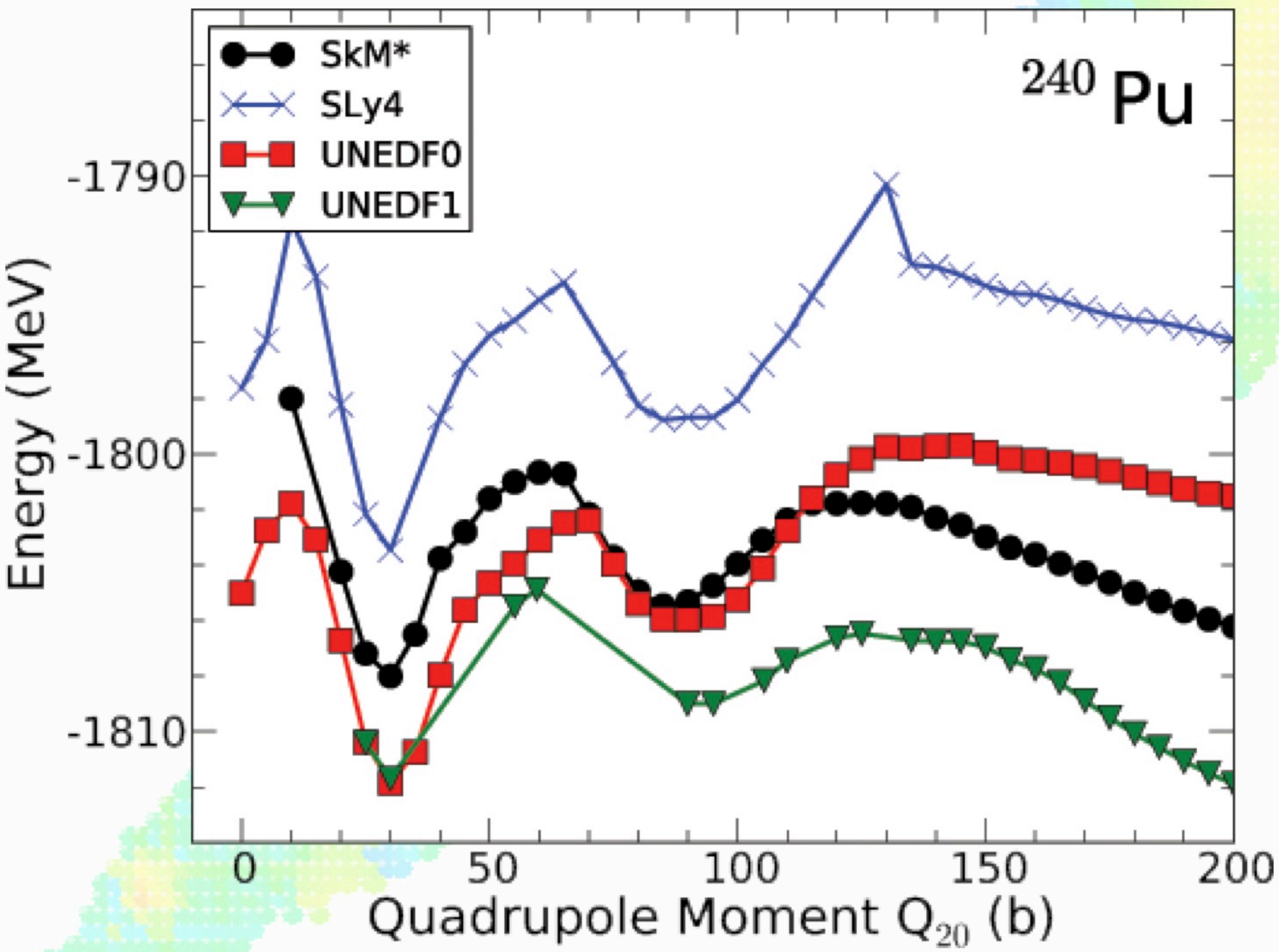
Z	N	E (MeV)	w (MeV)
92	146	-1800.98110	2.0
94	146	-1812.70387	2.0
96	146	-1822.56507	2.0

Super deformed isomers added

Z	N	E (MeV)	w(MeV)
92	144	2.750	0.5
92	146	2.557	0.5
94	146	2.800	0.5
96	146	1.900	0.5

Center of mass correction removed





Pu(240)

Functional	Binding Energy	First Barrier Height
SLy4	1801.5	11.9
SkM*	1804.3	9.4
UNEDF0	1811.8	9.6
UNEDF1	1811.8	6.8
Exp	1813.5	6.1

See the talk of N. Schunck

NEXT UNEDF FUNCTIONAL
Single-Particle Energies

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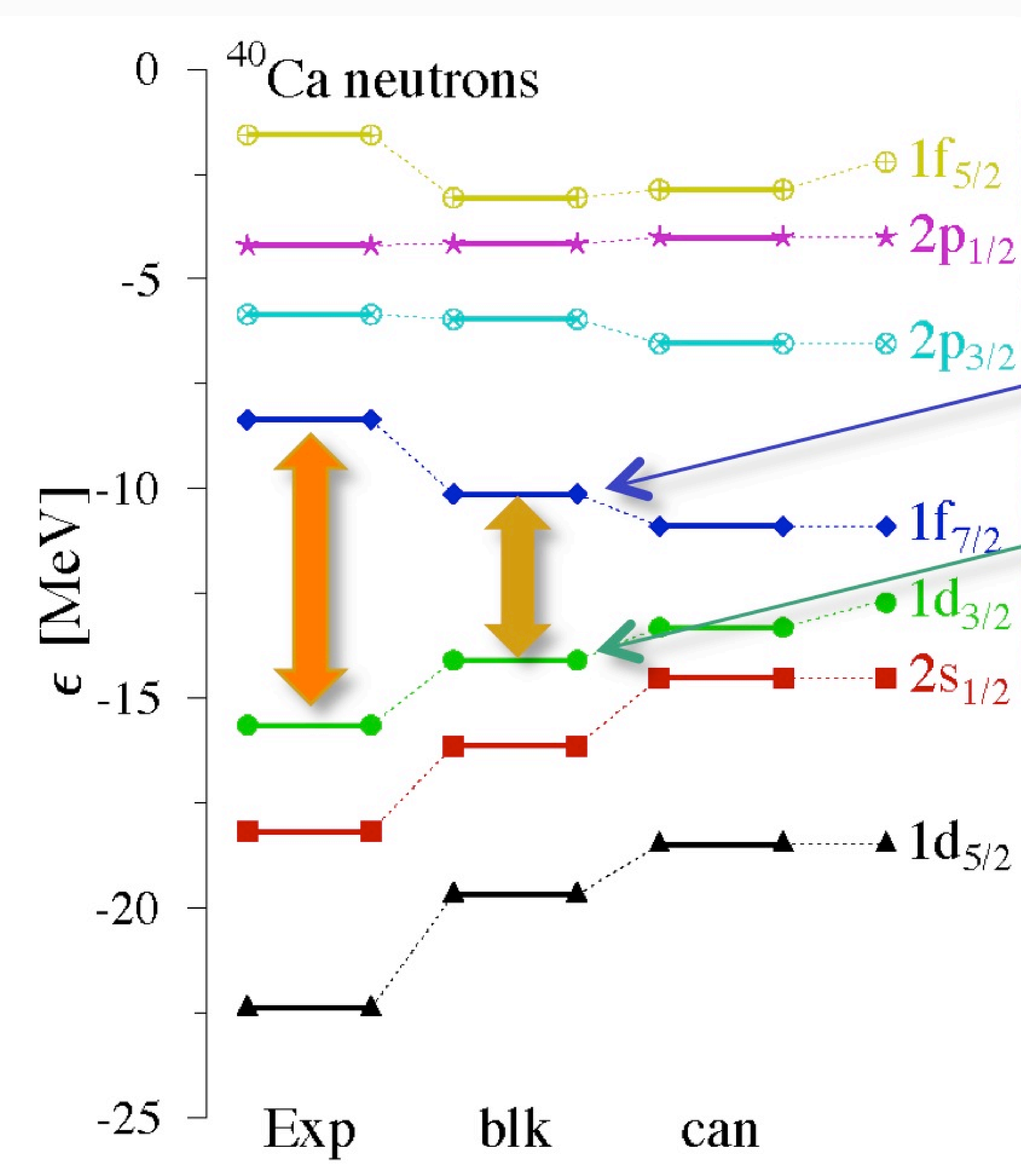
Single-particle splitting candidates

Neutrons	Protons
^{40}Ca f5/2 - f7/2	^{40}Ca f7/2 - d3/2
^{40}Ca f7/2 - d3/2	
^{48}Ca f5/2 - f7 /2	^{48}Ca f5/2 - f7/2
^{132}Sn h9/2 - h11/2	^{132}Sn g7/2 - g9/2
^{208}Pb i11/2 - i13/2	^{208}Pb h9/2 - h11/2



Goal:

- Improving spectroscopic properties of the functional
- Resolving the ability to optimize spin-orbit and tensor terms simultaneously

Using odd-even mass differences after applying a blocking procedure

Calculating:

$$e_{f7/2} = E_{HFB}[^{40}Ca] - E_{HFB}[^{41}Ca + \text{blocking: } f7/2]$$

$$e_{d3/2} = E_{HFB}[^{40}Ca] - E_{HFB}[^{39}Ca + \text{blocking: } d3/2]$$

Fitting:

$$\Delta e = e_{f7/2} - e_{d3/2}$$

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NEXT UNEDF FUNCTIONALS
Single-Particle Energies

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NEXT UNEDF FUNCTIONAL
Neutron Drops and Giant Resonances

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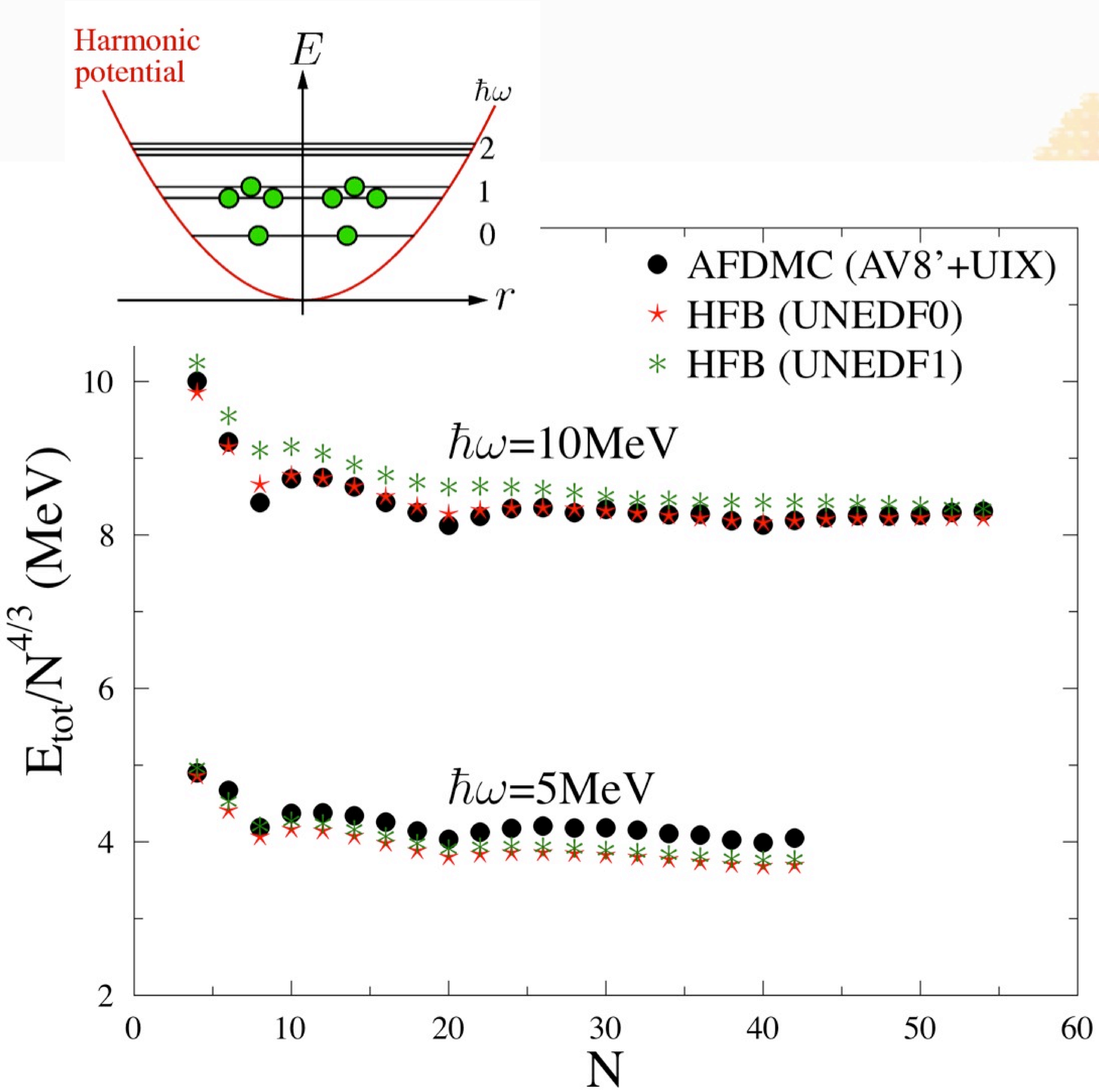
Including pseudo data form neutron drops in a trap

- Small strength of the HO trap (or Woods-Saxon trap ?)
- Large number N of the neutrons (CC-results ?)
- Total energies
- RMS radii
- Neutron infinite nuclear matter at low densities



See the talk of M. Kortelainen

Including experimental data from giant resonances

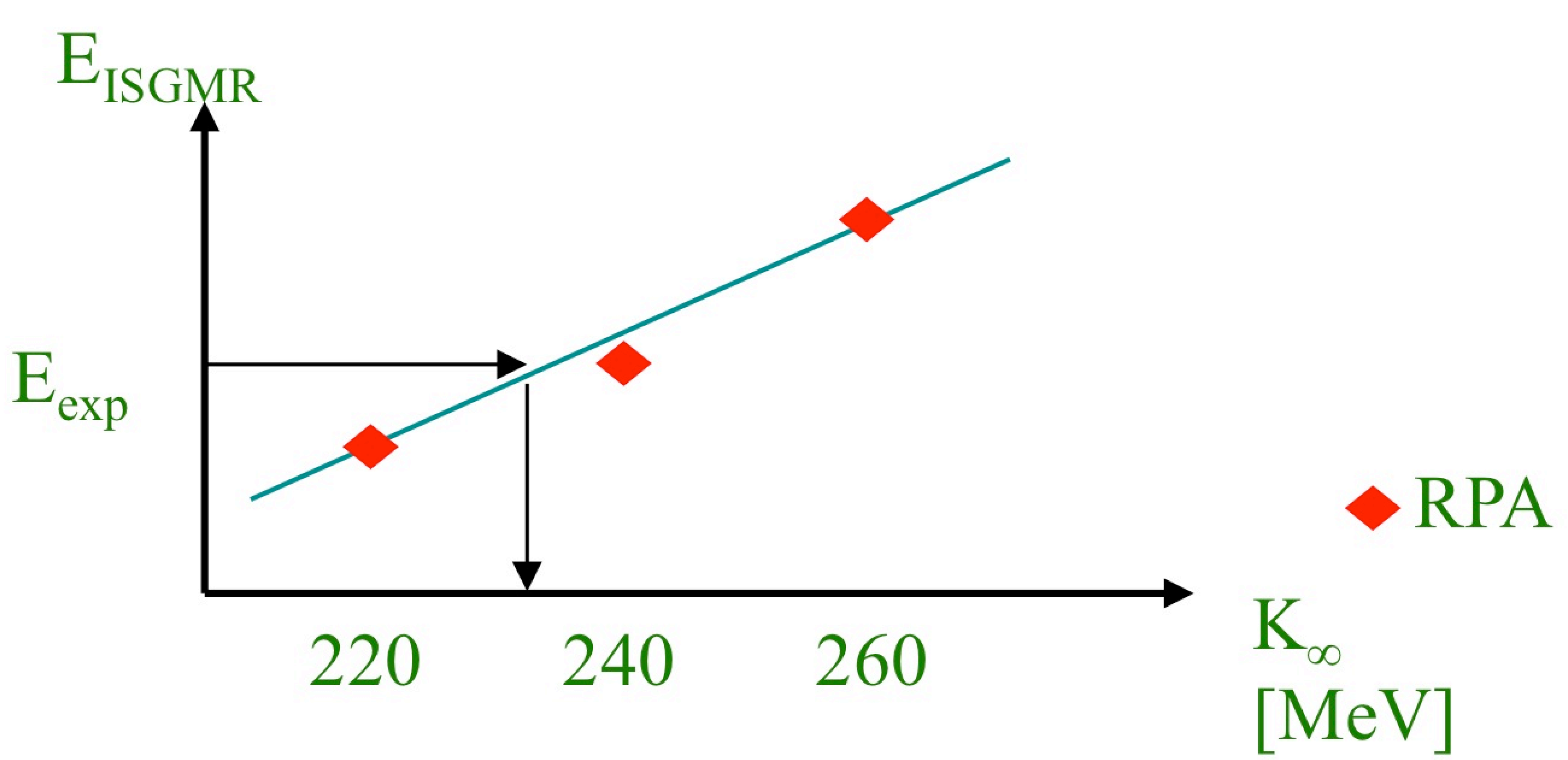
RPA SUM RULE APPROACH

Work in progress: E. Olsen

$$E_{\mathrm{ISGMR}} = \sqrt{\frac{m(1)}{m(-1)}}$$

$$H' = H + \lambda r^2,$$

$$m(-1) = -\frac{1}{2}\frac{\delta\langle r^2\rangle}{\delta\lambda} = \frac{1}{2}\frac{\delta^2\langle H\rangle}{\delta\lambda^2}$$



NEXT UNEDF FUNCTIONAL
DME Functional Optimization

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Analytical Expressions
LO, NLO, N2LO

Dick Furnstahl, Scott Bogner, Biruk Gebremariam, Thomas Duguet

VOLUME PART
Expressed in terms of Infinite NM

All seven volume parameters $\{C^{\rho\rho}_{t0}, C^{\rho\rho}_{tD}, C^{\rho\tau}_{t}, \gamma\}$ expressed in terms of $\rho_c, \frac{E^{NM}}{A}, K^{NM}, M^{*NM}_{s}, a^{NM}_{sym}, L^{NM}, M^{*NM}_{v}$ M.S.

IMPLEMENTATION TO FINITE NUCLEI

M. Kortelainen

Implemented in HFBRAD
- fast (seconds per nucleus)
- spherical nuclei
- $k_F(r) \sim \rho_0(r)^{1/3}$

LO, NLO, N2LO

M.S.

Implemented in HFBTHO
- about 10 min per nucleus
- spherical & axially deformed
- $k_F(r) \sim \rho_0(r)^{1/3}$ + gradients

LO, NLO, N2LO

Done

Optimization

SVD Optimization
HFBTHO using energies and pairing gaps on spherical and deformed nuclei

Genetic Algorithm
Spherical nuclei (HFBRAD)
T. Lesinski, N. Schunck

ADVANCE STAGE

ANL Algorithm
Deformed nuclei (HFBTHO)
J. Moré, J. Sarich, S. Wild

IN PREPARATION

New Mass Table

PHYSICS

HFBTHO ENHANCEMENT

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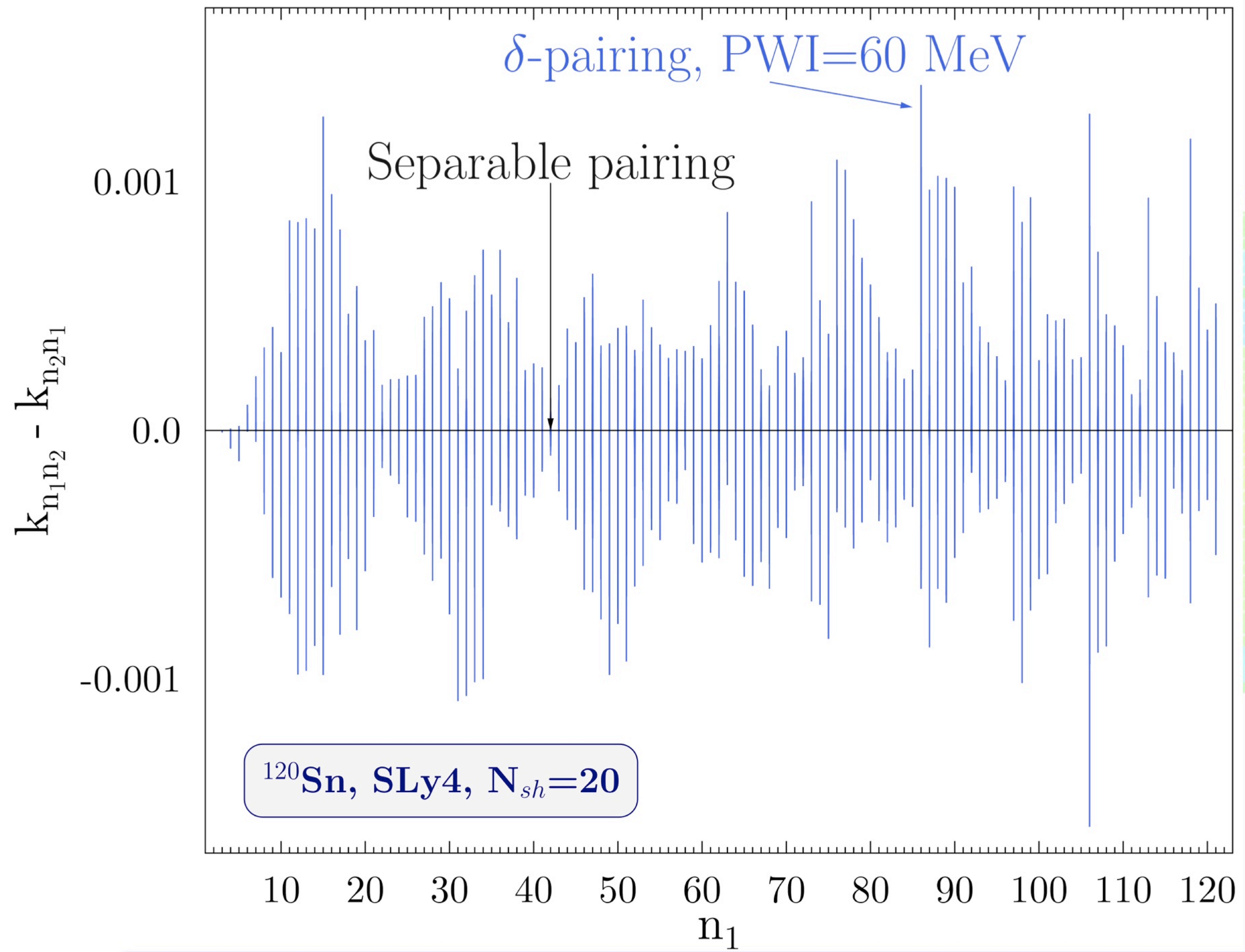
- ✓ Reflection symmetry restriction removed – remains optional
- ✓ Blocking individual quasi-particle state implemented
- ✓ General functionals implemented - including DME functional
- ✓ Handle neutron drops in a trap – optional
- ✓ Separable pairing interaction implemented - optional
- ✓ FAM QRPA implemented – optional
- ✓ Improved performance:

Single core: - 3.5 sec CPU time per iteration at N_{sh}=20
- about 20-30 iterations to converge

Open MP: Jason Sarich is working to reinforce the OpenMP implementation he did for the previous version (additional acceleration of 5-6 times expected)

See the talk of J. Sarich

SEPARABLE PAIRING



The computational overhead is about 1 sec CPU time per iteration mainly due to the full HFB space used

$$< k|V_{sep}|k' >= -Gp(k)p(k')$$

$$p(k) = e^{-a^2k^2}$$

Y. Tian, Z. Ma, P. Ring, Phys.Rev. C 80, 024313 (2009)

Avoids the non-unitarity of the Bogoliubov transformation due to the quasi-particle space truncation

J. Dobaczewski, P. Borycki, W. Nazarewicz, M. Stoitsov, EPJ A25 (2005) 541

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FAM QRPA

For years there is intensive effort to develop efficient tool for performing QRPA calculations for deformed nuclei. Finite Amplitude Method (FAM) is such a tool suggested by T. Nakatsukasa

SHORT HISTORY

Demonstration of FAM efficiency in RPA calculations

T. Nakatsukasa, T. Inakura and K. Yabana, Phys. Rev. C 76 024318 (2007).
T. Inakura, T. Nakatsukasa and K. Yabana, Phys. Rev. C 80 044301 (2009).

Demonstration of FAM efficiency in QRPA calculations for spherical nuclei

P. Avogadro, T. Nakatsukasa, Finite amplitude method for the quasi-particle random-phase approximation, arXiv:1104.3692 (2011)

PRESENT DEMONSTRATION

M.S., M. Kortelainen, T. Nakatsukasa, W. Nazarewicz, C. Losa

- ✧ New efficient way of solving FAM equations based on Broyden method
- ✧ Complete implementation within HFBTHO solver
- ✧ Benchmark comparison with standard QRPA results with pairing and deformation

FAM QRPA

QRPA:

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \omega \begin{pmatrix} X \\ -Y \end{pmatrix}$$

FAM QRPA:

$$(E_\mu + E_\nu)\, X_{\nu\mu} + \delta H^{20}_{\nu\mu}(\omega) = \omega X_{\nu\mu},$$

$$(E_\mu + E_\nu)\, Y^*_{\nu\mu} + \overline{\delta H}^{20}_{\nu\mu}(\omega) = -\omega Y^*_{\nu\mu},$$

$$\delta H^{20}(\omega) = U^\dagger \delta h(\omega) V^* - V^\dagger \overline{\delta h}^{\,*}(\omega) U^* - V^\dagger \overline{\delta \Delta}^{\,*}(\omega) V^* + U^\dagger \delta\Delta(\omega) U^*,$$

$$\overline{\delta H}^{20}(\omega) = U^\dagger \overline{\delta h}(\omega) V^* - V^\dagger \delta h^*(\omega) U^* - V^\dagger \Delta^*(\omega) V^* + U^\dagger \overline{\delta\Delta}(\omega) U^*,$$

$$\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}$$

HFB

$$\rho_\eta = (V + \eta U^* X^*)^* (V + \eta U^* Y)^T,$$

$$k_\eta = -(U + \eta V^* Y)(V + \eta U^* X^*)^\dagger,$$

$$\bar{\rho}_\eta = (V + \eta U^* Y)^* (V + \eta U^* X^*)^T,$$

$$\bar{k}_\eta = -(U + \eta V^* X^*)(V + \eta U^* Y)^\dagger.$$

$$\delta h(\omega) = \frac{h[\rho_\eta, k_\eta] - h[\rho, k]}{\eta},$$

$$\overline{\delta h}(\omega) = \frac{h[\bar{\rho}_\eta, \bar{k}_\eta] - h[\rho, k]}{\eta},$$

$$\delta\Delta(\omega) = \frac{\Delta[\rho_\eta, k_\eta] - \Delta[\rho, k]}{\eta},$$

$$\overline{\delta\Delta}(\omega) = \frac{\Delta[\bar{\rho}_\eta, \bar{k}_\eta] - \Delta[\rho, k]}{\eta},$$

FAM QRPA EQUATIONS - SOLUTION

FAM QRPA EQUATIONS

$$(E_\mu + E_\nu - \omega)\, X_{\nu\mu} = -\delta H^{20}_{\nu\mu}(\omega) - F_{\nu\mu},$$

$$(E_\mu + E_\nu + \omega)\, Y_{\nu\mu} = -\overline{\delta H}^{20*}_{\nu\mu}(\omega) - F_{\nu\mu},$$

$$X_{\mu\nu} = -\frac{\delta H^{20}_{\mu\nu}(\omega) - F^{20}_{\mu\nu}}{E_\mu + E_\nu - \omega},$$

$$Y_{\mu\nu} = -\frac{\overline{\delta H}^{20*}_{\mu\nu}(\omega) - F^{20*}_{\mu\nu}}{E_\mu + E_\nu + \omega}.$$

SELF-CONSISTENT ITERATIONS
(Broyden mixing as in HFB)

$$X^{(0)}_{\mu\nu} = Y^{(0)}_{\mu\nu} = 0 \Longrightarrow \delta H^{20(0)}(\omega),\, \overline{\delta H}^{20(0)}(\omega) \Longrightarrow X^{(1)}_{\mu\nu},\, Y^{(1)}_{\mu\nu} \Longrightarrow \delta H^{20(1)}(\omega),\, \overline{\delta H}^{20(1)}(\omega),\quad \ldots$$

COMPLEX FREQUENCY

$$\omega \rightarrow \omega + i\gamma$$

Lorenz smoothing

$$\Gamma = 2\gamma$$

FAM QRPA - NUMBER OF ITERATIONS

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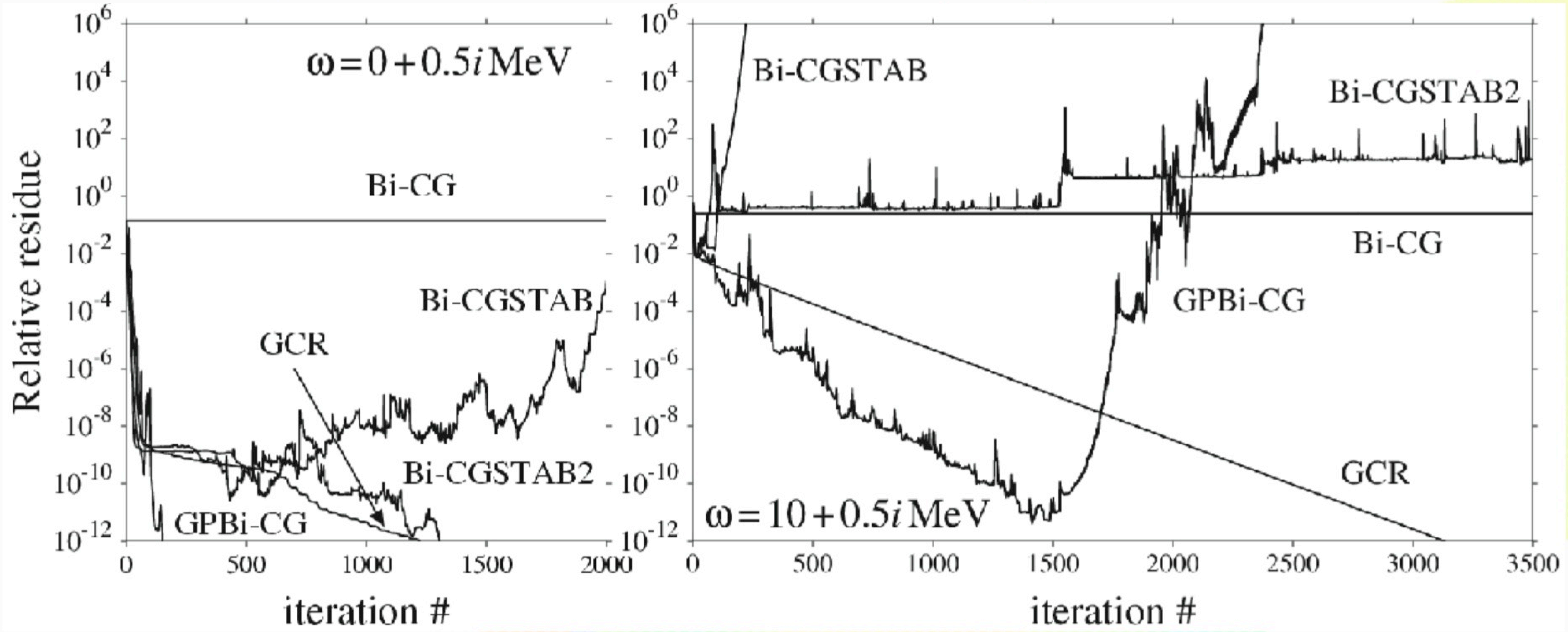
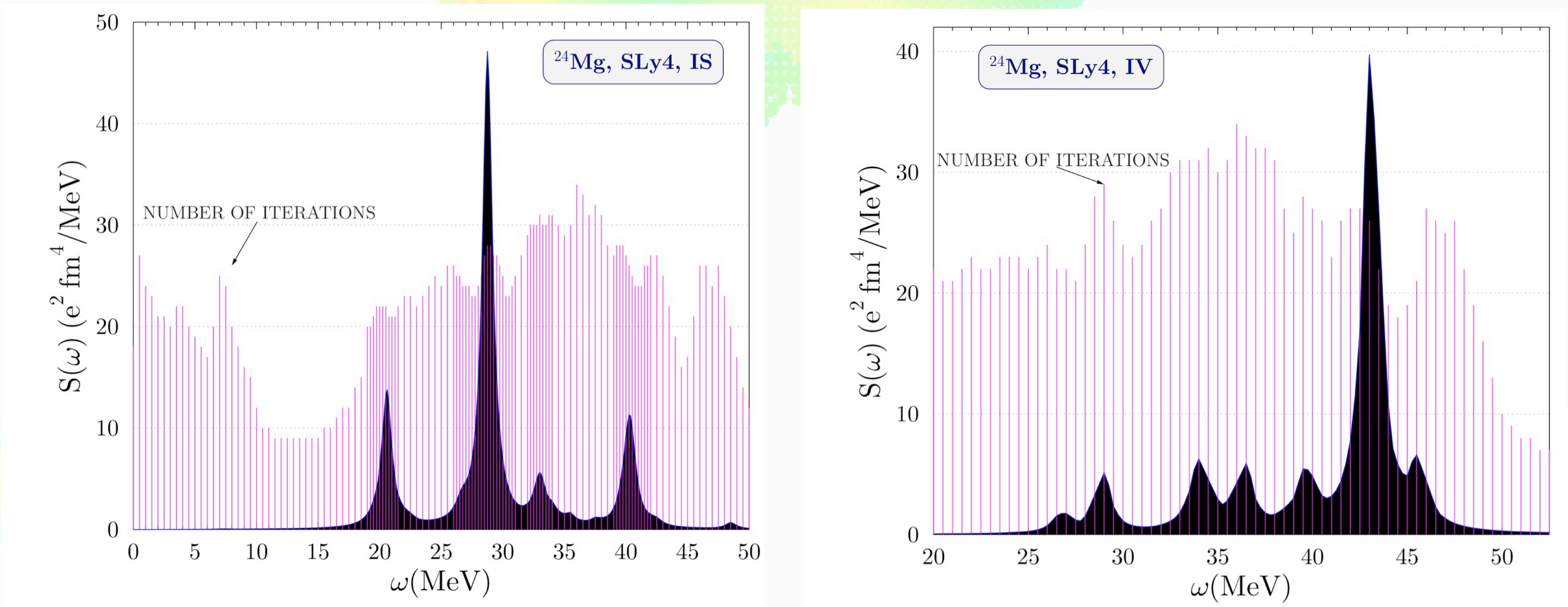
T. Inakura, T. Nakatsukasa and K. Yabana, Phys. Rev. C 80 044301 (2009).



PRESENT METHOD



FAM QRPA - ACCURACY

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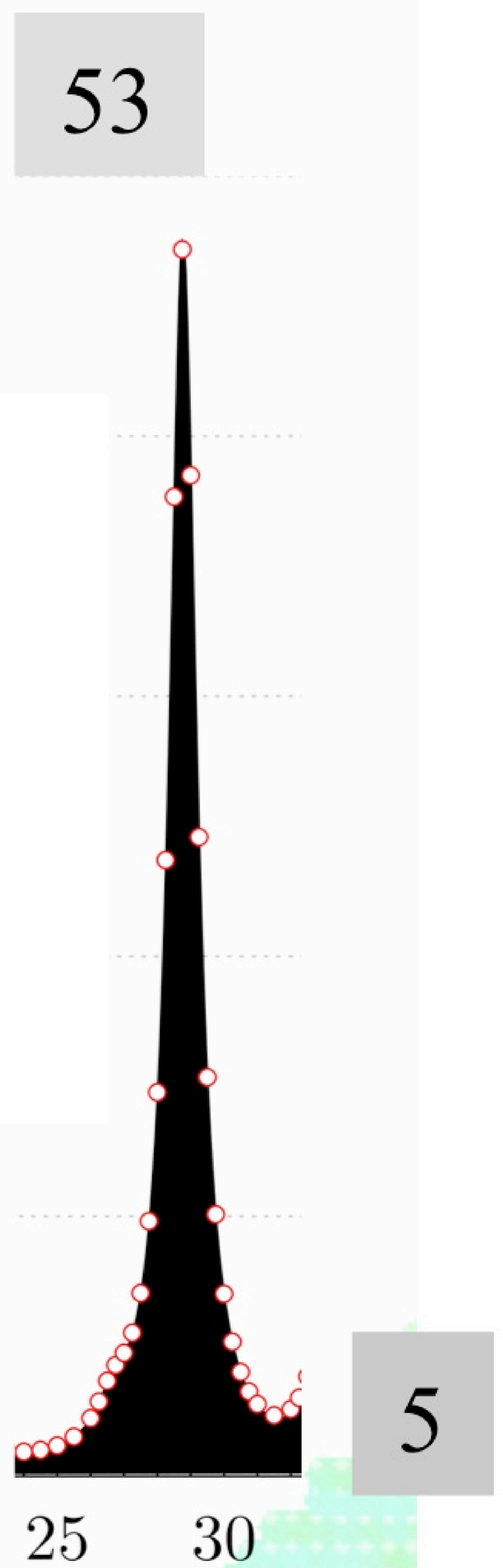

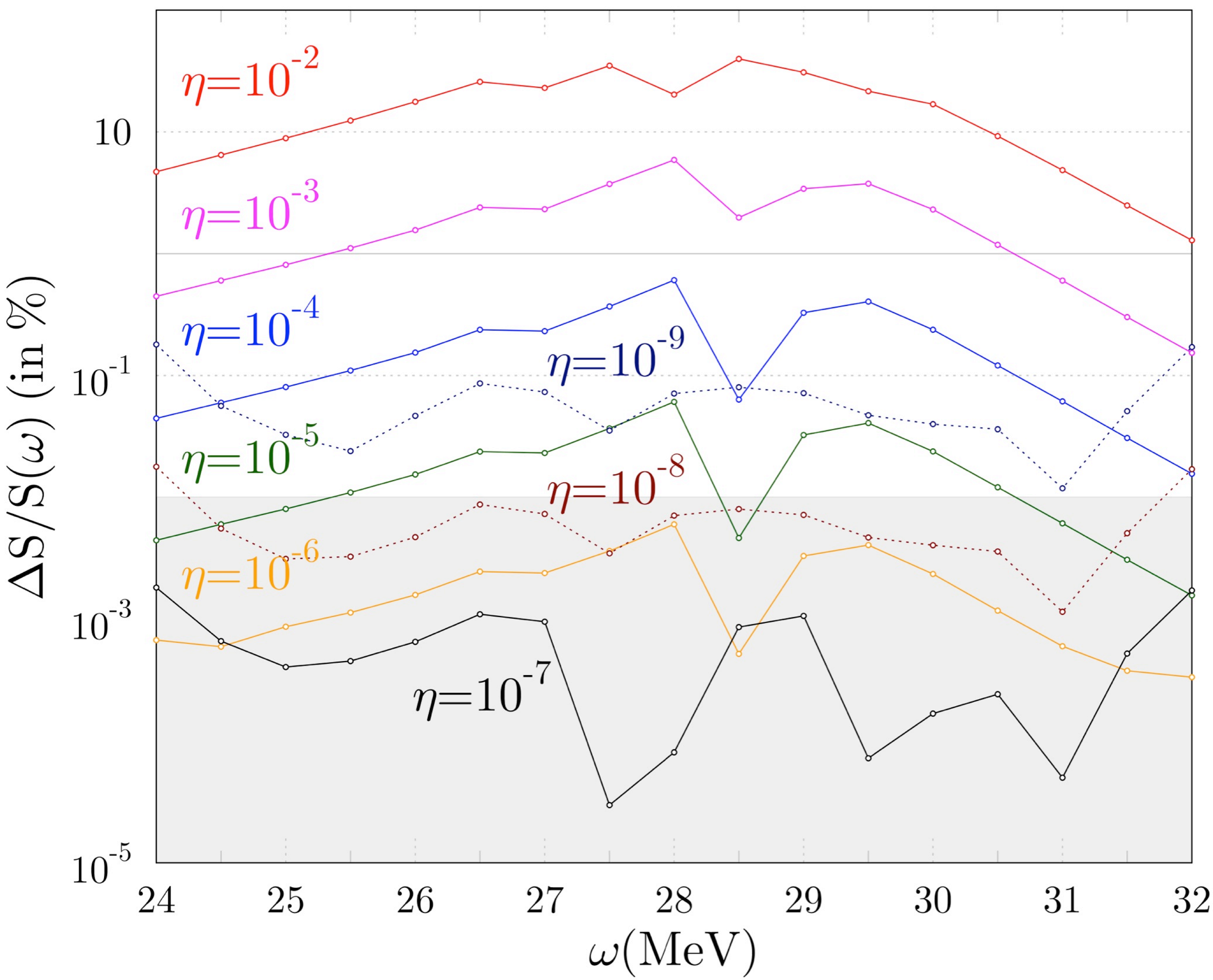

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QRPA – FAM (COMPARISON)

QRPA:

Calculating and diagonalizing A,B matrices in the canonical basis following from the HFB solution obtained by the HFBTHO solver

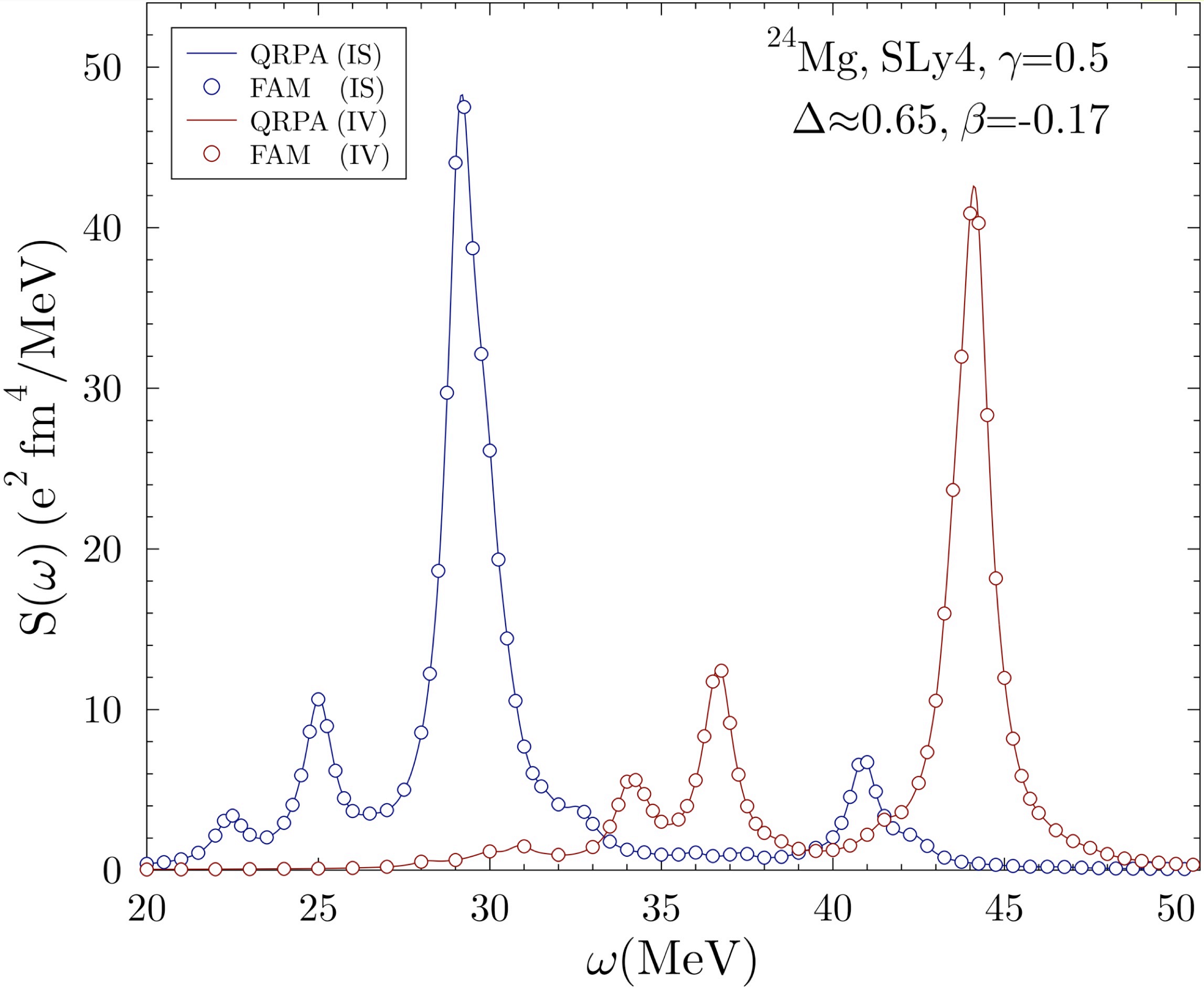
C. Losa, A. Pastore, T. Dossing, E. Vigezzi, R.A. Broglia, Phys. Rev. C 81, 064307 (2010).

FAM:

FAM QRPA module build on the top of HFBTHO solver

SLY4, VOLUME PAIRING, ISGMR, IVGMR

QRPA versus FAM
NUMERICALLY IDENTICAL RESULTS



QRPA TRUNCATIONS

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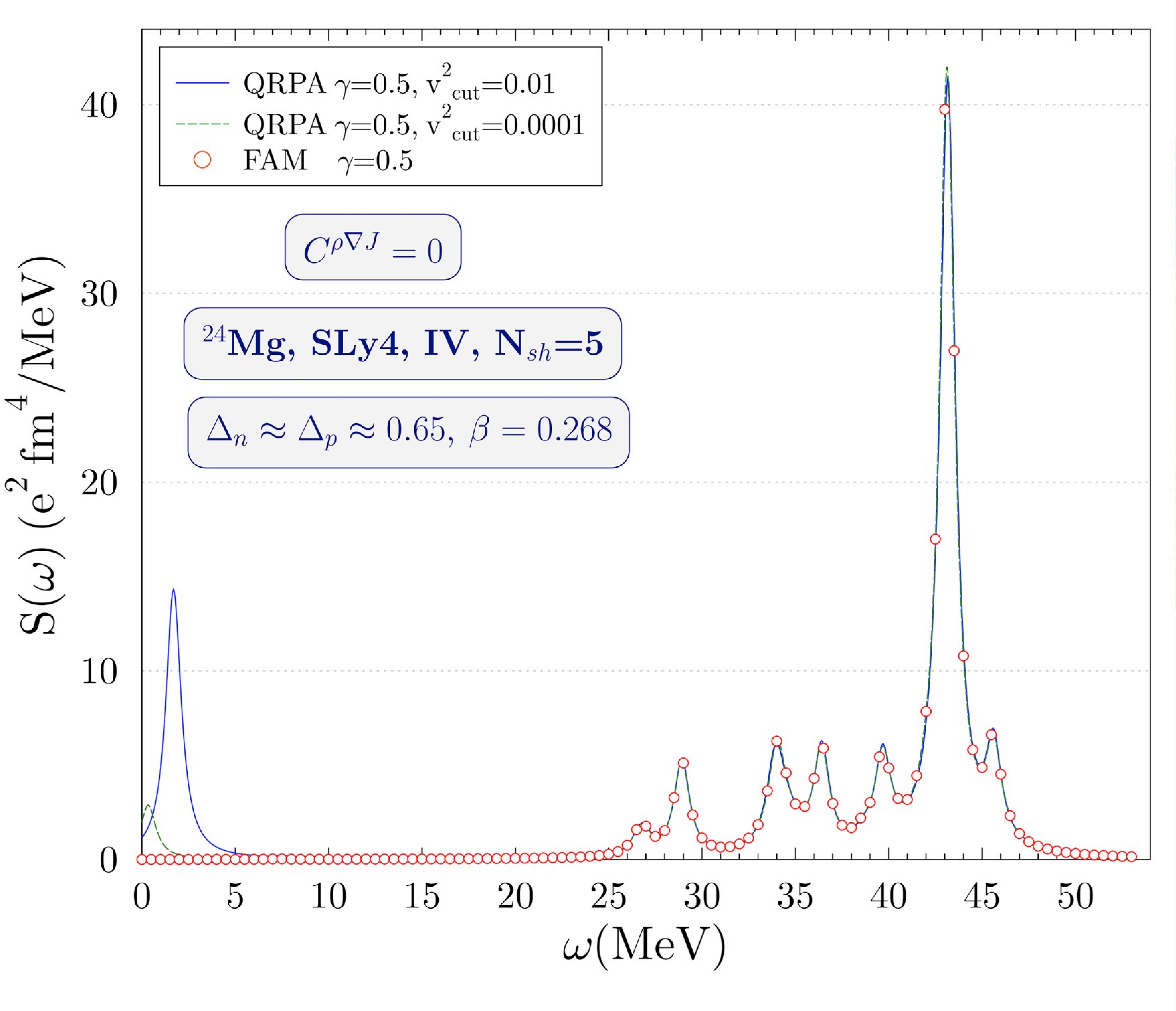

QRPA			FAM
v_{crit}	Size of A, B matrices	Memory (in GB)	Memory (in GB)
^{40}Mg			
10^{-3}	32039 × 32039	16.4	
10^{-4}	53386 × 53386	45.6	
10^{-5}	53823 × 53823	46.35	
10^{-10}	130936 × 130936	274.31	
10^{-15}	189271 × 189271	473.18	
10^{-20}	211159 × 211159	713.41	0.572
^{100}Zr			
10^{-3}	83970 × 83970	112.81	
10^{-4}	140229 × 140229	314.63	
10^{-5}	160633 × 160633	412.85	
10^{-10}	189500 × 189500	574.56	
10^{-15}	230274 × 230274	848.41	
10^{-20}	230304 × 230304	848.64	0.572

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FAM QRPA RESULTS: ^{100}Zr

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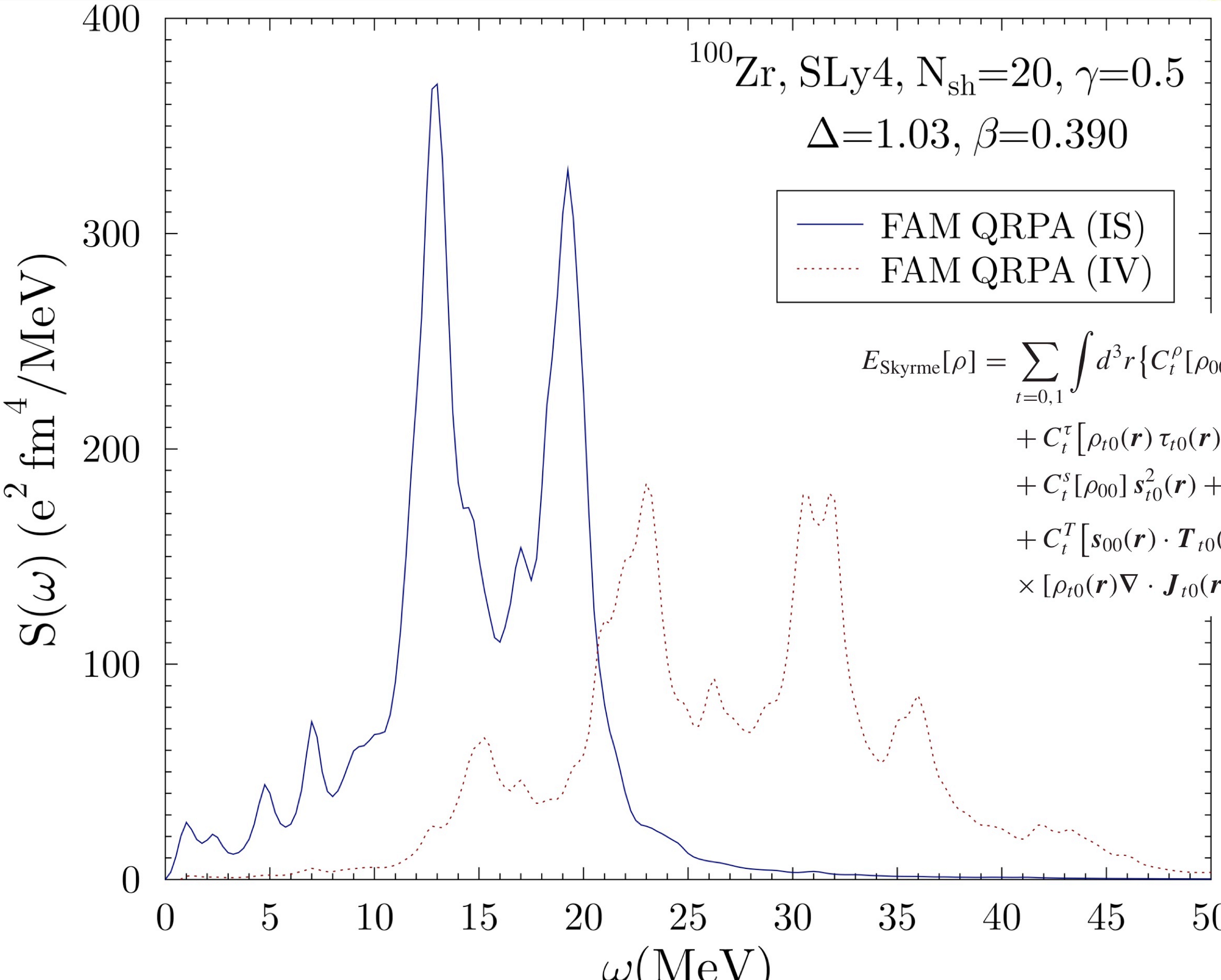

$$E_{\text{Skyrme}}[\rho] = \sum_{t=0,1} \int d^3r \{ C_t^{\rho}[\rho_{00}]\, \rho_{t0}^2(\boldsymbol{r}) + C_t^{\Delta\rho} \rho_{t0}(\boldsymbol{r}) \Delta\rho_{t0}(\boldsymbol{r})$$
$$+ C_t^{\tau} \left[\rho_{t0}(\boldsymbol{r})\, \tau_{t0}(\boldsymbol{r}) - \boldsymbol{j}_{t0}^2(\boldsymbol{r}) \right]$$
$$+ C_t^{s}[\rho_{00}]\, \boldsymbol{s}_{t0}^2(\boldsymbol{r}) + C_t^{\Delta s} \boldsymbol{s}_{t0}(\boldsymbol{r}) \cdot \Delta \boldsymbol{s}_{t0}(\boldsymbol{r})$$
$$+ C_t^{T} \left[\boldsymbol{s}_{00}(\boldsymbol{r}) \cdot \boldsymbol{T}_{t0}(\boldsymbol{r}) - \overset{\leftrightarrow}{J}{}_{t0}^2(\boldsymbol{r}) \right] + C_t^{\nabla J}$$
$$\times [\rho_{t0}(\boldsymbol{r}) \nabla \cdot \boldsymbol{J}_{t0}(\boldsymbol{r}) + \boldsymbol{s}_{t0}(\boldsymbol{r}) \cdot \nabla \times \boldsymbol{j}_{t0}(\boldsymbol{r})] \}.$$

QRPA for the Zr-chain
K. Yoshida, Phys. Rev. C 82, 034324 (2010)

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FAM QRPA RESULTS: ^{240}Pu

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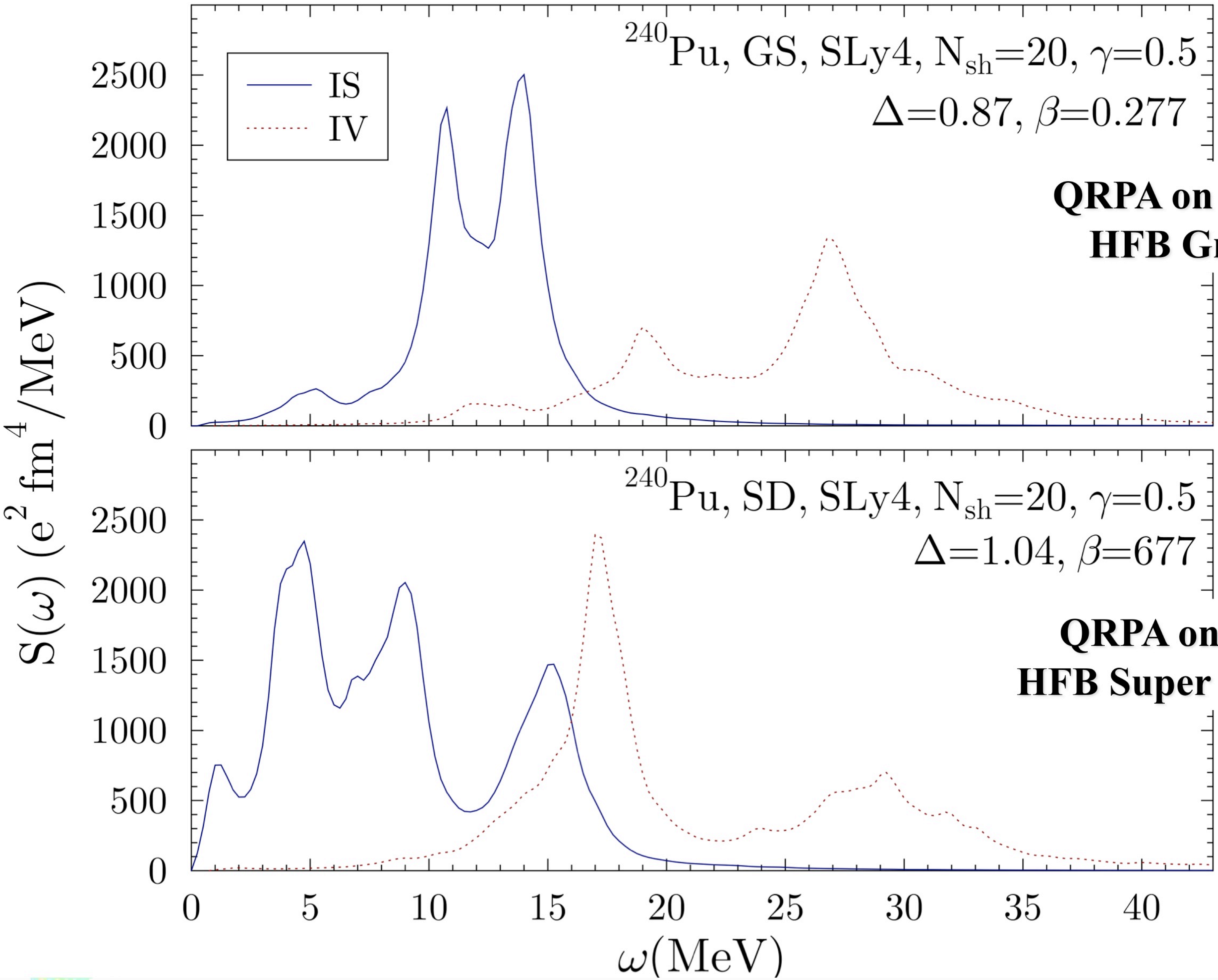

QRPA on the top of the HFB Ground State

QRPA on the top of the HFB Super Deformed State

CLACULATIONS PERFORMED ON A LAPTOP

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SUMMARY

NEXT STEPS TO THE UNEDF FUNCTIONAL

- Optimization adding single-particle energies
- Optimization adding neutron drops ‘data’
- Optimization adding giant resonances data

Hopefully all Skyrme parameters will be constrained

- Optimization using DME functional

Considering exploring the separable pairing

Complete mass table QRPA calculations