The QRPA approach within the Gogny EDF framework : some success and current limitations

S. Péru

CEA, DAM, DIF

Hirschegg, January 18-24, 2026

1. the HFB+QRPA approach in the Gogny-EDF context

HFB formalism

$$F(\rho,\kappa) = \sum_{\alpha\beta} t_{\alpha\beta}\rho_{\beta\alpha} + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|\mathcal{V}(\rho)|\widetilde{\gamma\delta}\rangle \rho_{\gamma\alpha}\rho_{\delta\beta} + \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|\mathcal{V}(\rho)|\widetilde{\gamma\delta}\rangle \kappa^*_{\beta\alpha}\kappa_{\gamma\delta}$$

$$\delta F = \sum_{\alpha\beta} \frac{\partial F}{\partial\rho_{\beta\alpha}}\delta\rho_{\alpha\beta} + \frac{1}{2}\sum_{\alpha\beta}\left(\frac{\partial F}{\partial\kappa_{\beta\alpha}}\delta\kappa_{\alpha\beta} + \frac{\partial F}{\partial\kappa^*_{\beta\alpha}}\delta\kappa^*_{\alpha\beta}\right)$$

$$\boxed{[H_B, \mathcal{R}] = 0}$$

$$H_B = \begin{pmatrix} e & \Delta \\ -\Delta^* & -e^* \end{pmatrix} \qquad e_{\alpha\beta} = \frac{\partial F}{\partial\rho_{\beta\alpha}} \qquad \Delta_{\alpha\beta} = \frac{\partial F}{\partial\kappa^*_{\alpha\beta}} \qquad \mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & (1-\rho^*) \end{pmatrix}$$

Proton Chemical Potential

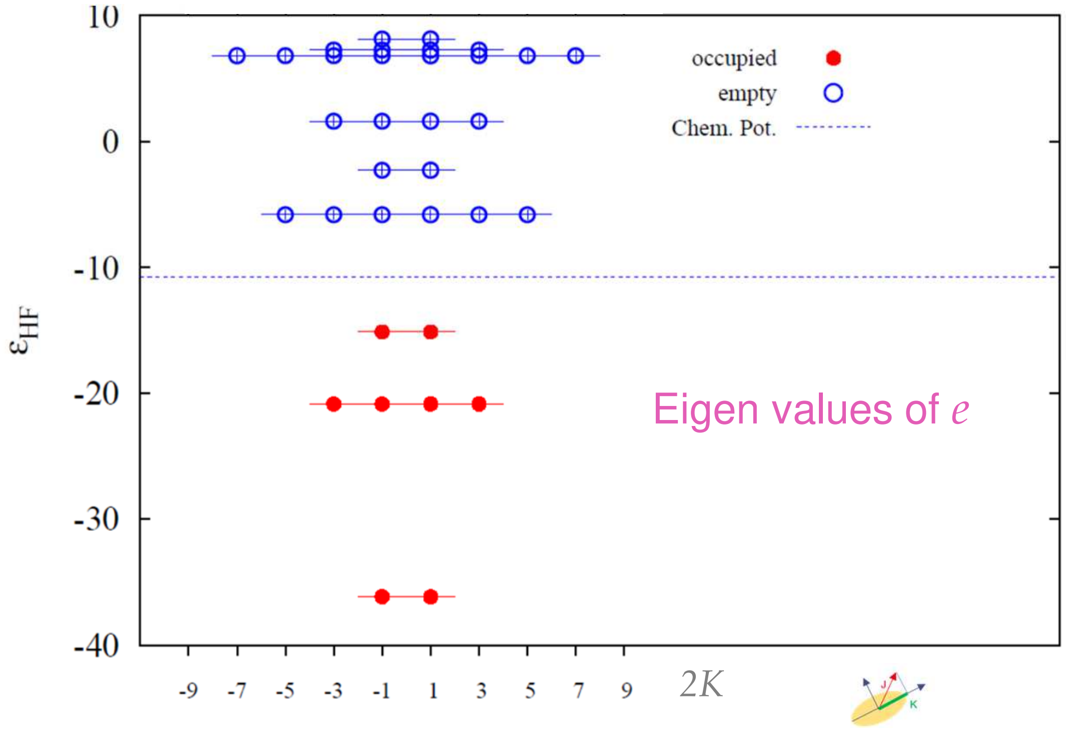
$$\delta\langle\Phi_q|\hat{H} - \lambda_N\hat{N} - \lambda_Z\hat{Z} - \sum_i \lambda_i\hat{Q}_i|\Phi_q\rangle = 0,$$

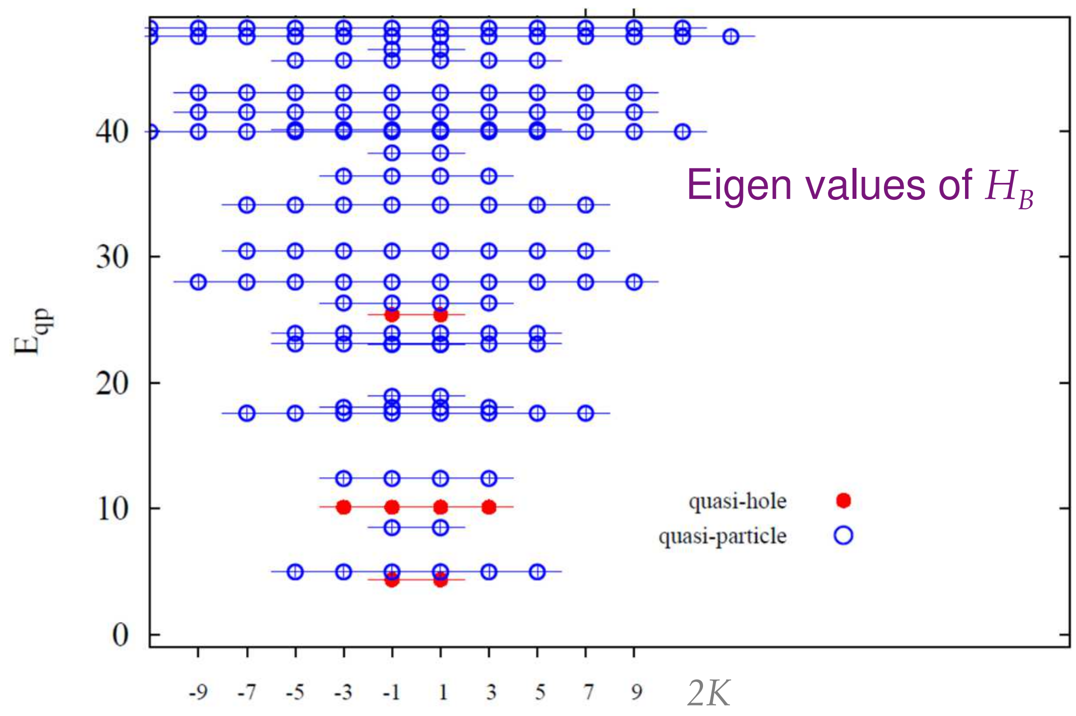
Neutron Chemical Potential

HFB neutron single particle levels for ^{16}O

$$H_B = \boxed{\begin{pmatrix} \boxed{e} & \Delta \\ -\Delta^* & -e^* \end{pmatrix}}$$

For ^{16}O $\Delta=0$





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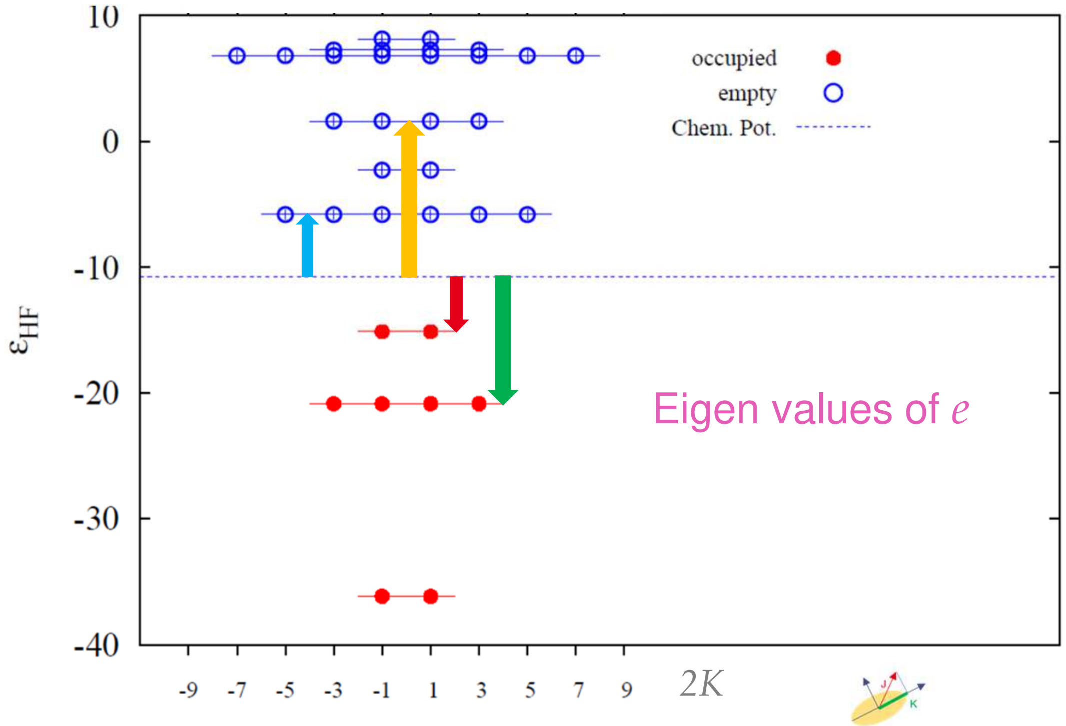

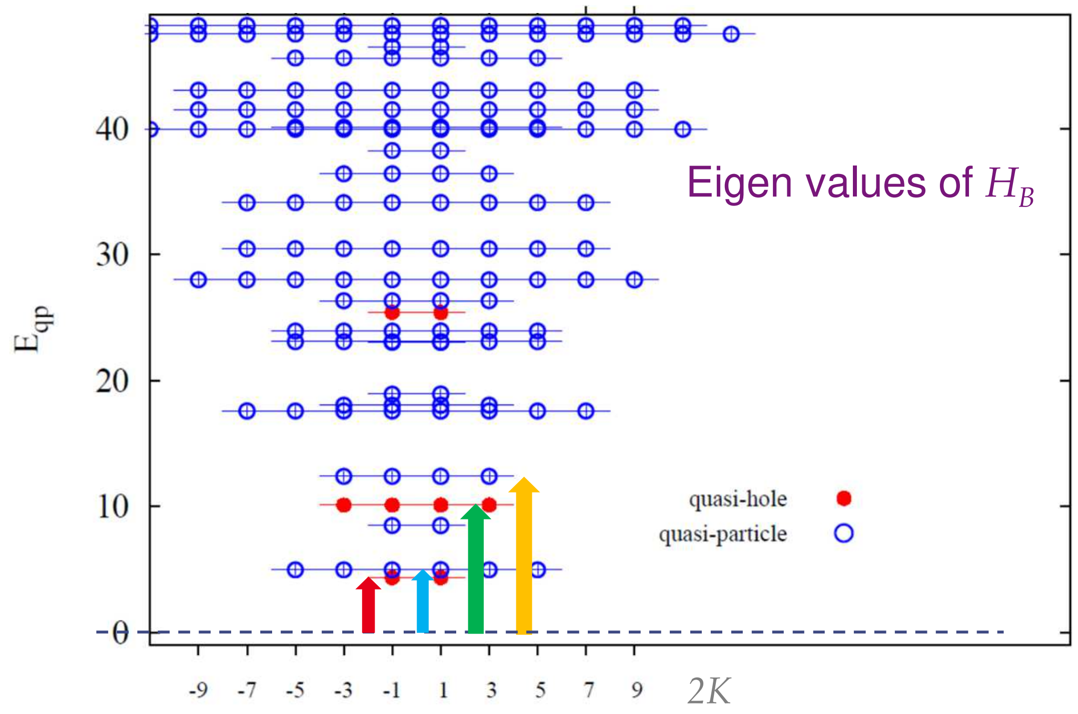

Neutron Chemical Potential = -10.75 MeV

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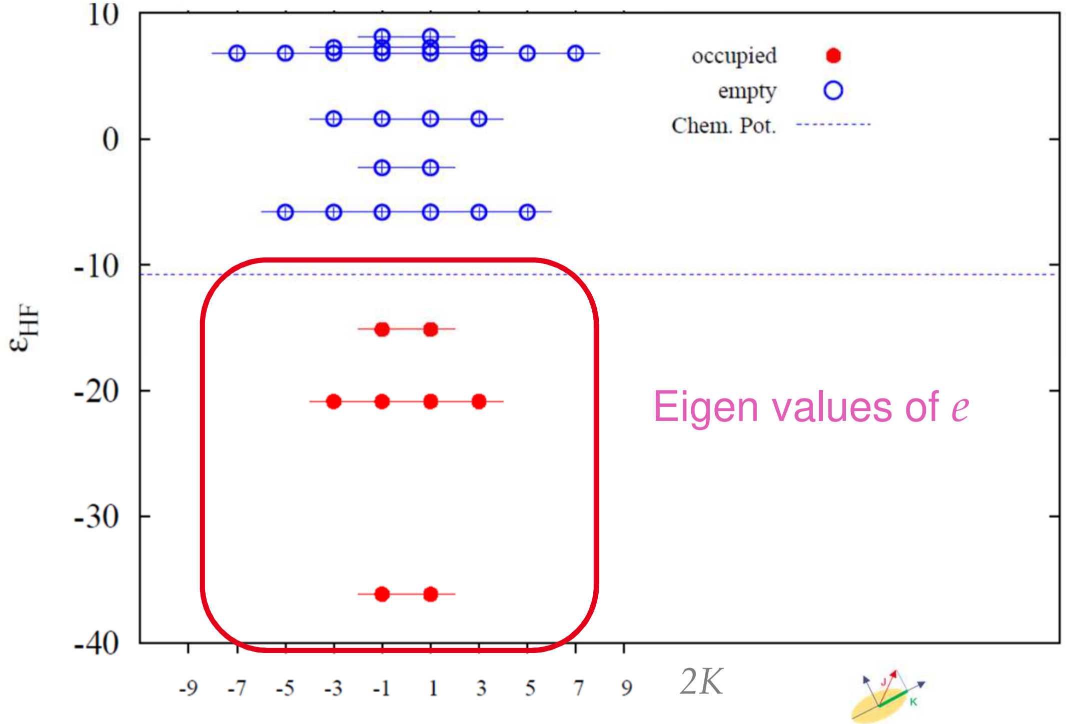

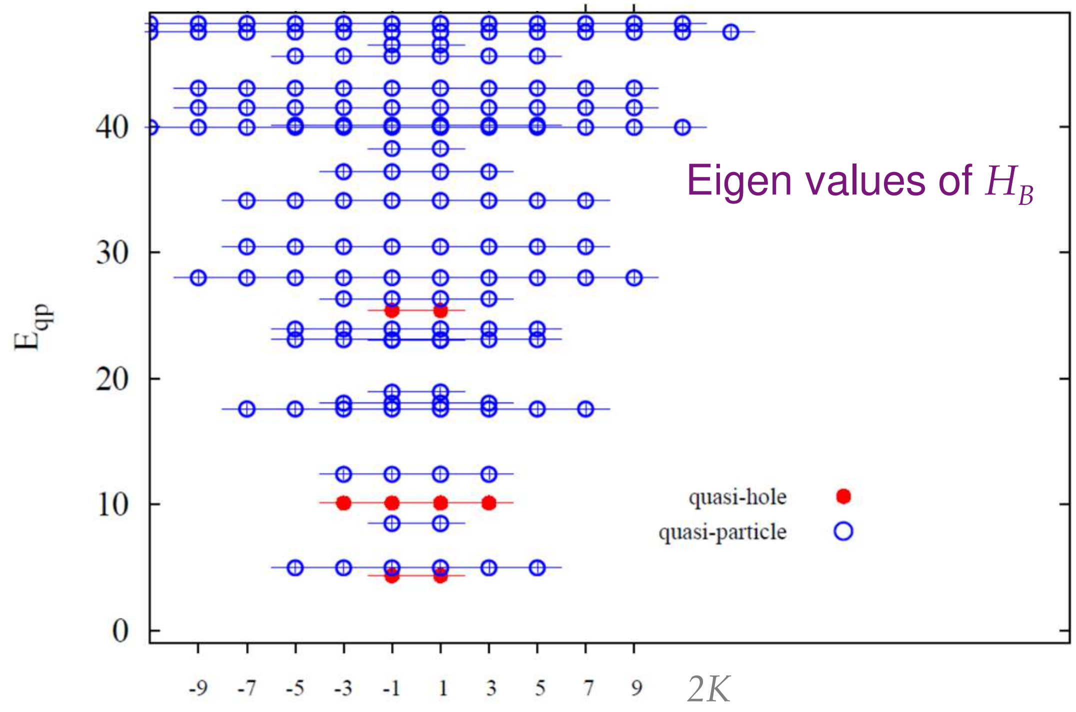

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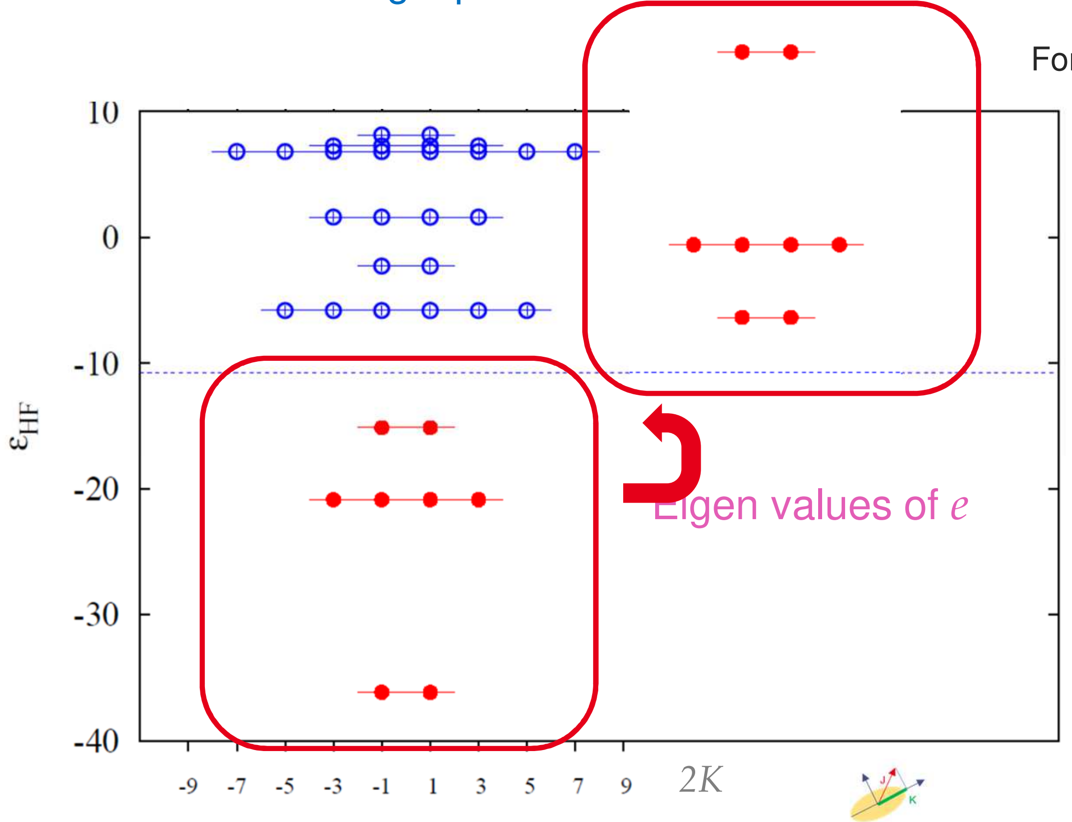

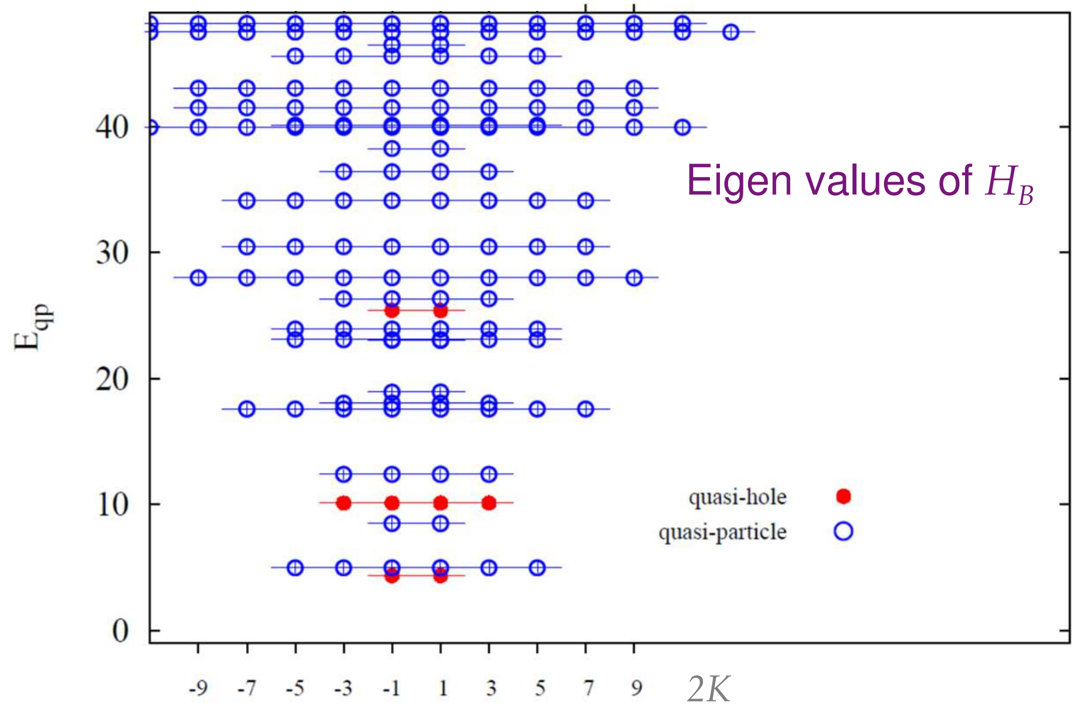

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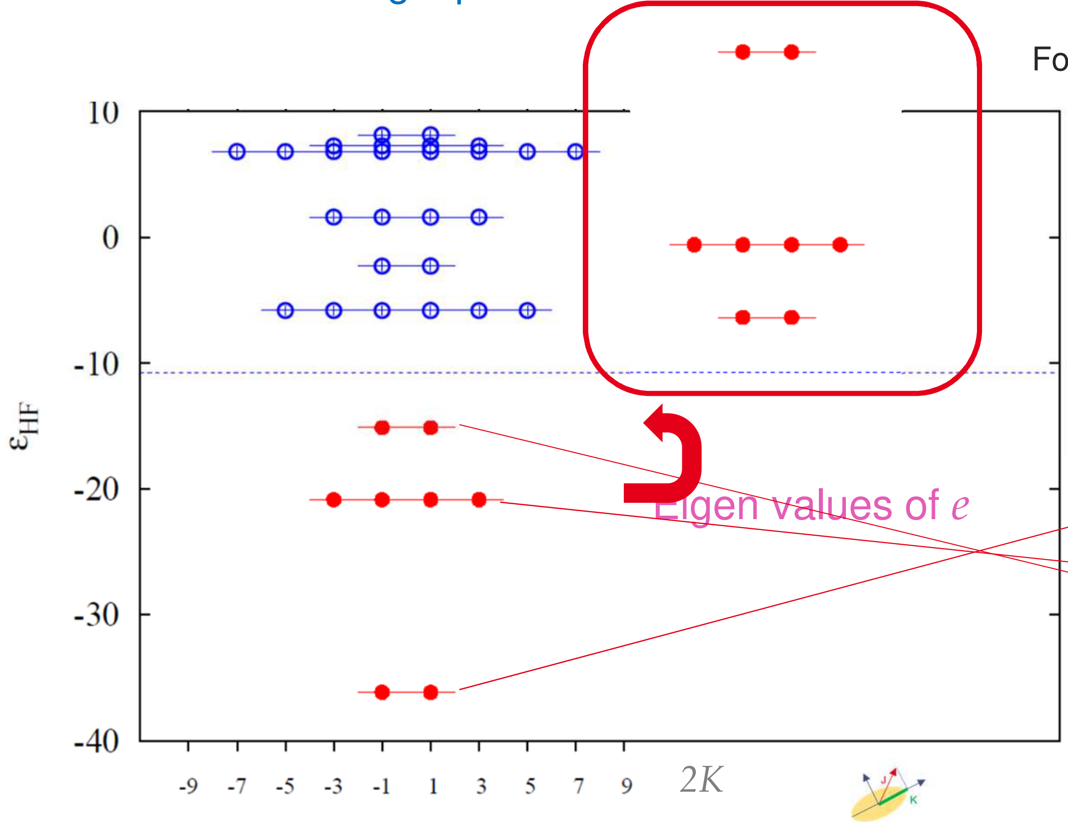

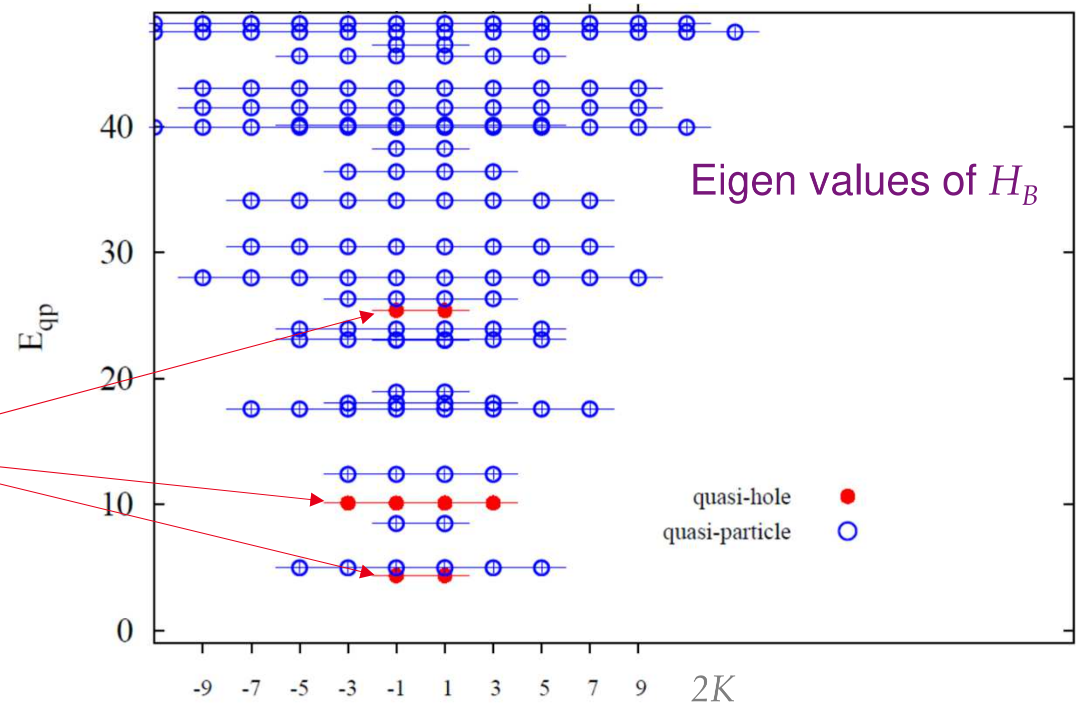

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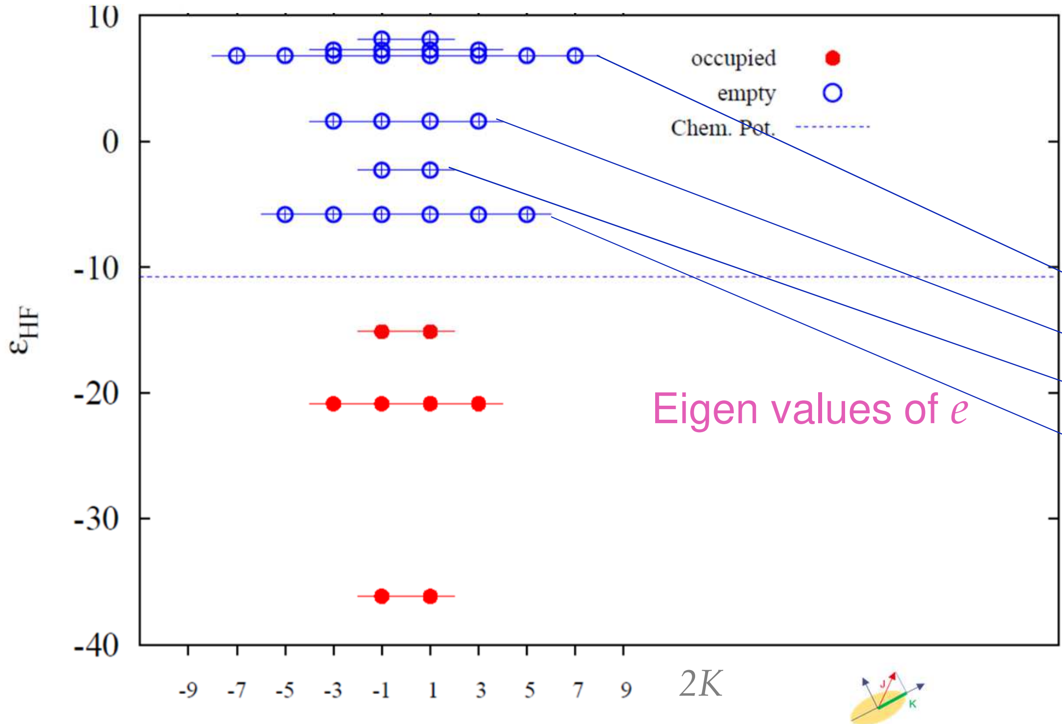

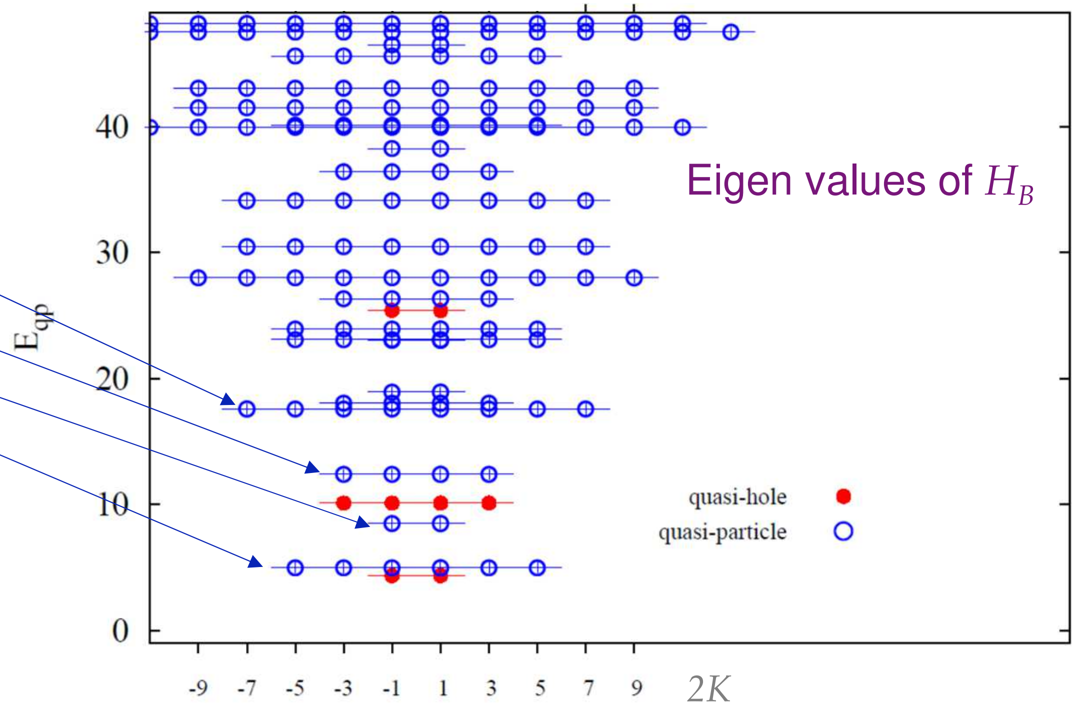

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HFB neutron single particle levels for ^{18}O

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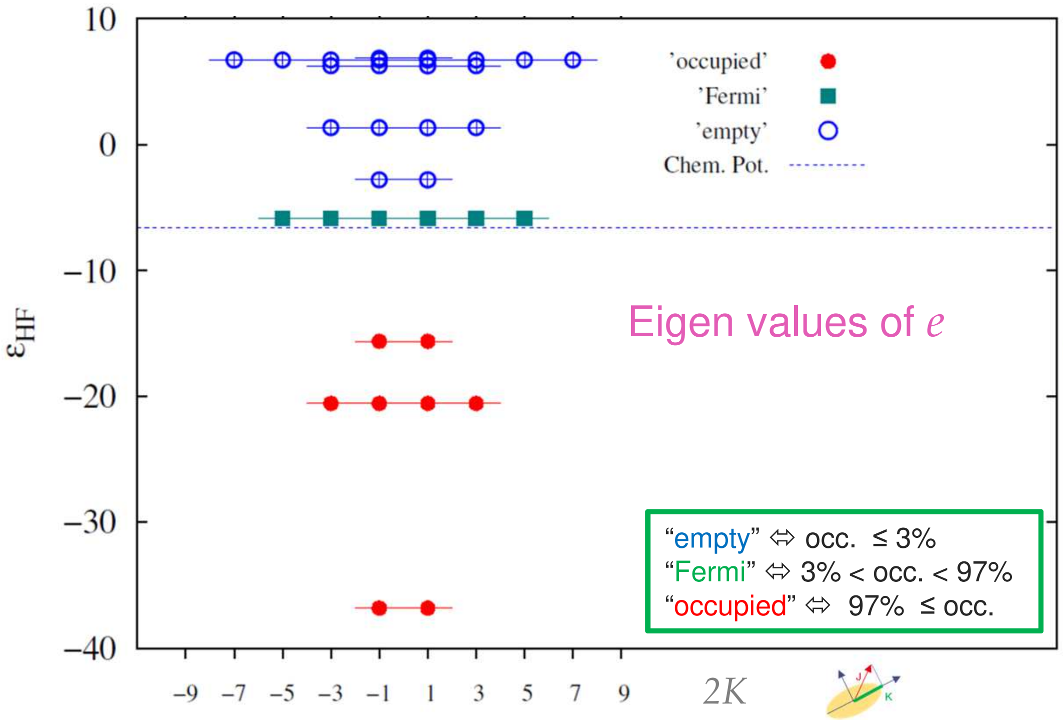

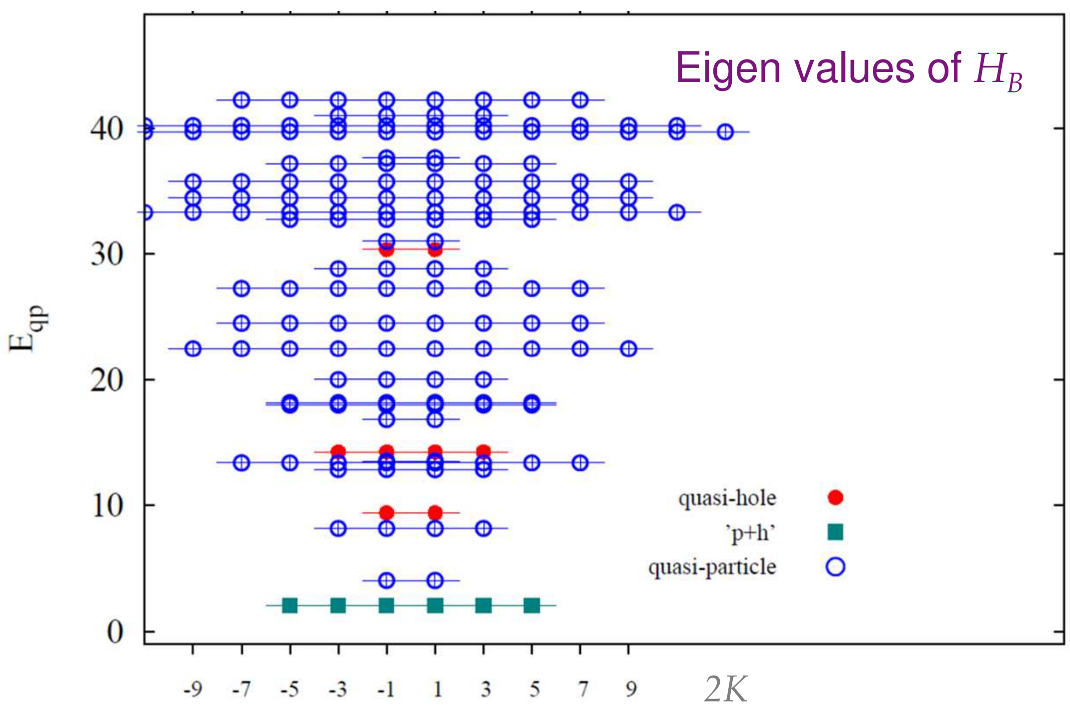

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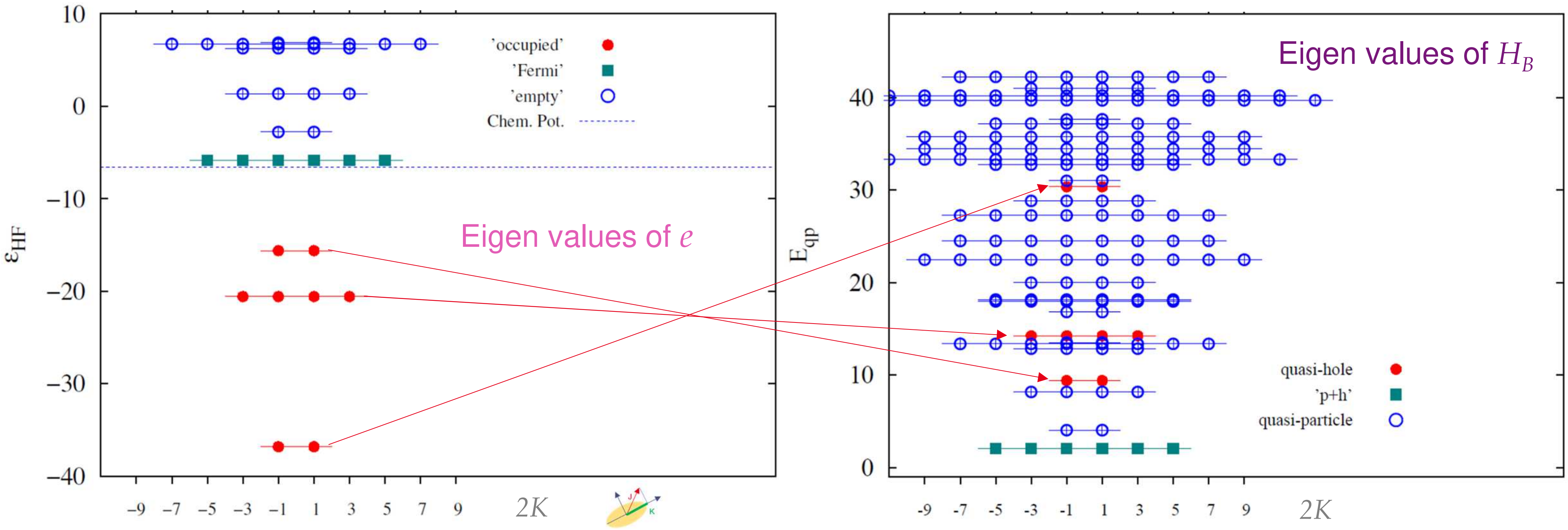

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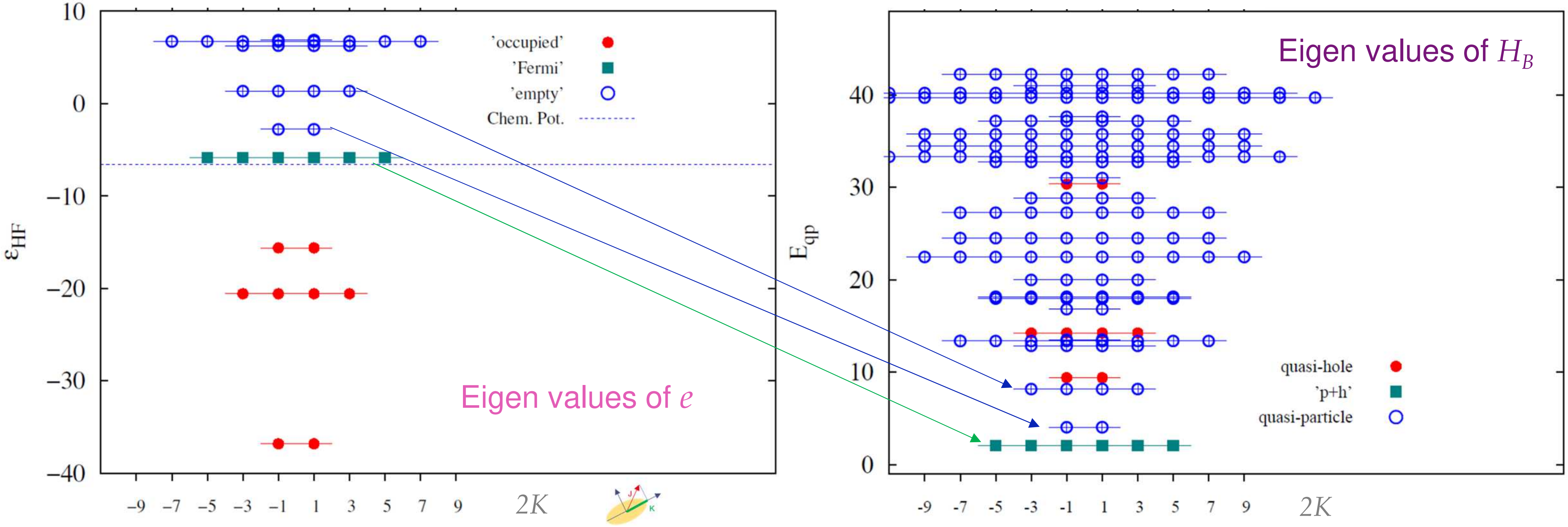

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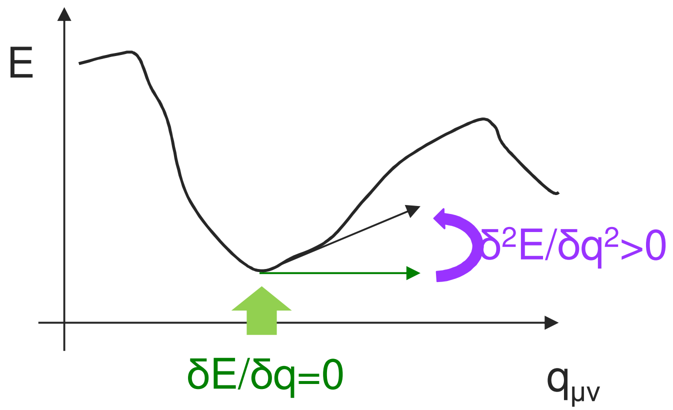
What is the standard QRPA approach ?

The (Q)RPA methods describe nuclear excited states for all multipoles and both parities whatever the intrinsic deformation of the ground state.

No rotational motion included even for deformed nuclei !

Main approximation:
Linear response, i.e. harmonic potential approximation



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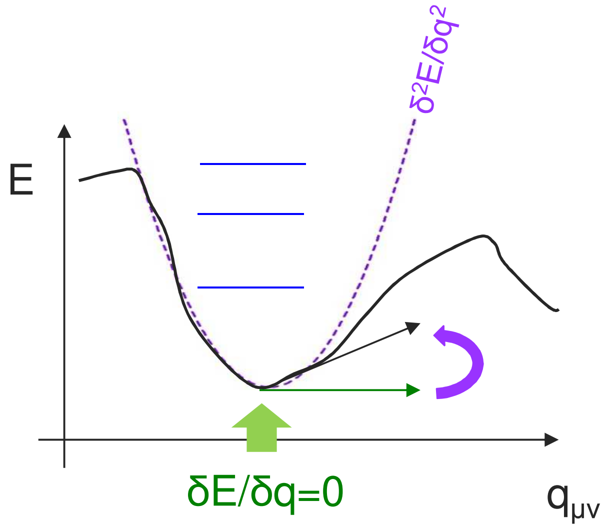

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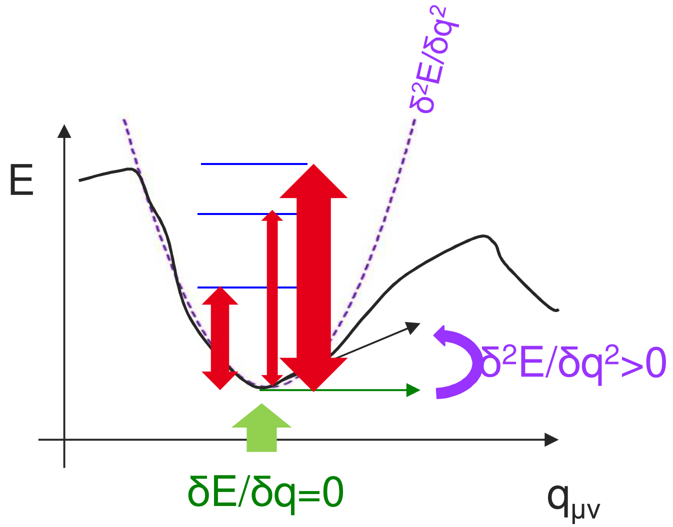

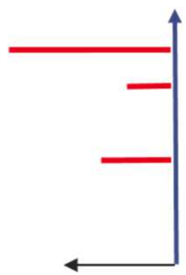

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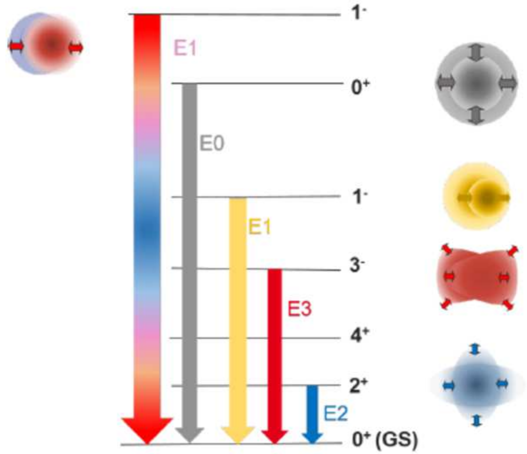
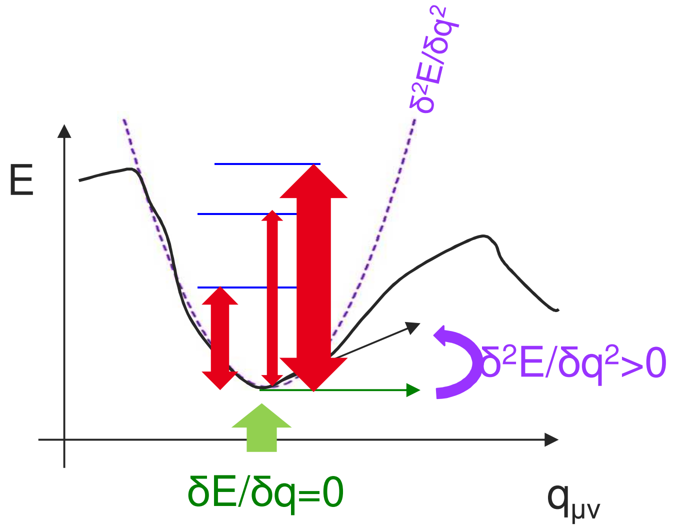
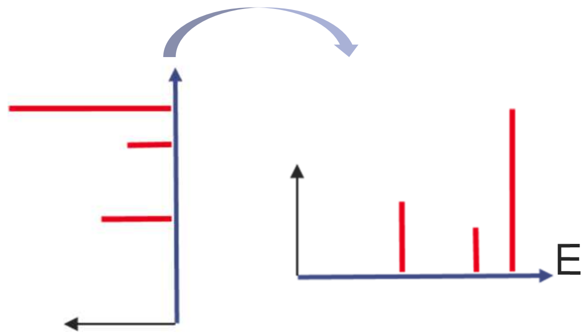
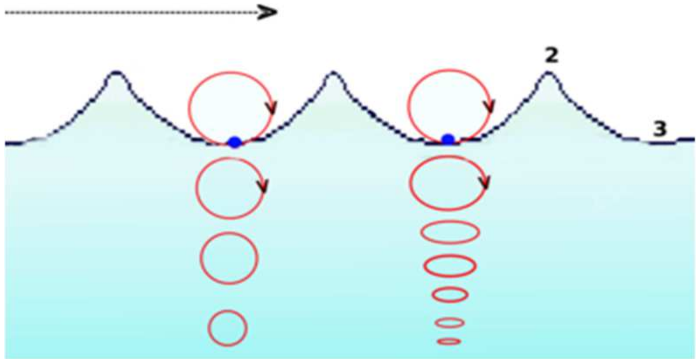


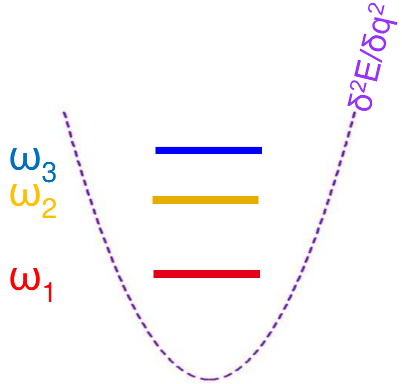
S. Péru. *et al*,
EPJ Web of Conferences **322**,06003(2025),CNR*24





The QRPA approaches :
collectivity and single particles excitations.





$$\theta_3^+ = \sum_{ij} X_{ij}^3 \beta_i^+ \beta_j^+ + \sum_{ij} Y_{ij}^3 \beta_j \beta_i$$

$$\theta_2^+ = \sum_{ij} X_{ij}^2 \beta_i^+ \beta_j^+ + \sum_{ij} Y_{ij}^2 \beta_j \beta_i$$

$$\theta_1^+ = \sum_{ij} X_{ij}^1 \beta_i^+ \beta_j^+ + \sum_{ij} Y_{ij}^1 \beta_j \beta_i$$

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

(Q)RPA equations

$$F\left(\rho,\kappa\right)=\sum_{\alpha\beta}\ t_{\alpha\beta}\rho_{\beta\alpha}+\frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\mathcal{V}(\rho)|\widetilde{\gamma\delta}\rangle\rho_{\gamma\alpha}\rho_{\delta\beta}+\frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\mathcal{V}(\rho)|\widetilde{\gamma\delta}\rangle\kappa^*_{\beta\alpha}\kappa_{\gamma\delta}$$

$$\delta F_2=\frac{1}{2}\sum_{\alpha\beta}\left[\delta\rho_{\alpha\beta}\sum_{\gamma\delta}\left(V^{CM}_{\beta\alpha,\delta\gamma}\delta\rho_{\gamma\delta}+V^{M}_{\beta\alpha,\delta\gamma}\delta\kappa_{\gamma\delta}\right)+\delta\kappa_{\alpha\beta}\sum_{\gamma\delta}\left(V^{M*}_{\beta\alpha,\delta\gamma}\delta\rho_{\gamma\delta}+V^{P}_{\beta\alpha,\delta\gamma}\delta\kappa_{\gamma\delta}\right)\right]$$

$$V^{CM}_{\beta\alpha,\gamma\delta}=\frac{1+\delta_{\alpha\beta}}{2}\frac{1+\delta_{\gamma\delta}}{2}\frac{\partial^2F}{\partial\rho_{\alpha\beta}\partial\rho_{\gamma\delta}}$$

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$$V^{P}_{\beta\alpha,\gamma\delta}=\frac{1+\delta_{\alpha\beta}}{2}\frac{1+\delta_{\gamma\delta}}{2}\frac{\partial^2F}{\partial\kappa_{\alpha\beta}\partial\kappa_{\gamma\delta}}$$

$$A_{ph,p'h'}=(\epsilon_p-\epsilon_h)\delta_{pp'}\delta_{hh'}+\frac{\partial^2F}{\partial\rho_{hp}\partial\rho_{p'h'}}$$

$$B_{ph,p'h'}=\frac{\partial^2F}{\partial\rho_{hp}\partial\rho_{h'p'}}$$

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

S. Péru, M. Martini, EPJA (2014) 50:88

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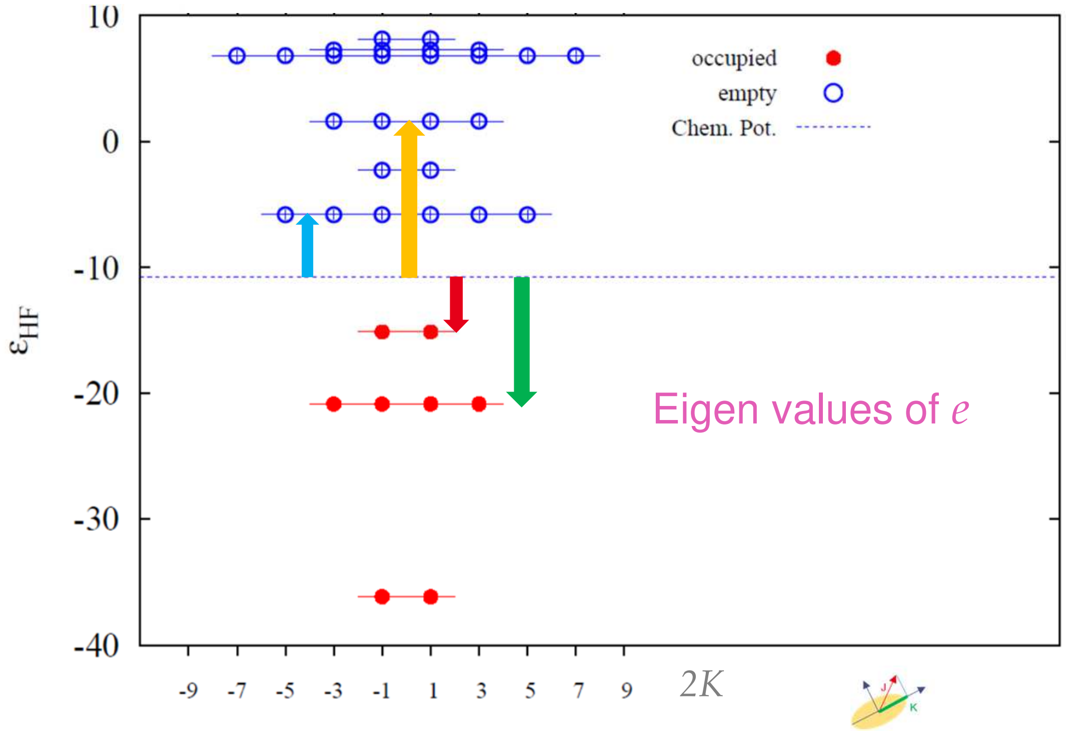

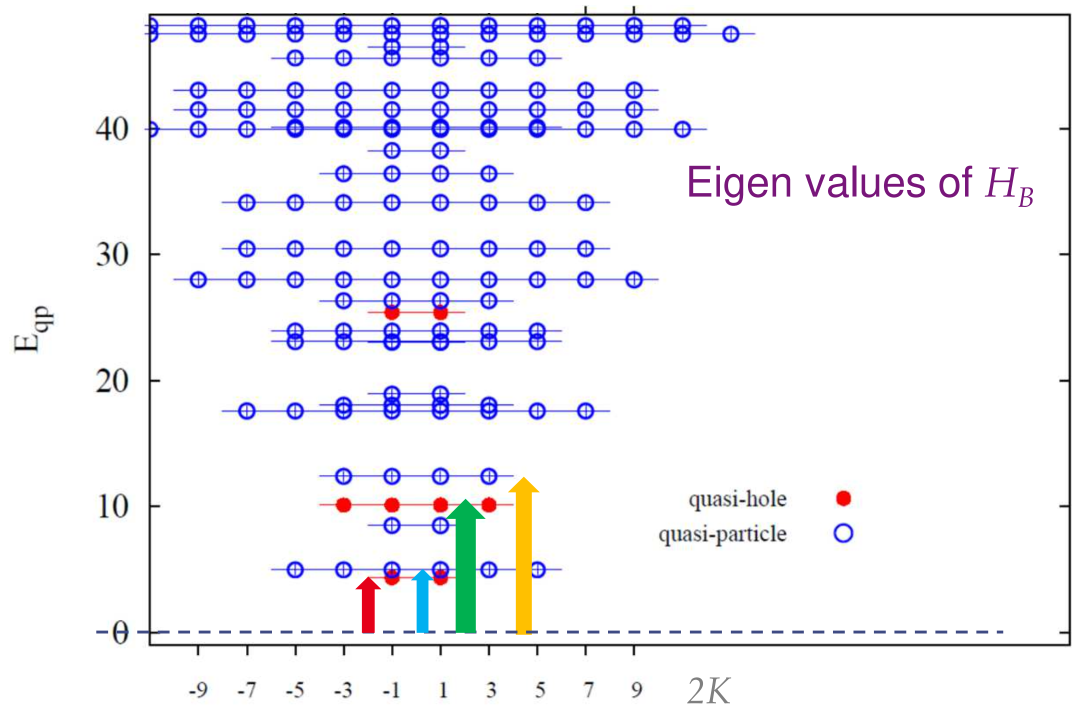

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Sophie Péru, CEA,DAM, DIF, sophie.peru-desenfants@cea.fr

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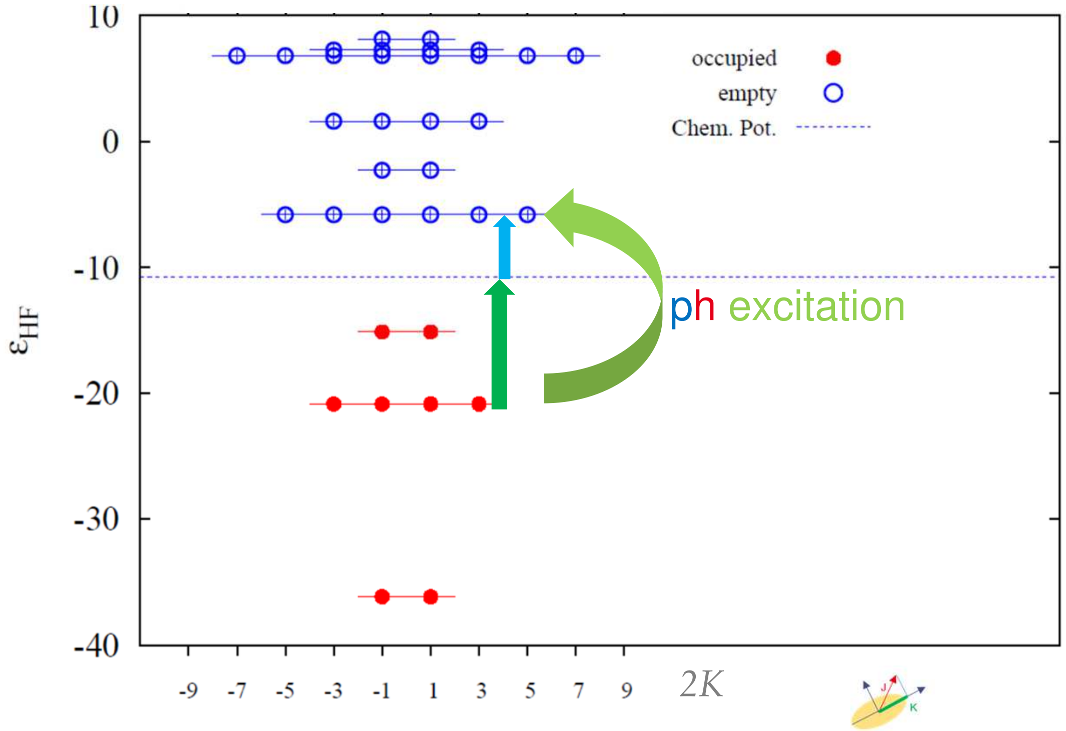

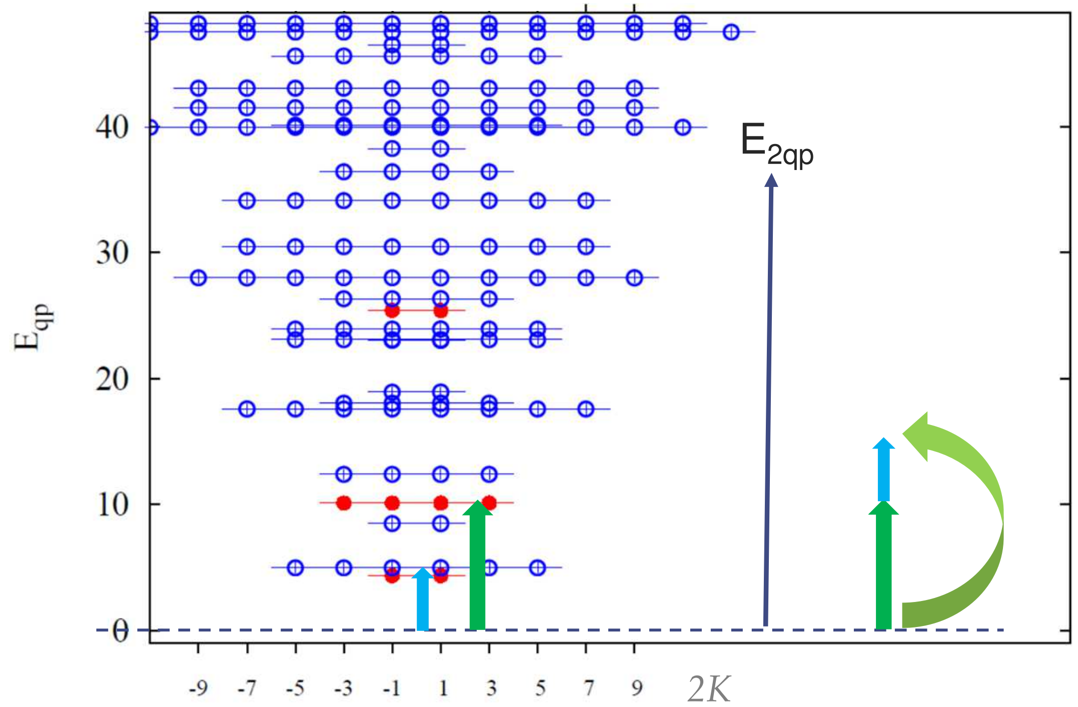

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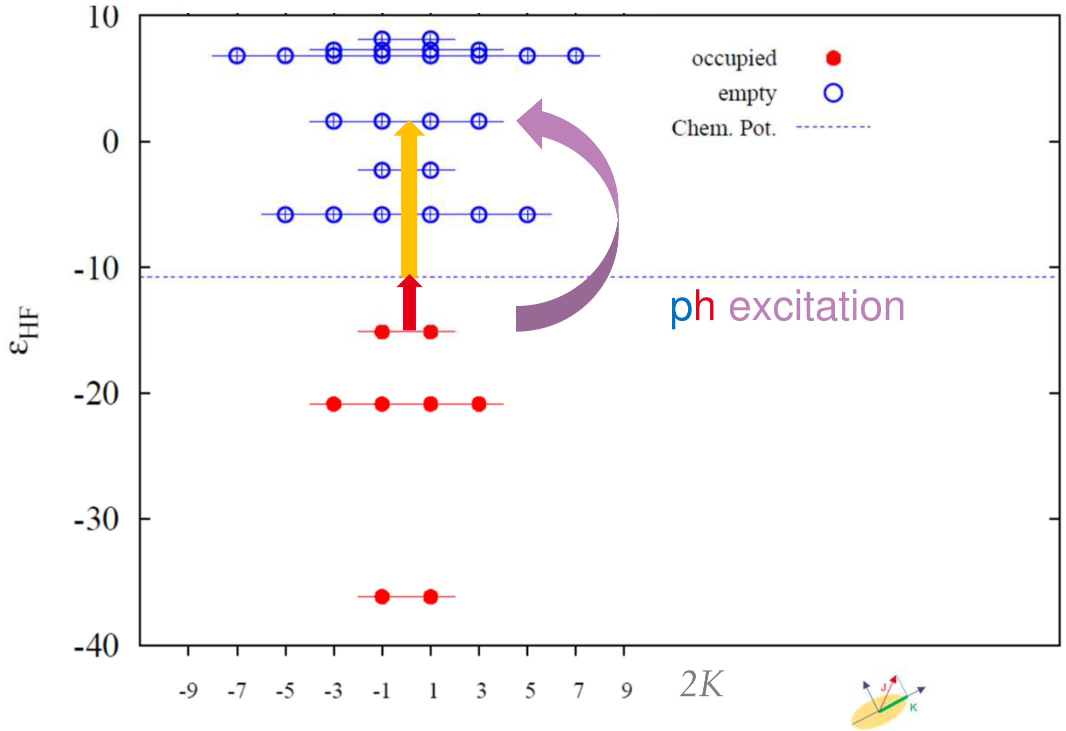

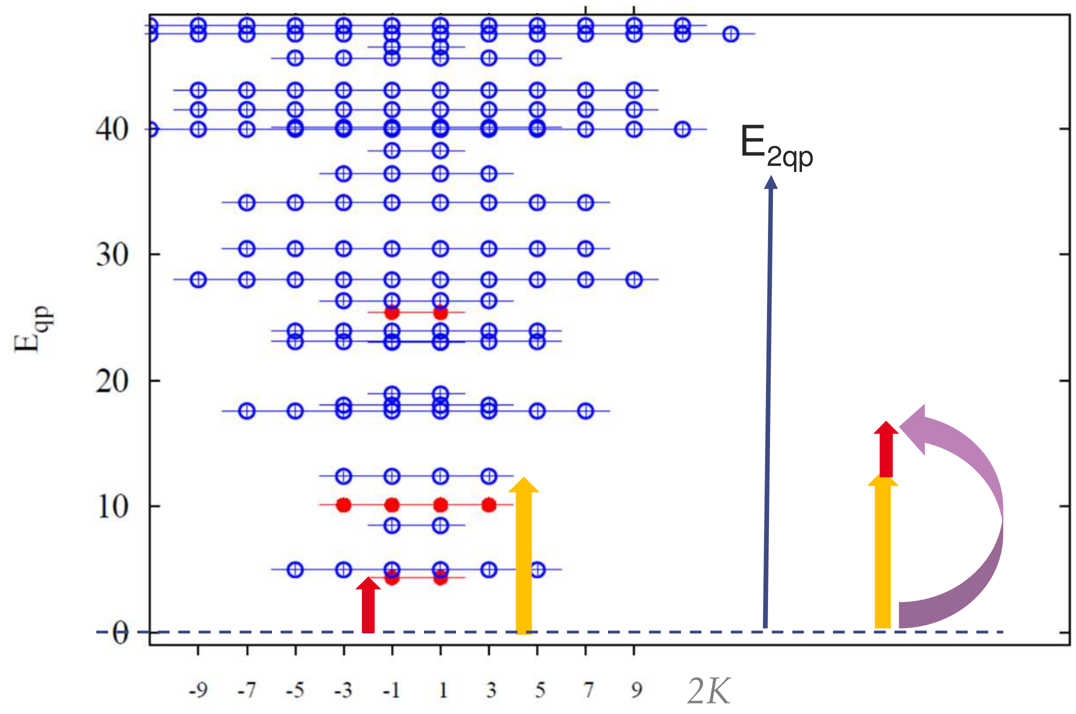

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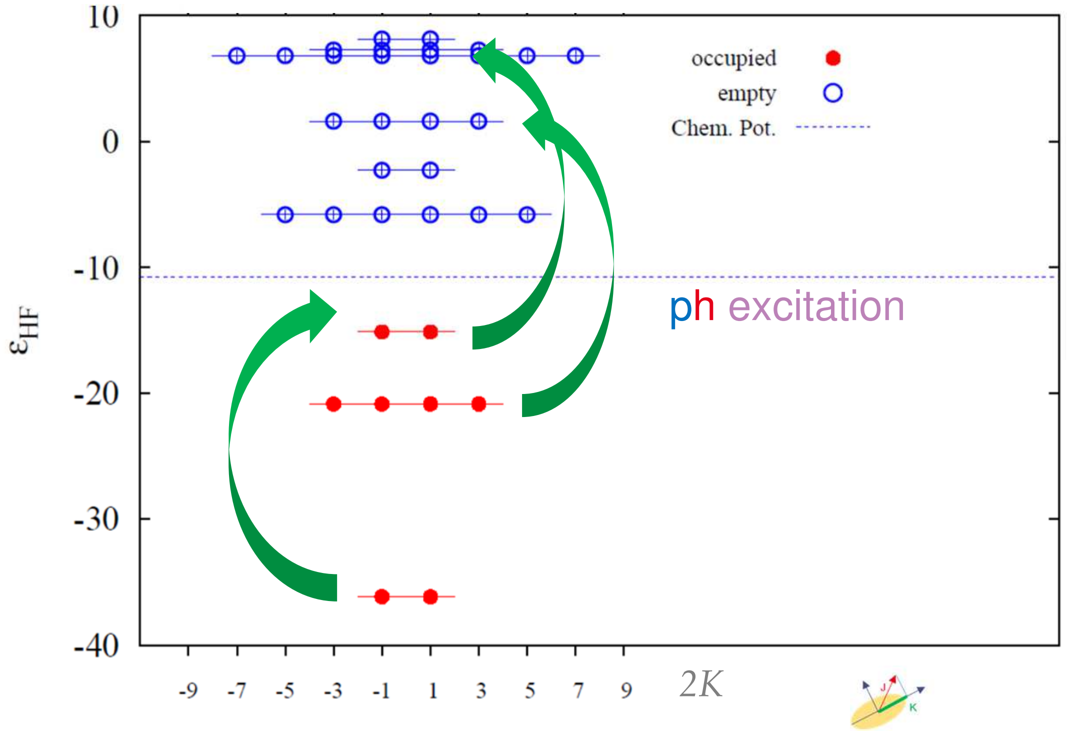

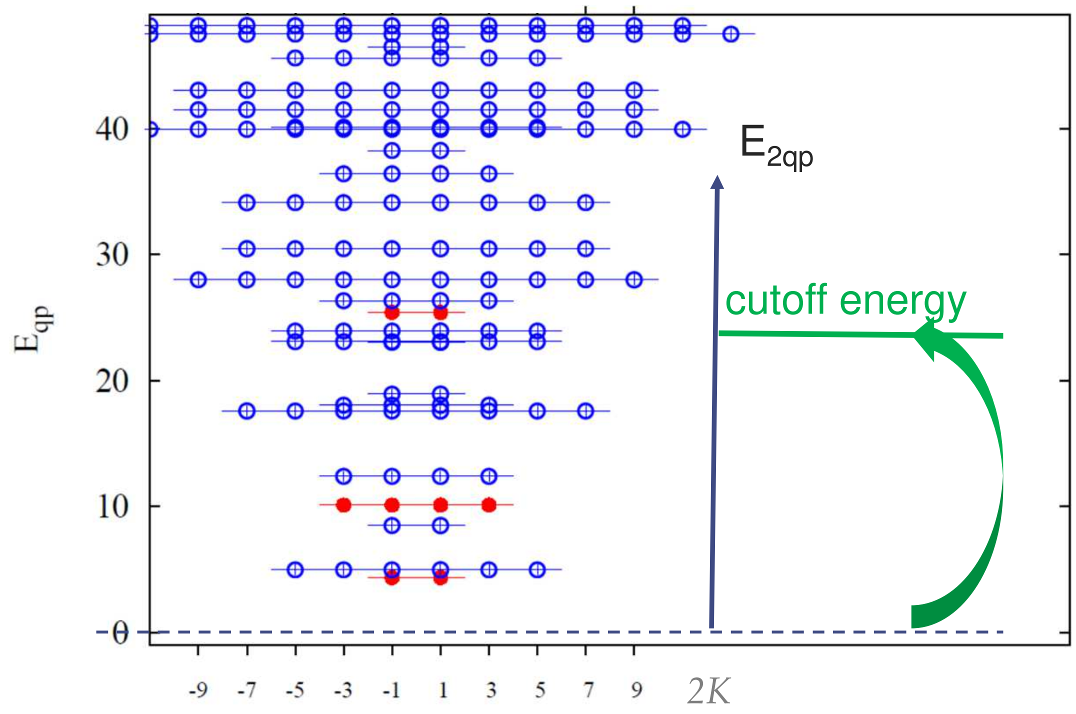

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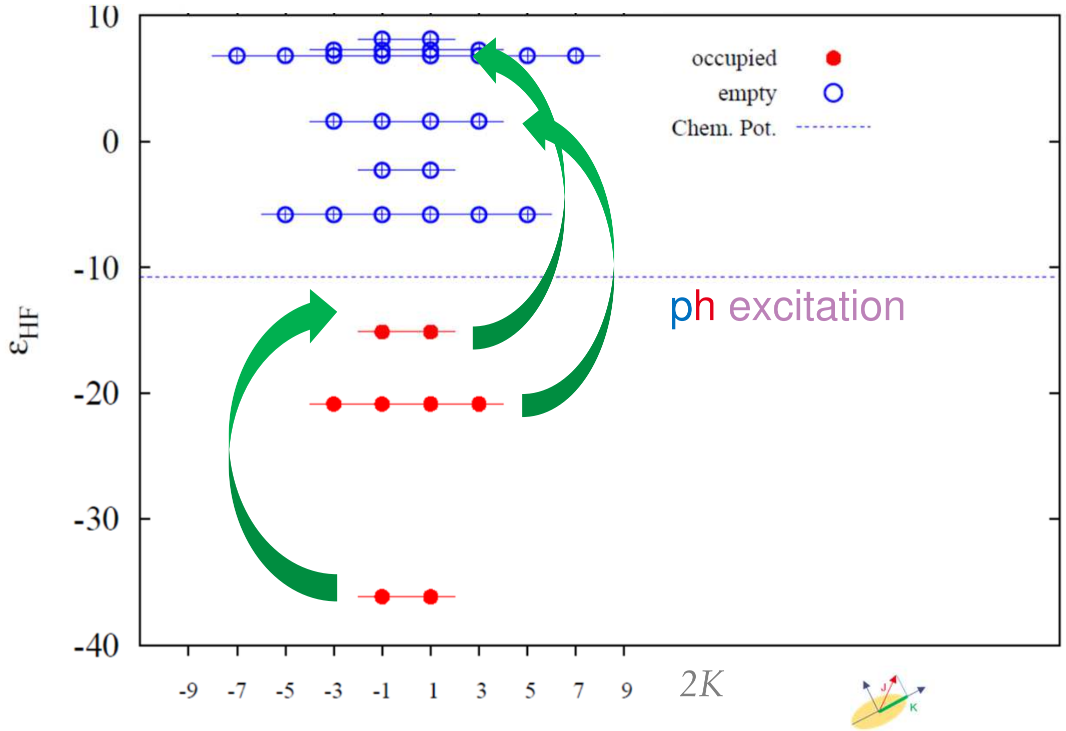

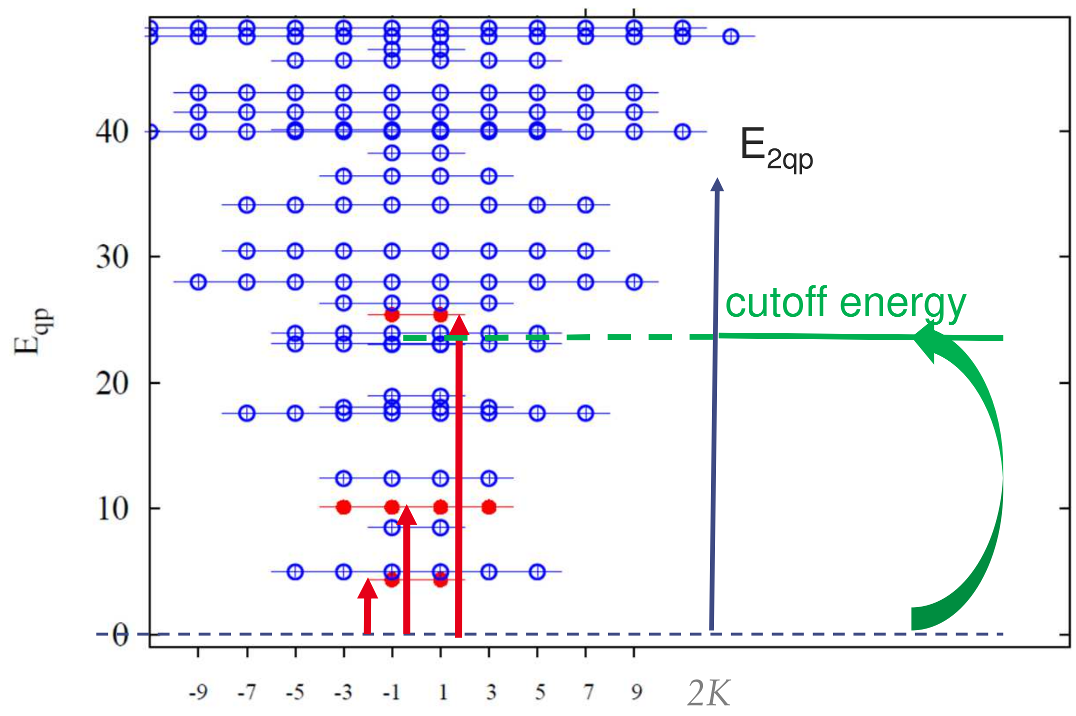

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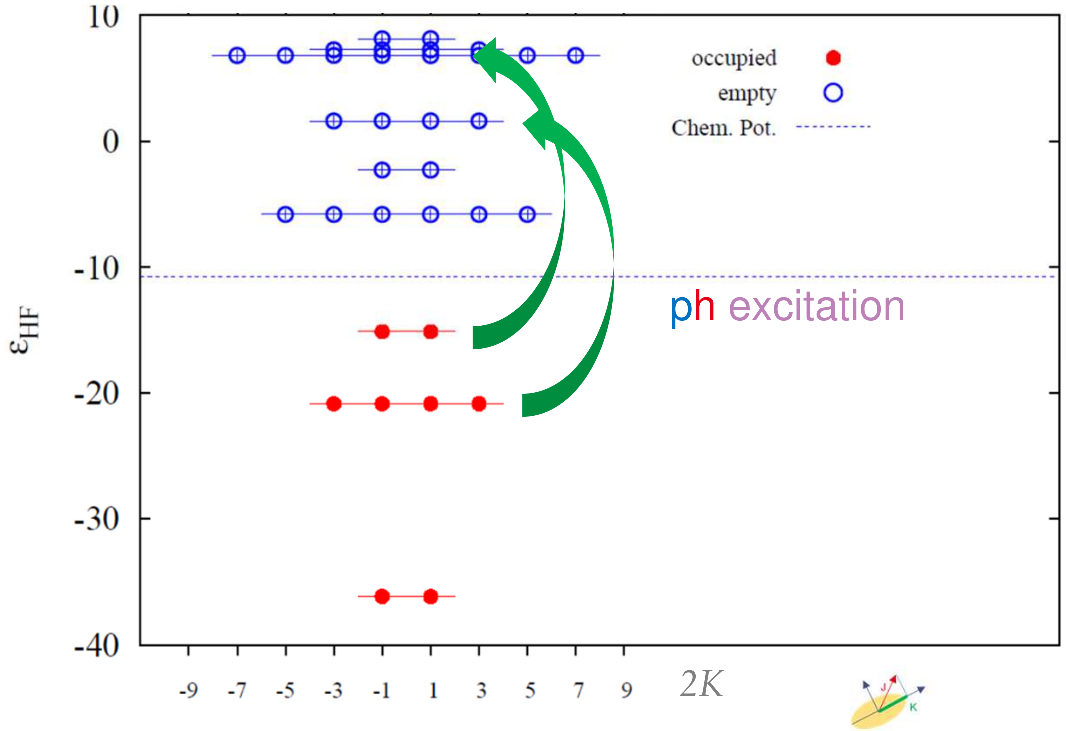

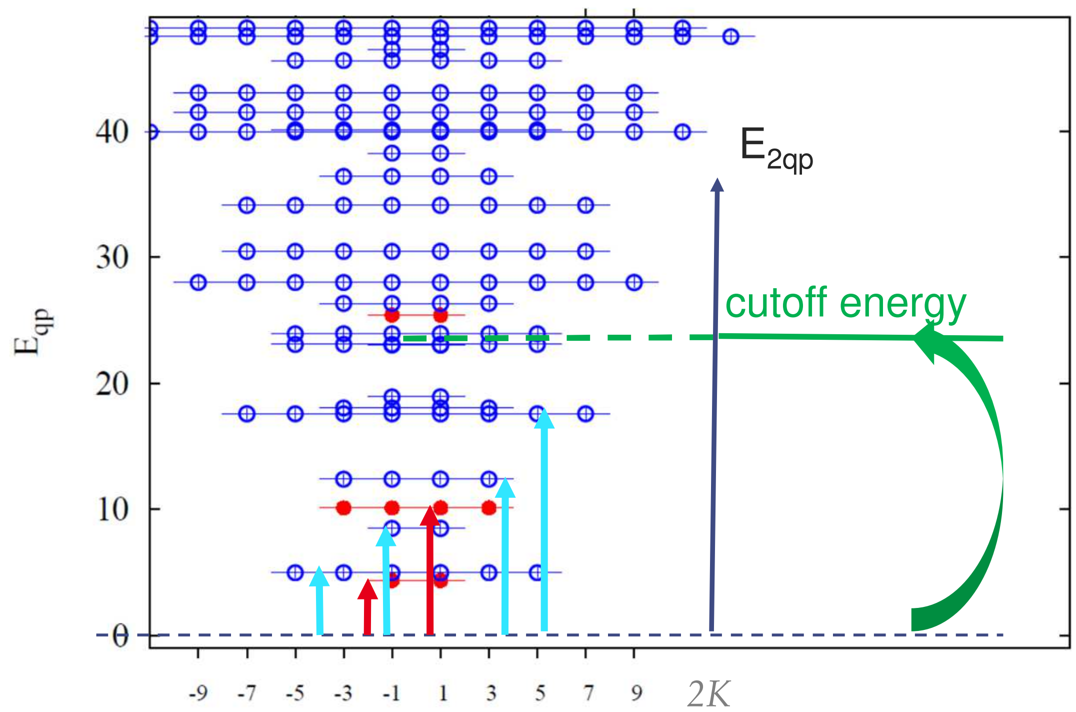

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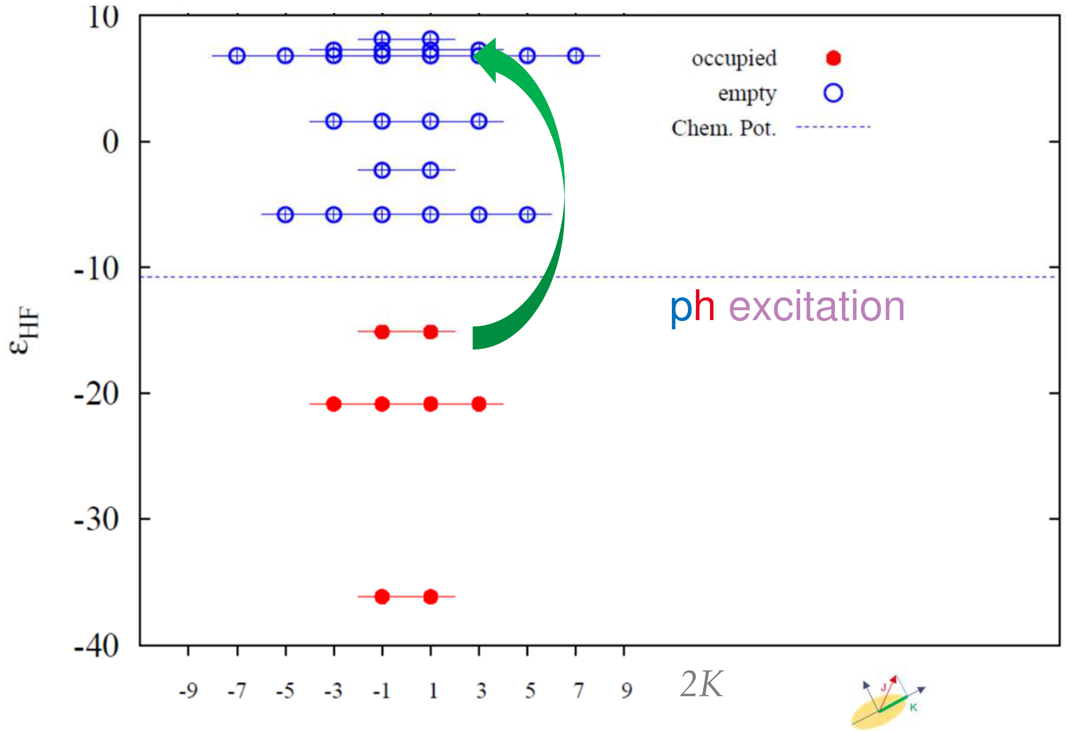

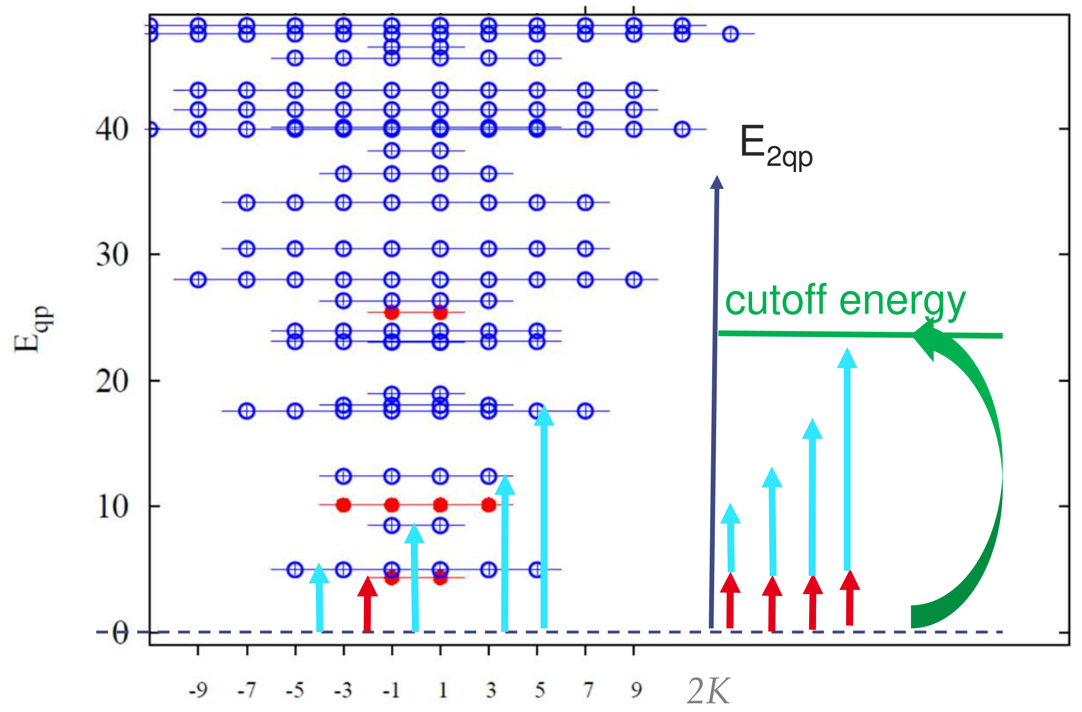

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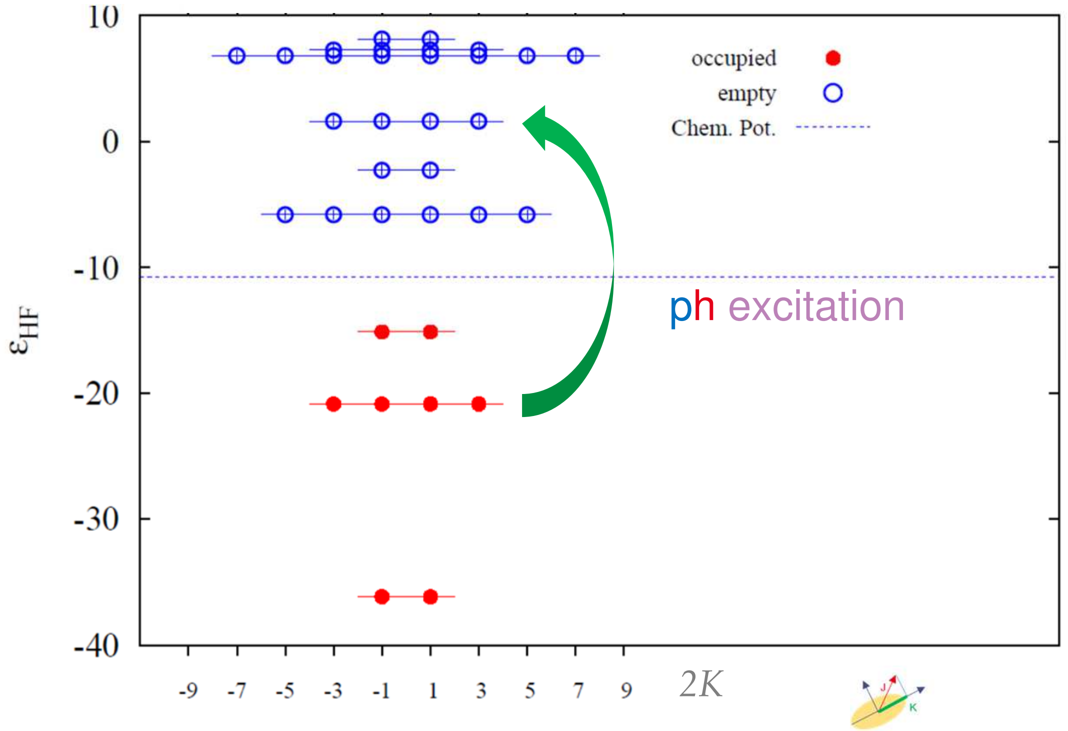

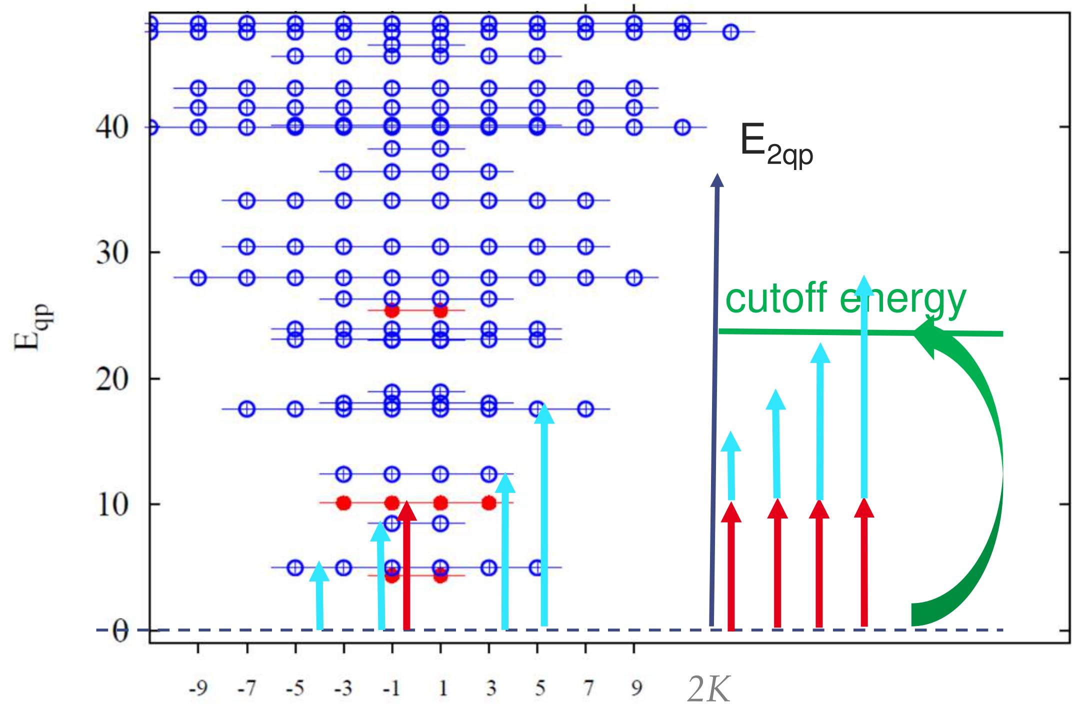

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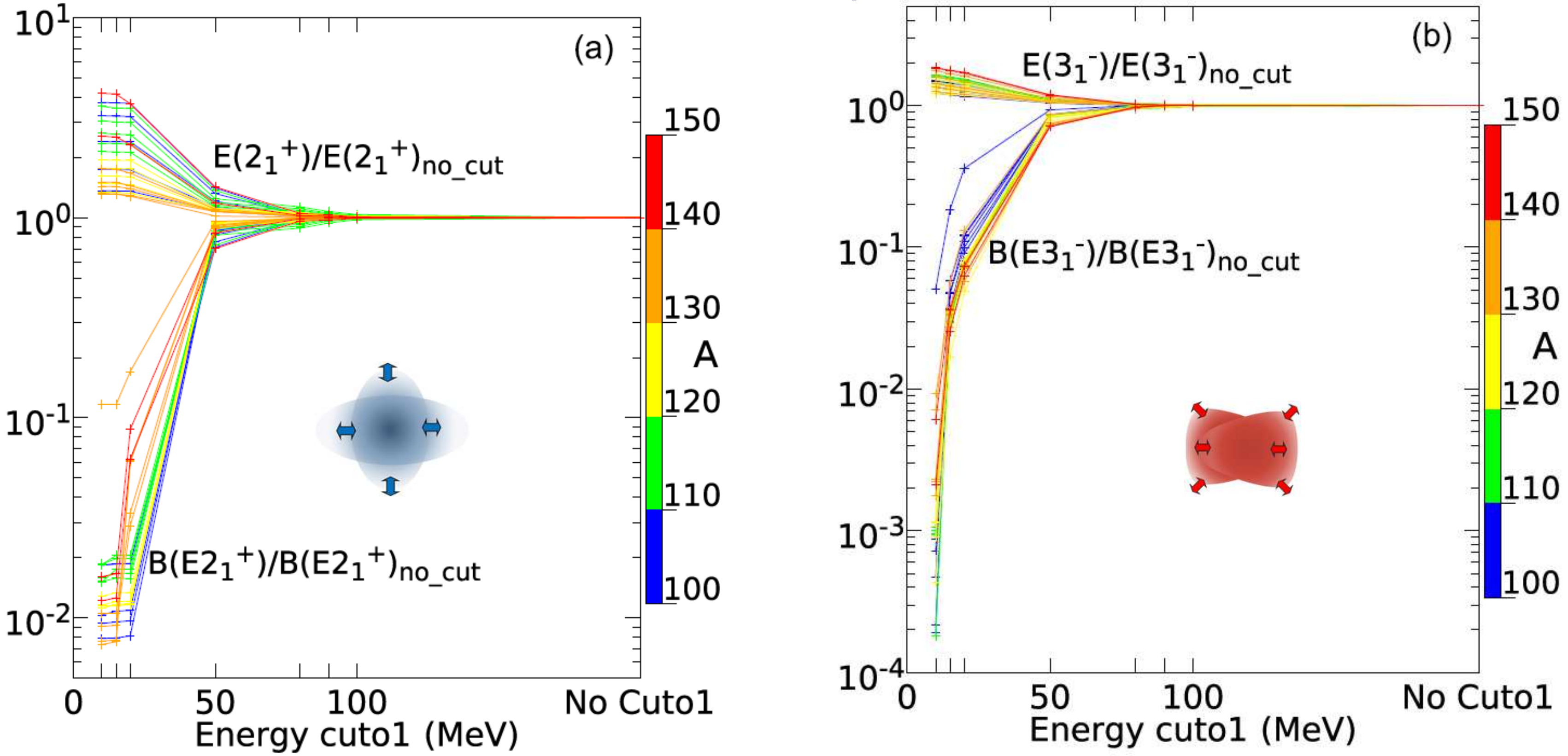
Impact of cutoff energy in 2qp excitation basis

Sn isotopes



F. Lechaftois, I. Deloncle, S. Péru, PRC92,034315 (2015)

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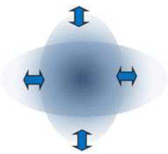
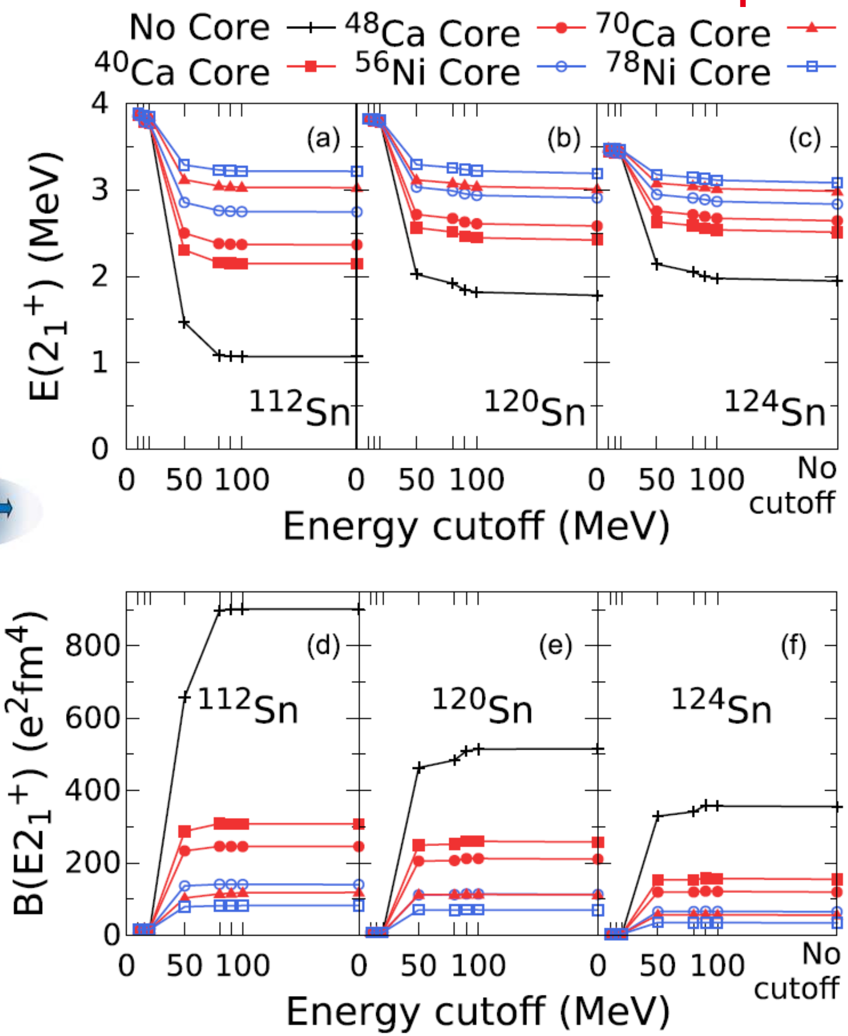
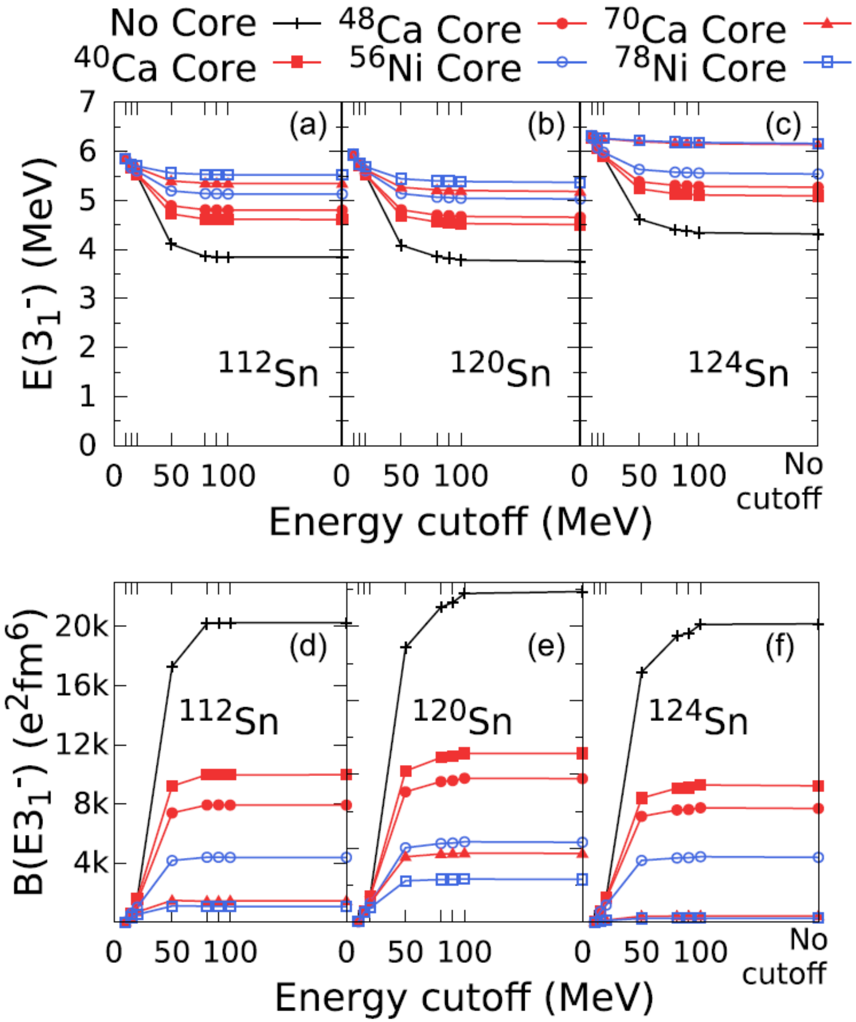
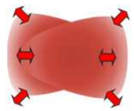
Impact of frozen core



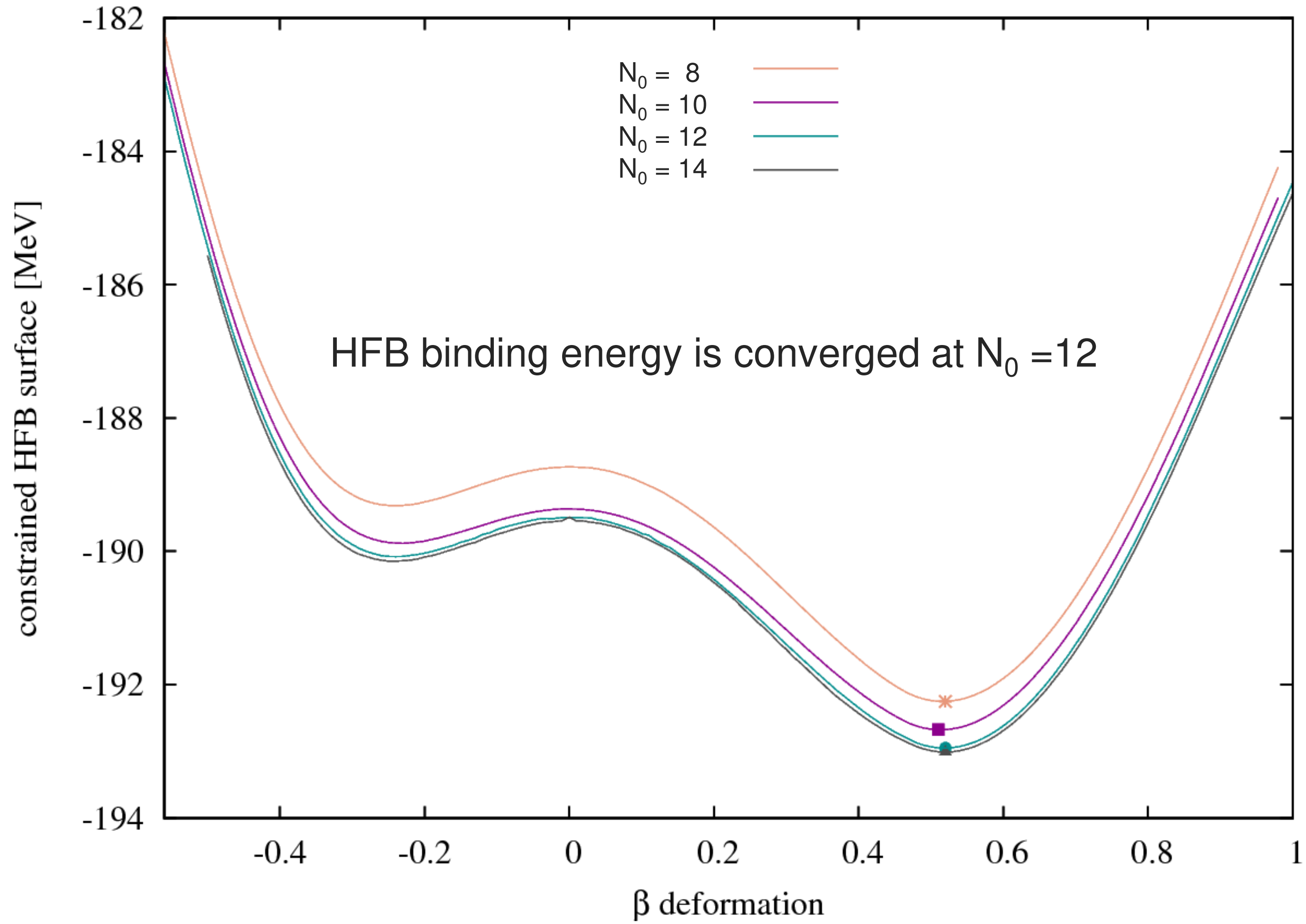






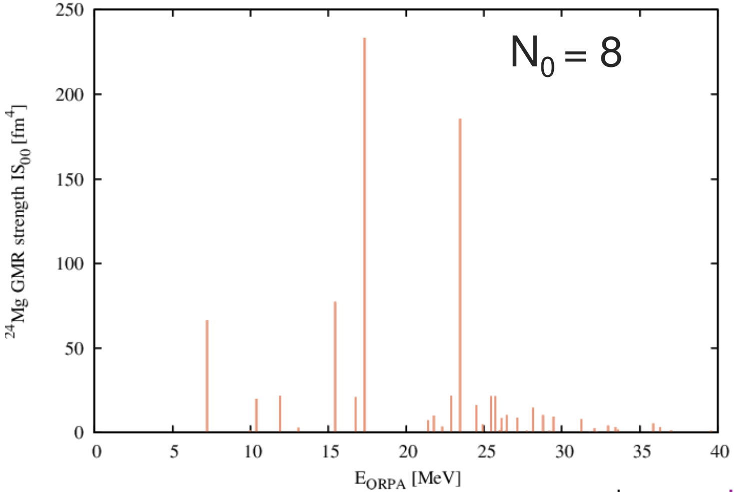
GMR in ^{24}Mg with the D1M interaction: tests on the size of the HO basis

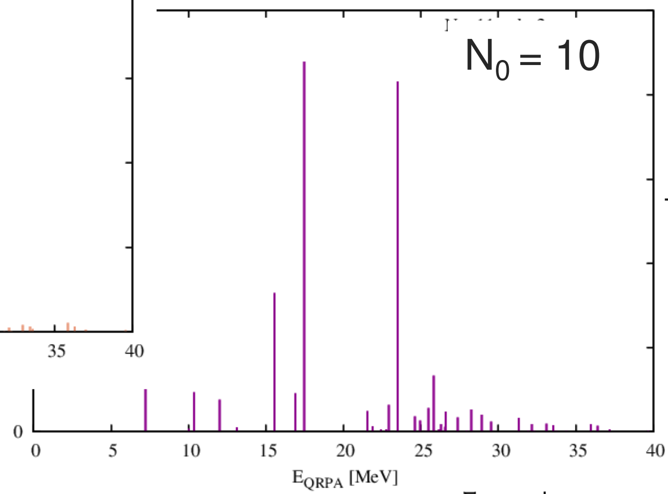
PhD Lysandra Batail, December 2021

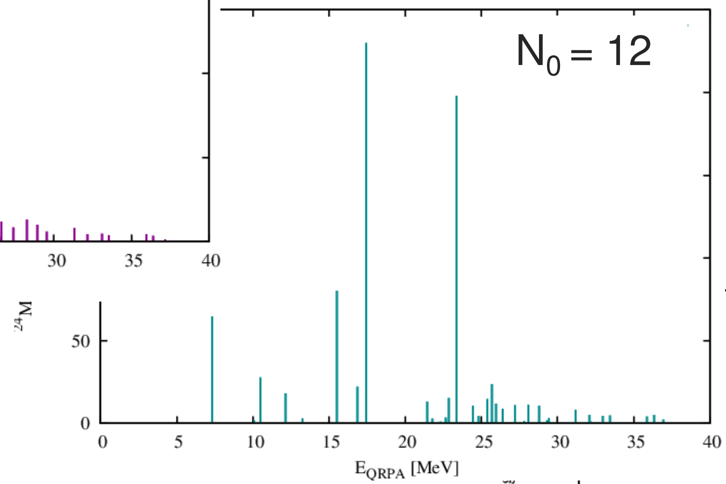


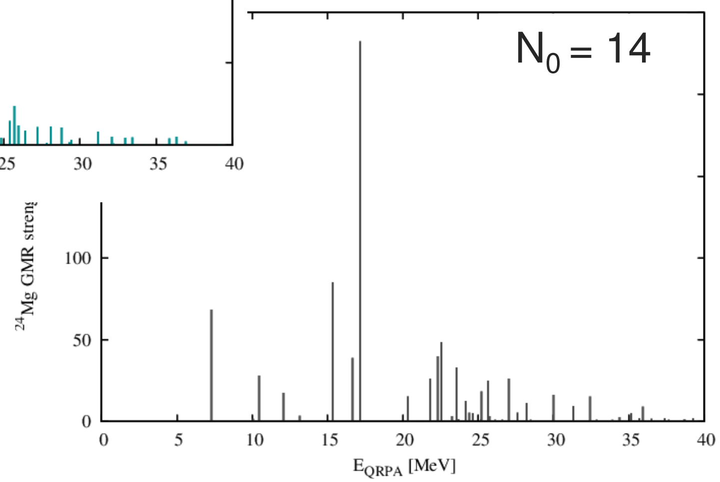
GMR in ^{24}Mg with the D1M interaction: tests on the size of the HO basis

PhD Lysandra Batail, December 2021







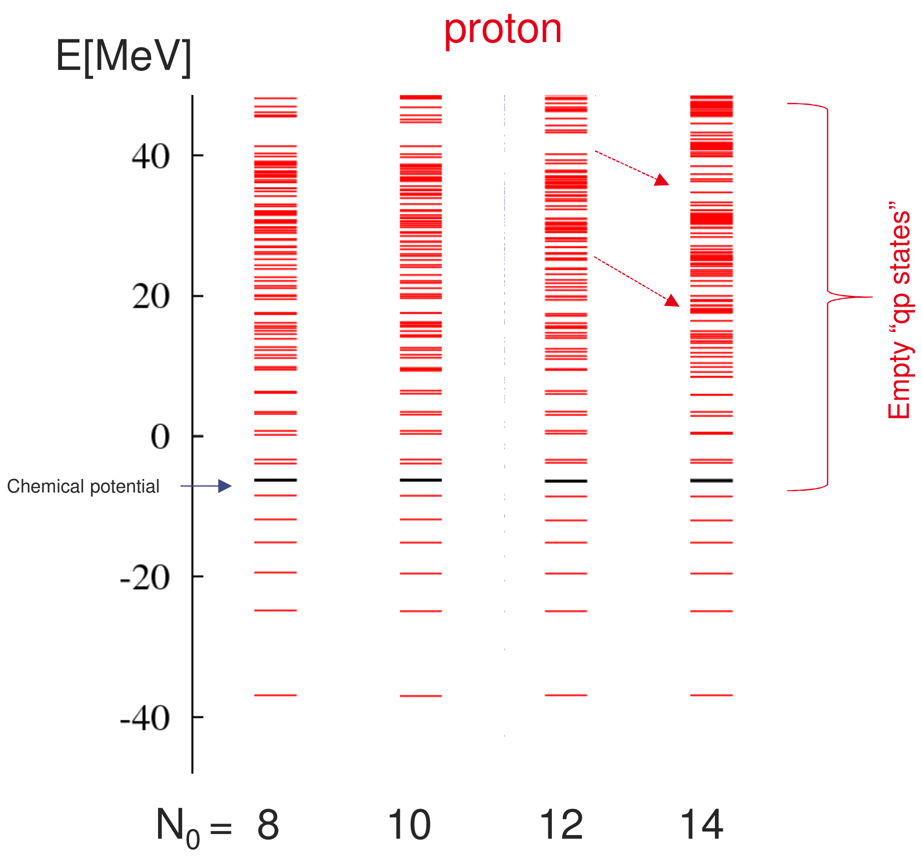


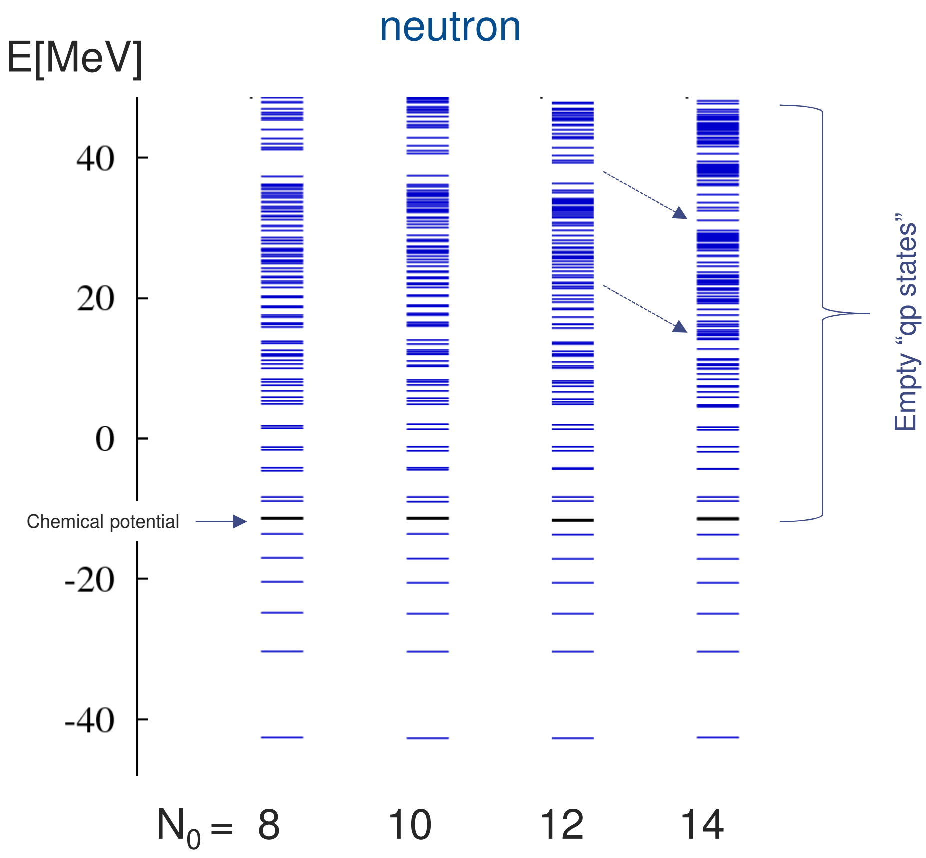
But the monopole strength is not converged at N_0=12!

GMR in ^{24}Mg with the D1M interaction: tests on the size of the HO basis

PhD Lysandra Batail, December 2021

The monopole strength is not converged at N_0=12 because the “empty” qp states are not!





GMR in ^{24}Mg with the D1M interaction: tests on the size of the HO basis

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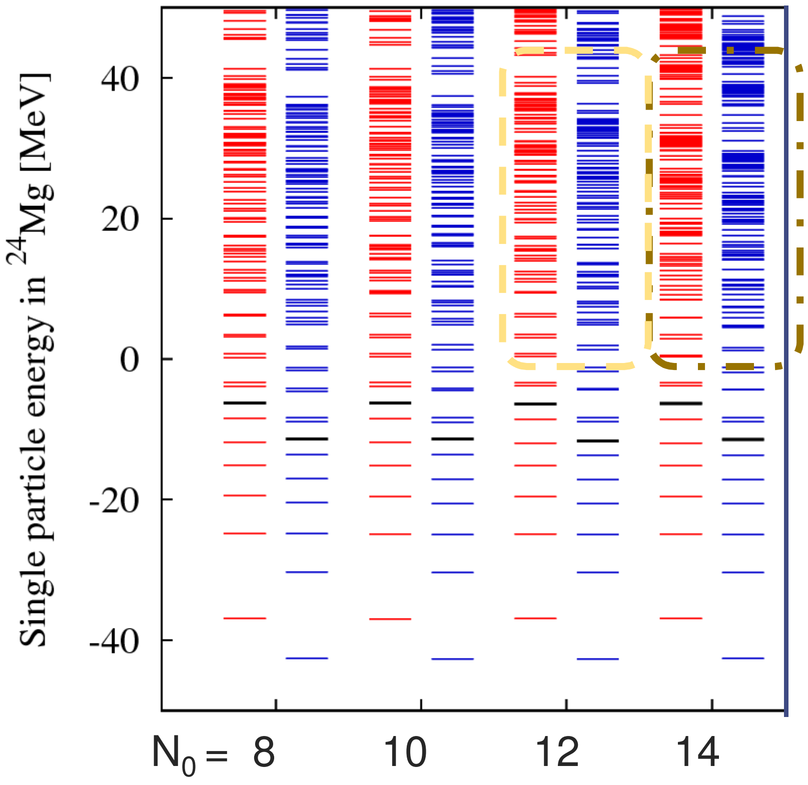
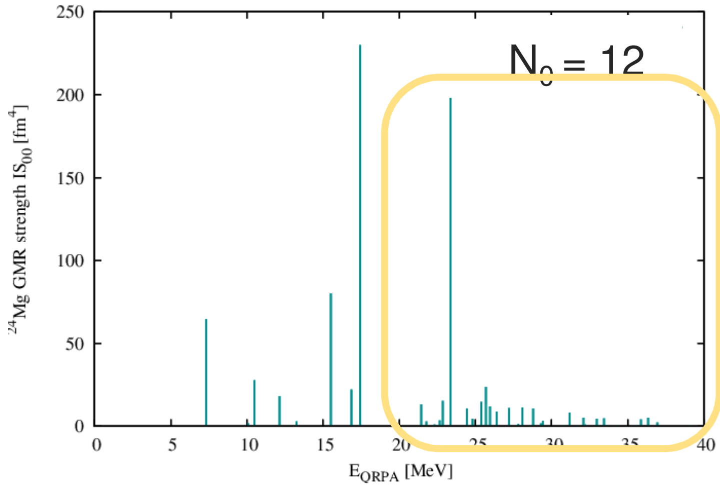
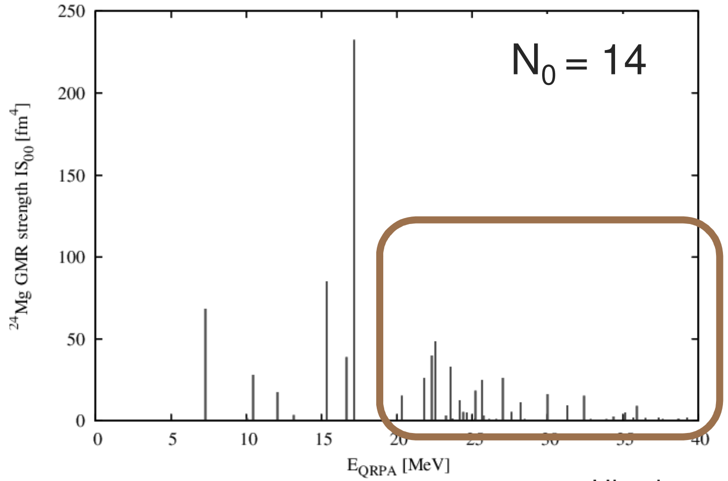


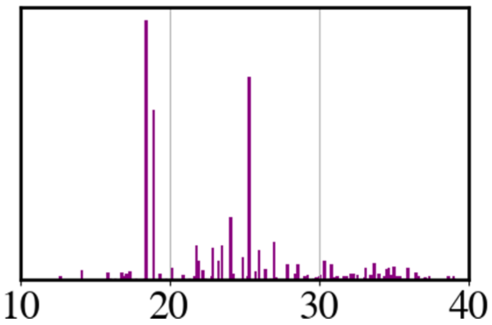




Alternative resolution of QRPA equations

Full matrix filling and diagonalization

Both excitations energies and phonon wave functions are obtained as eigenvalues and eigenvectors.



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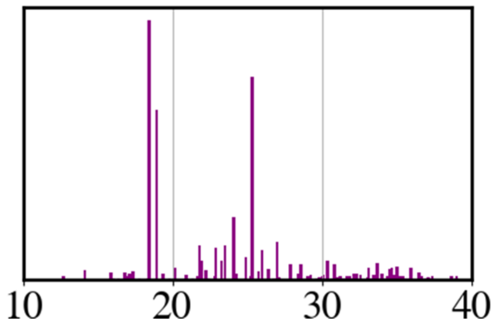
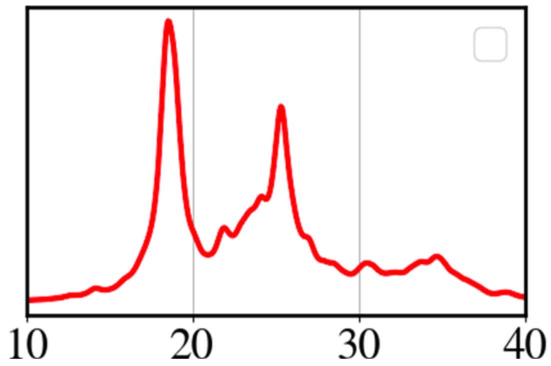


Finite amplitude method (FAM) :

Self-consistent Iterative process to provide multipolar smoothed response function

Each point of the curve is the solution of one QFAM run



See for example,

Y Beaujeault-Taudière et al Physical ReviewC,107(2):L021302, 2023.

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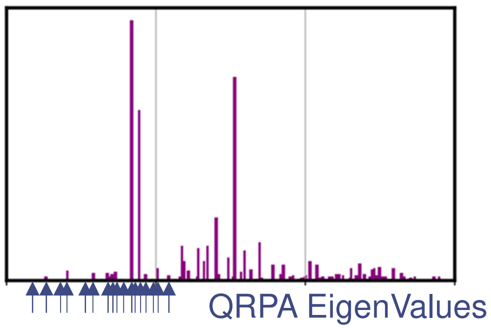

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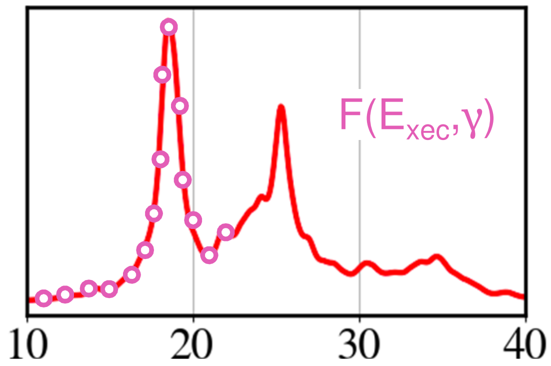

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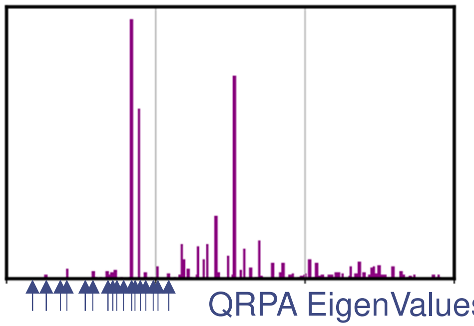

Require optimized codes running on supercomputers
to reduce the “human” computational time
and to share the available cpu memory.

Finite amplitude method (FAM) :
Self-consistent Iterative process to provide multipolar smoothed response function

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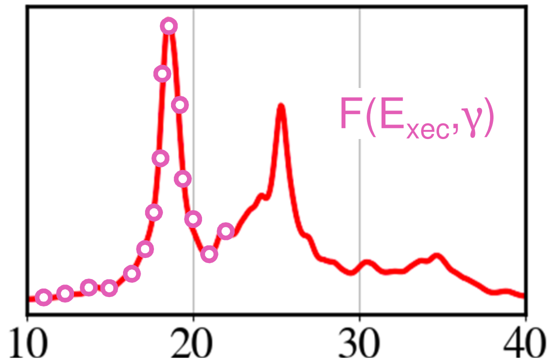


Smearing dependent !
$\omega \to \omega + i\gamma/2$

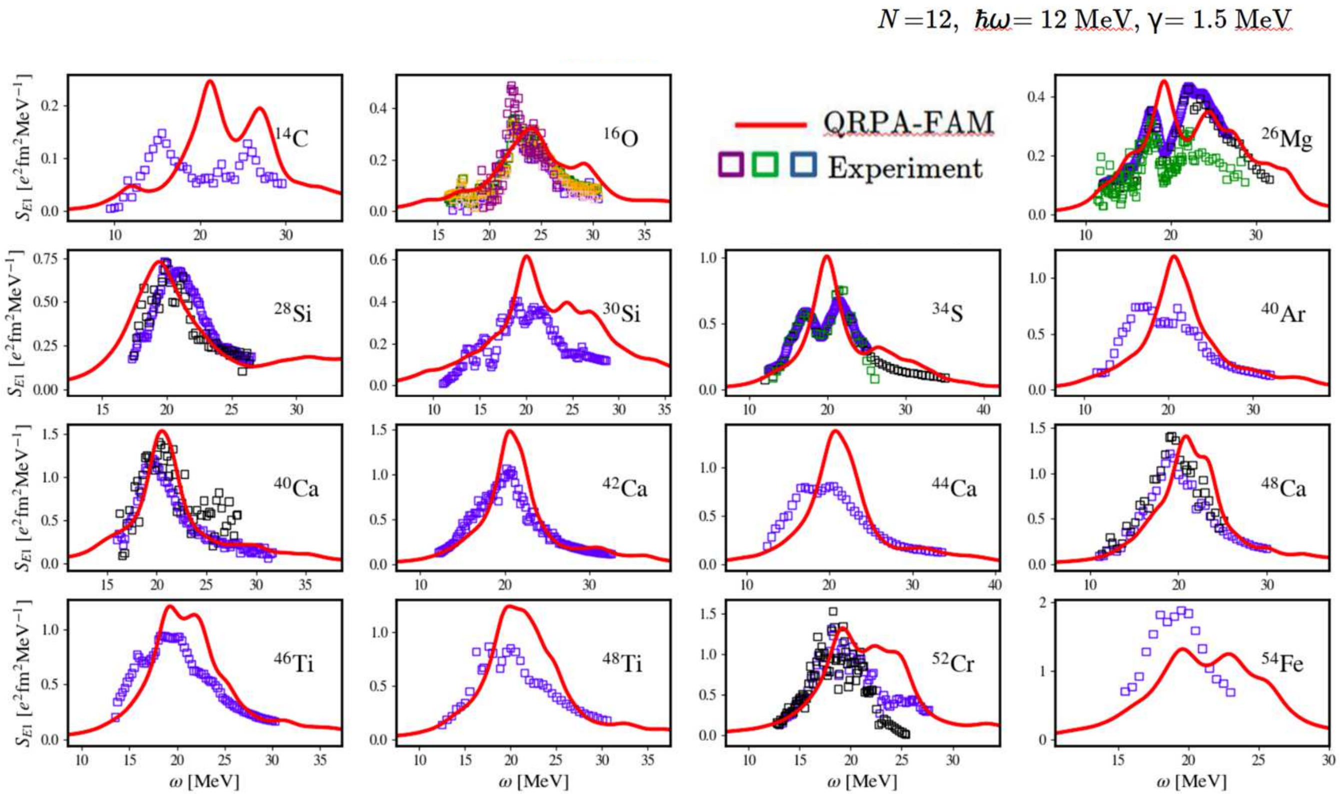
FAST production of multipolar response, but only the response.
Eigen mode wave functions require additional treatment.

See for example,
Y Beaujeault-Taudière et al Physical ReviewC,107(2):L021302, 2023.

“Ab-initio” interaction: Chiral QFAM results

PAN@CEA collaboration

Luis Gonzalez-Miret Zaragoza, PhD Nov2024



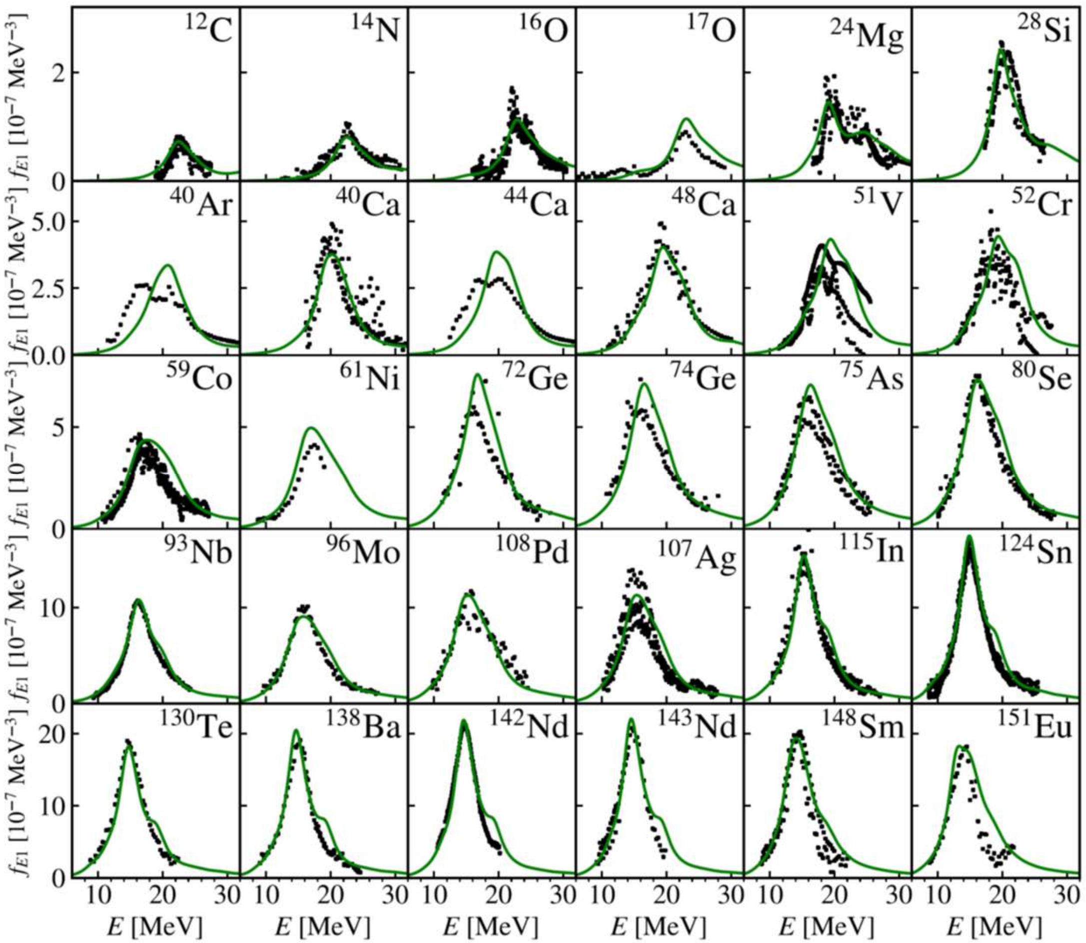
Chiral interaction: Hüther, T., Vobig, K., Hebeler, K., Machleidt, R., & Roth, R. (2020). Family of chiral two-plus three-nucleon interactions for accurate nuclear structure studies. Physics Letters B, 808, 135651.4

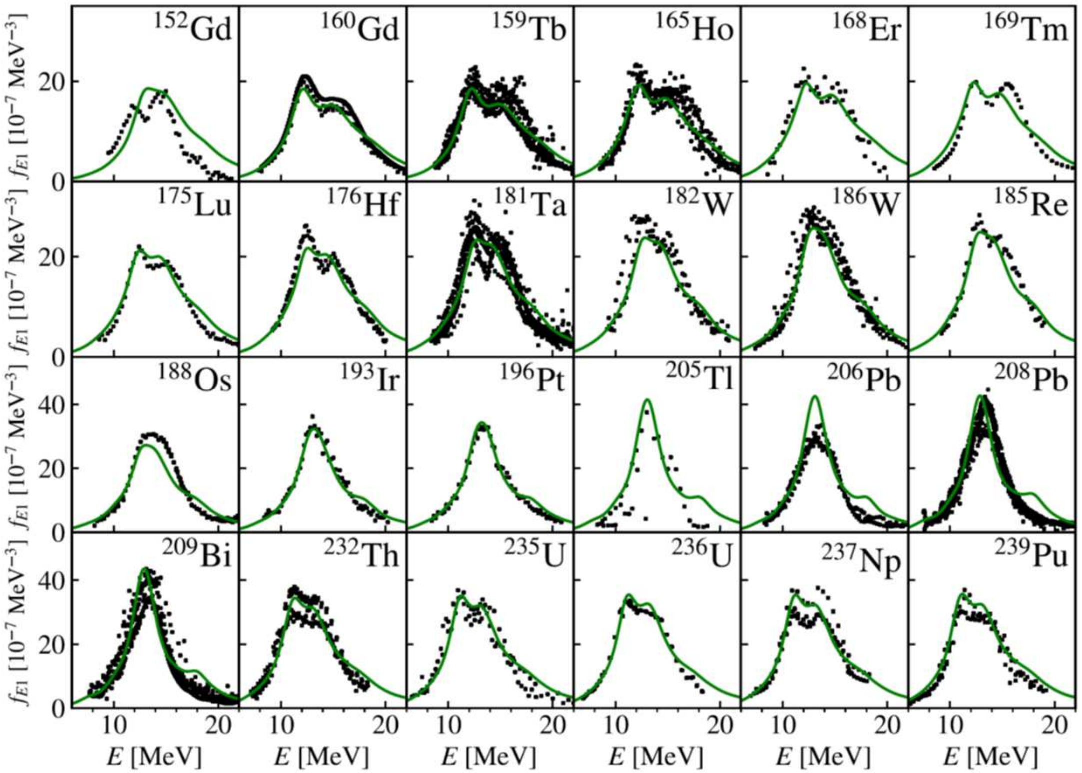
3-body to 2-body reduction method: Frosini, M., Duguet, T., Bally, B., Beaujeault-Taudière, Y., Ebran, J. P., & Somà, V. (2021). In-medium k-body reduction of n-body operators: A flexible symmetry-conserving approach based on the sole one-body density matrix. *The European Physical Journal A*, *57*(4), 151.

E1 photon strength function using a deformed covariant energy density functional approach

L. Gonzalez-Miret Zaragoza et al, PRC 112, 044303 (2025)

RHB +QFAM, DD-PC1 using the program DIRQFAM v2. 0.0 [Bjelčić, A., & Nikšić, T. (2023), *Computer Physics Communications*, *287*, 108689.]





RQFAMz(GLO) $\Delta(A) = \begin{cases} 0.065A - 3.4 \text{ MeV}, & \text{for } A < 60 \\ 0.5 \text{ MeV}, & \text{otherwise.} \end{cases}$

$$G(E, E_n, \Gamma) = \frac{2}{\pi} \frac{\Gamma E^2}{\Gamma^2 E^2 + (E^2 - E_n^2)^2}.$$

(Q)RPA approaches describe all multipolarities and all parities;
(Q)RPA describe low energy states
Some success of D1M QRPA …

Low energy states: Sn isotopes

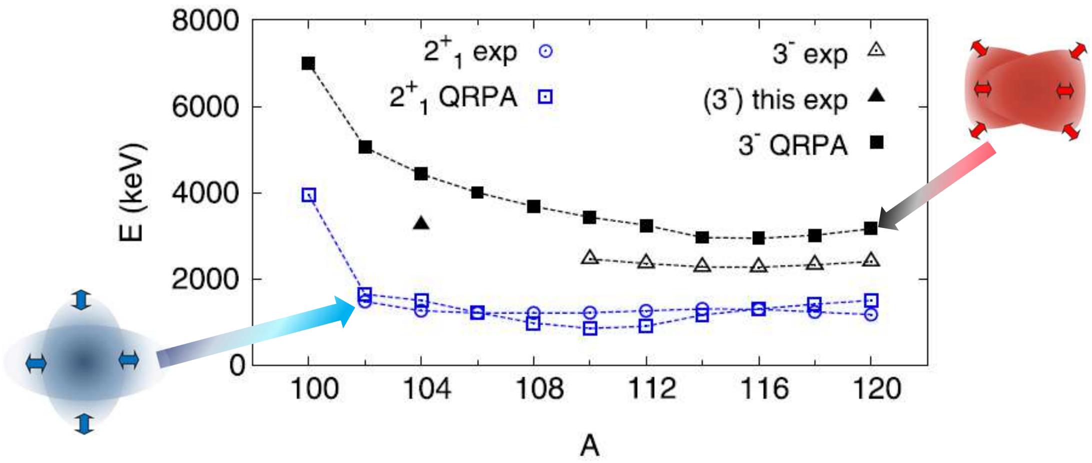
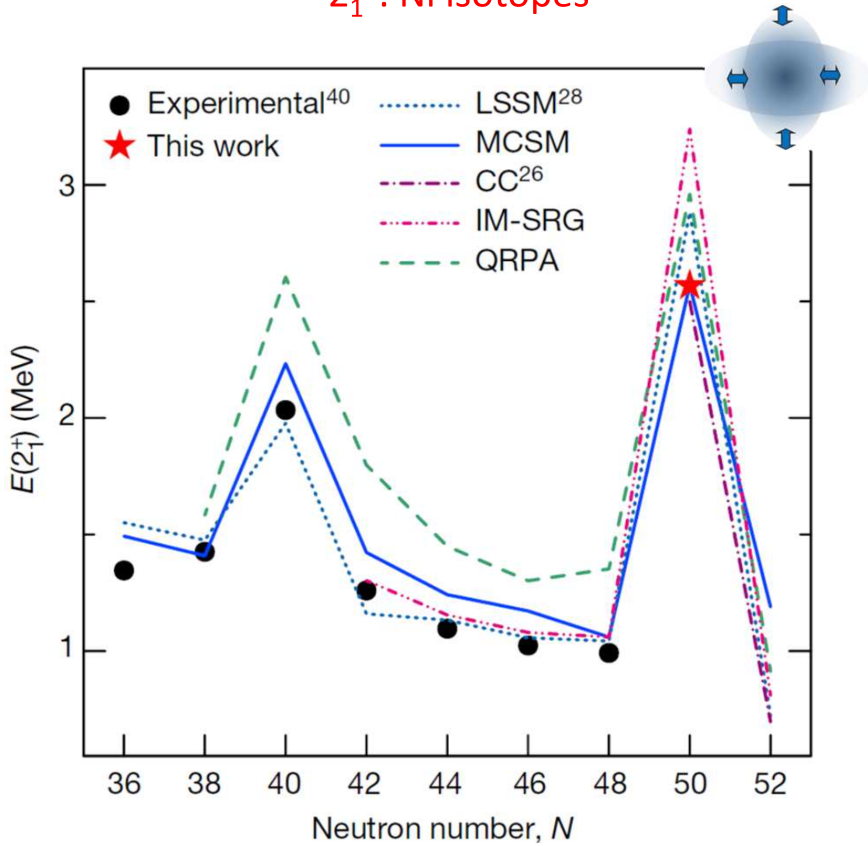


Fig. 3. (Color online.) Systematics of 2^+ and 3^- excitation energies in tin isotopes from experiment and HFB + QRPA calculations using the Gogny D1M interaction.

A. Corsi et al PLB 743 (2015) 451-455

2_1^+: Ni isotopes



R. Taniuchi *et al*, Nature 469 (2019) 53.

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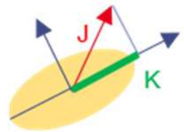
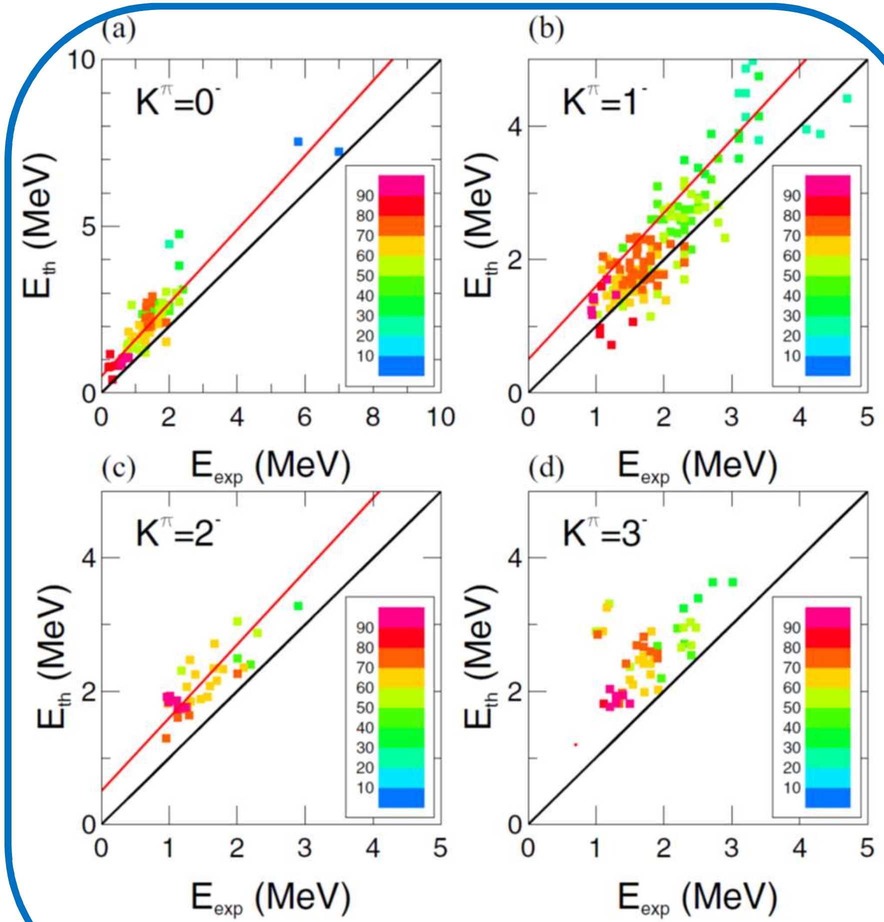
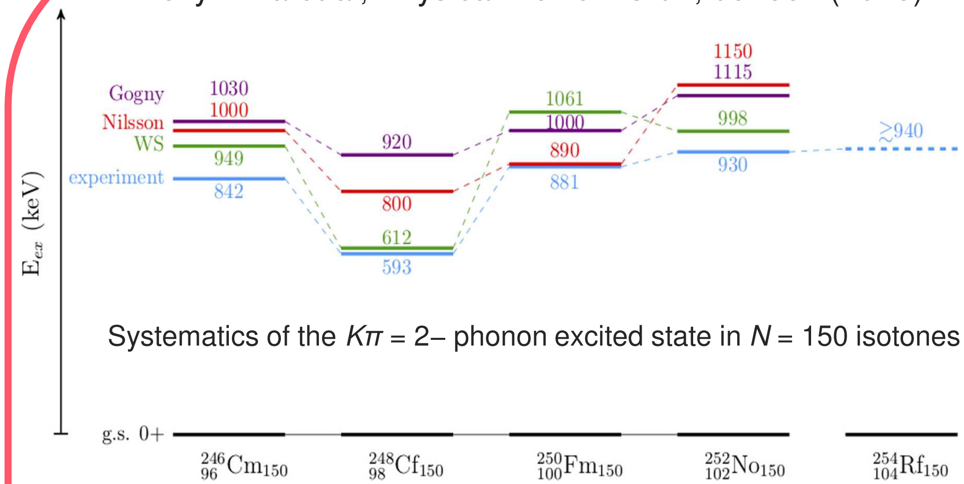




S. Goriely, S. Hilaire, S. Péru, and K. Sieja, Phys. Rev. C **98**, 014327 (2018)

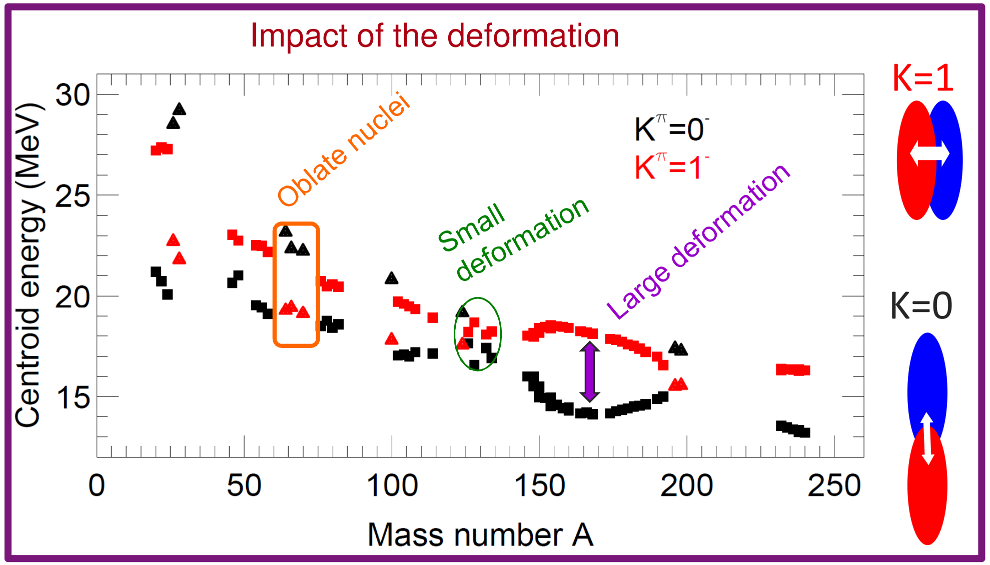
K. Rezynkina et al, Physical Review C 97, 054332 (2018)



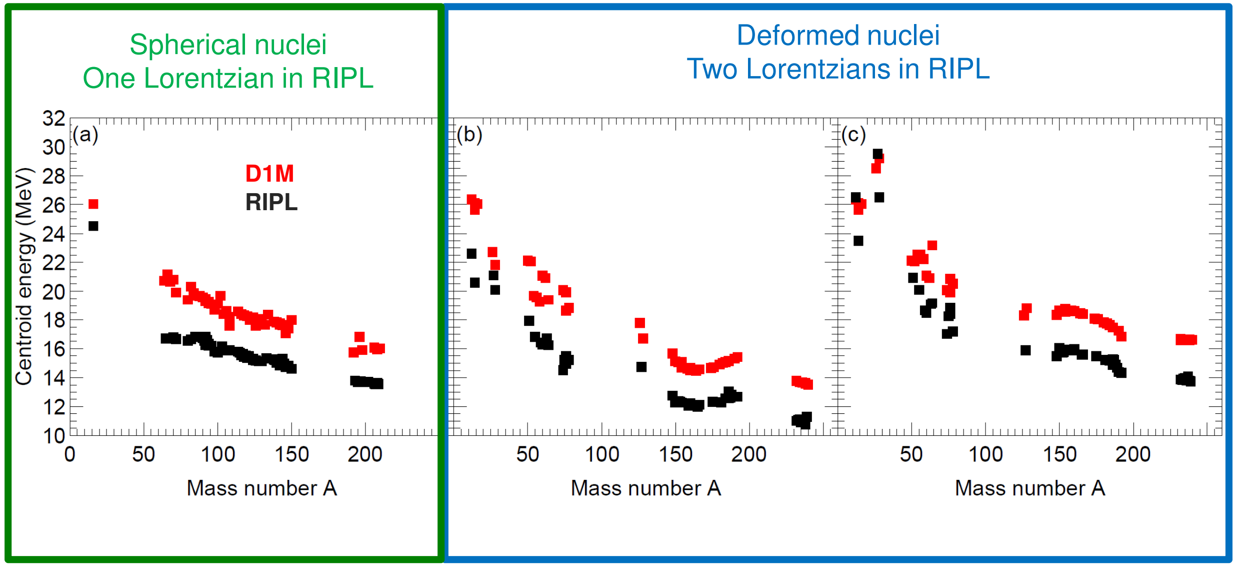
Nucleus	$E_{Exp.}$ keV	E_{D1M} keV	B(E3) $_{Exp.}$ W.u.	B(E3) $_{D1M}$ W.u.
^{246}Cm	842	1030	10,6	10,2
^{248}Cf	593	920		11,0
^{250}Fm	881	1000		10,0
^{252}No	930	1115		8,3

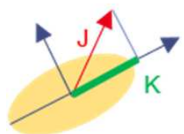
(Q)RPA approaches describe all multipolarities and all parities;
(Q)RPA describe Giant Resonances

D1M HFB+QRPA in axial symmetry applied to E1 strength



[M. Martini et al, PRC 94, 014304 (2016)]





Global 2 MeV overestimation

(Q)RPA approaches describe all multipolarities and all parities;
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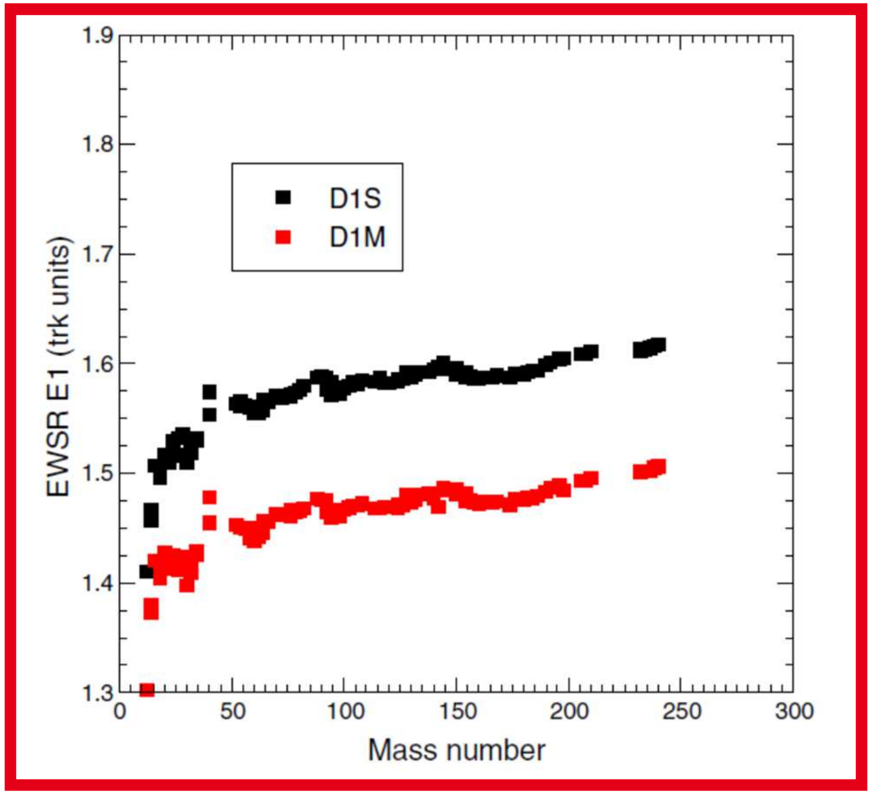
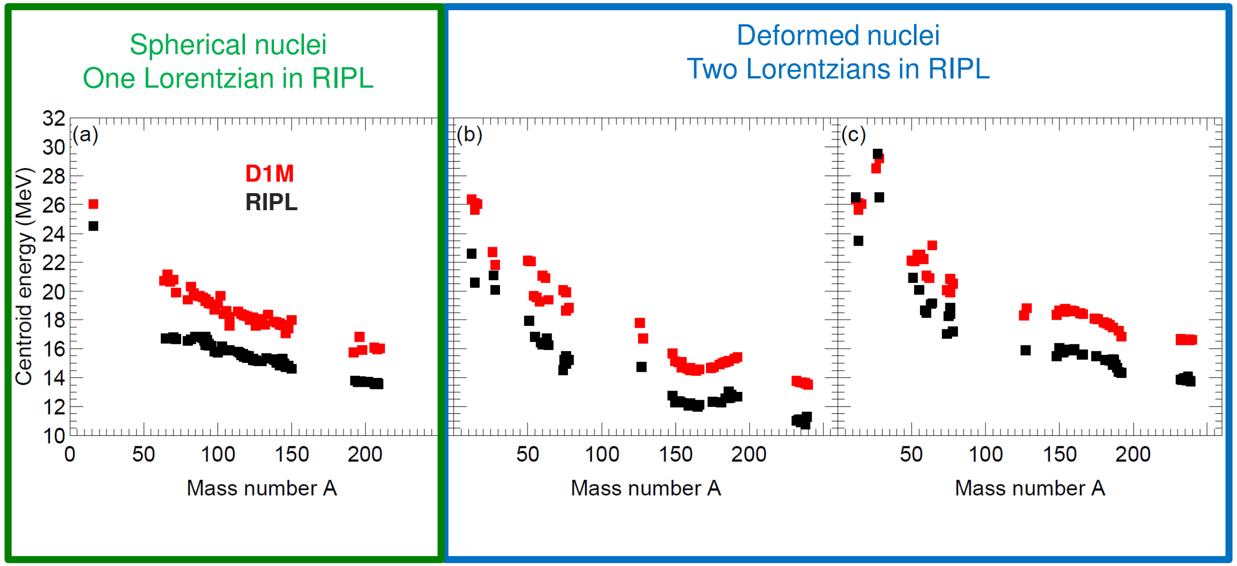
D1M HFB+QRPA in axial symmetry applied to E1 strength





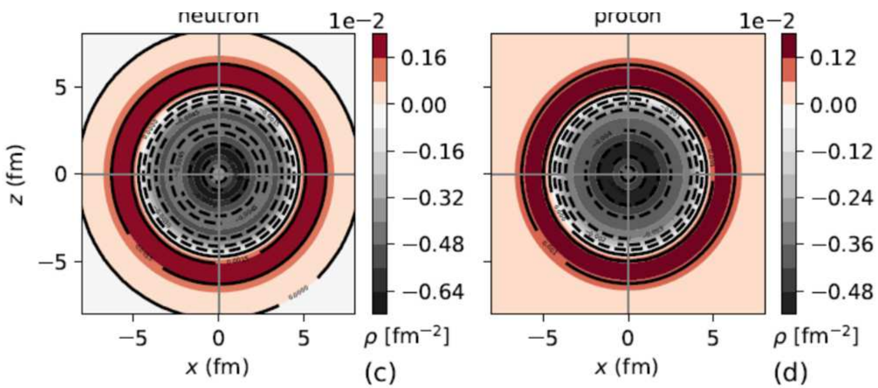
[M. Martini et al, PRC 94, 014304 (2016)]

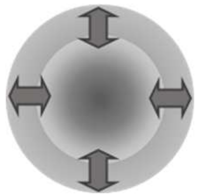
Global 2 MeV overestimation

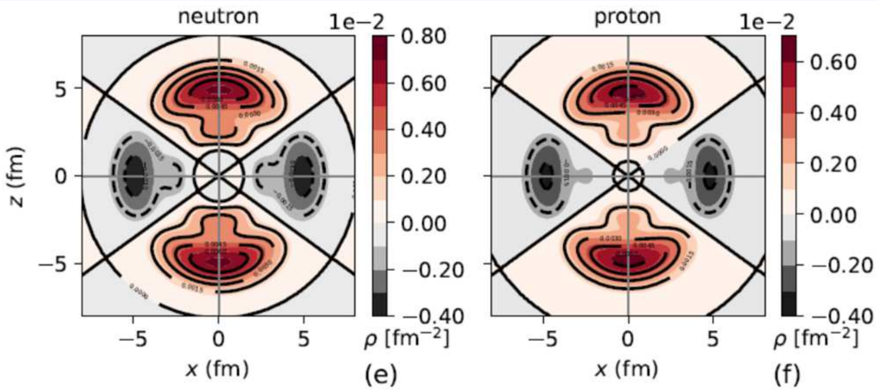
Transitions densities

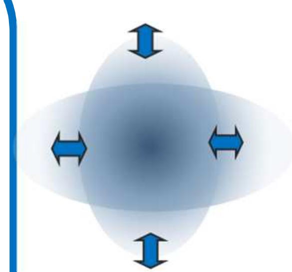
Spherical isotope ^{96}Zr

Pure monopole $K^{\pi}=0^{+}$, J=0 state at E_{QRPA}= 18.74 MeV

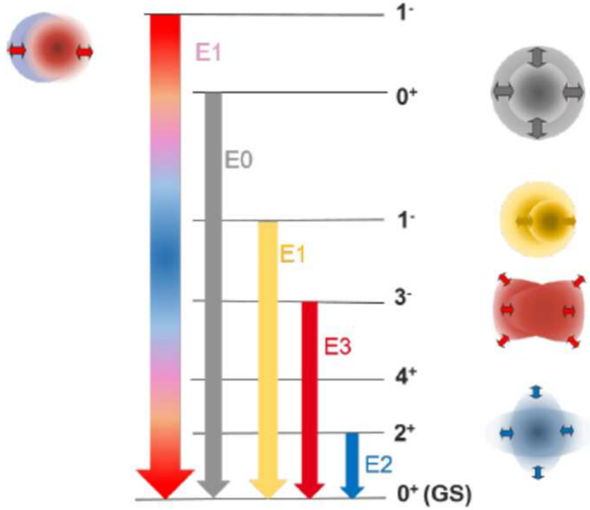








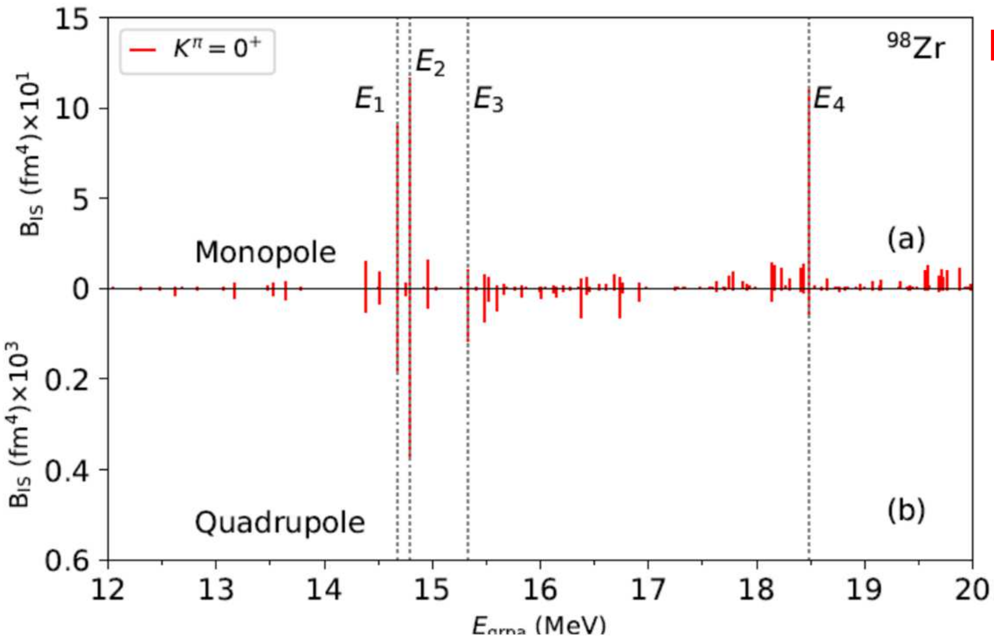
Pure quadrupole $K^{\pi}=0^{+}$, J = 2 state at E_{QRPA} = 15.08 MeV

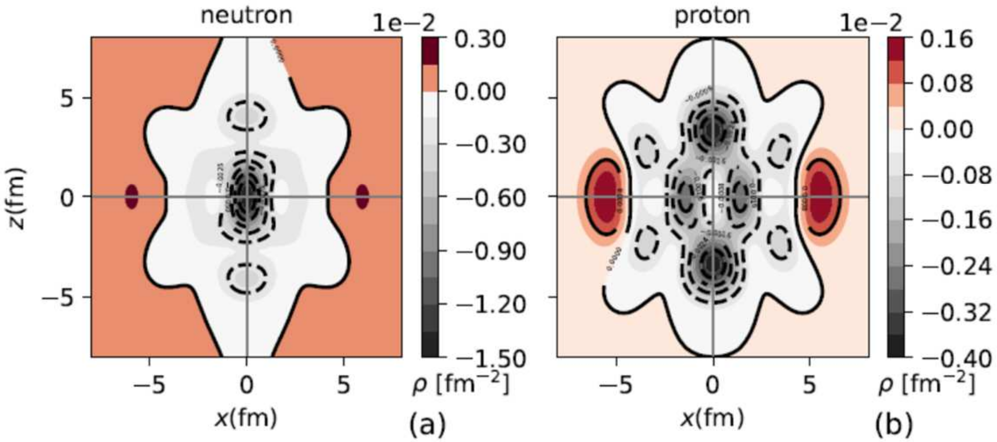


Isotope	J^{π}	QRPA (MeV)	Exp (MeV)
^{90}Zr	0_1^+	1.658	1.760
^{90}Zr	2_1^+	2.725	2.186
^{90}Zr	4_1^+	3.215	3.076
^{90}Zr	3_1^-	2.858	2.748
^{96}Zr	0_1^+	1.054	1.581
^{96}Zr	2_1^+	1.815	1.750
^{96}Zr	4_1^+	2.740	2.750
^{96}Zr	3_1^-	0.553 *	1.897

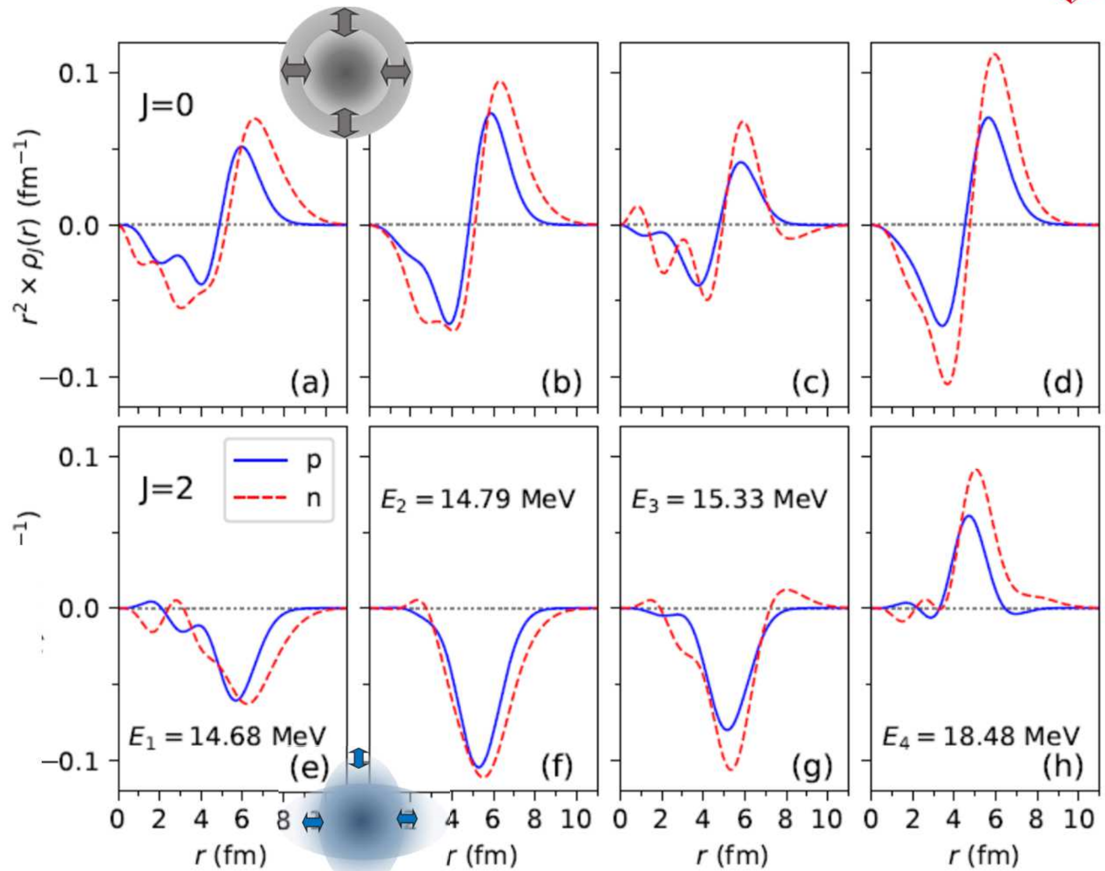
E.V. Chimanski et al, Phys. Rev. C 111, 054314 (2025)

Monopole-quadrupole coupling in deformed nuclei



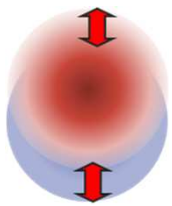


Intrinsic transition density for E_1=14,68 MeV.

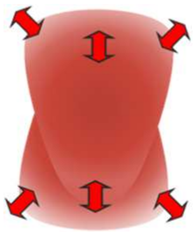


E.V. Chimanski et al, Phys. Rev. C 111, 054314 (2025)

E.V. Chimanski et al,
Phys. Rev. C 111, 054314 (2025)

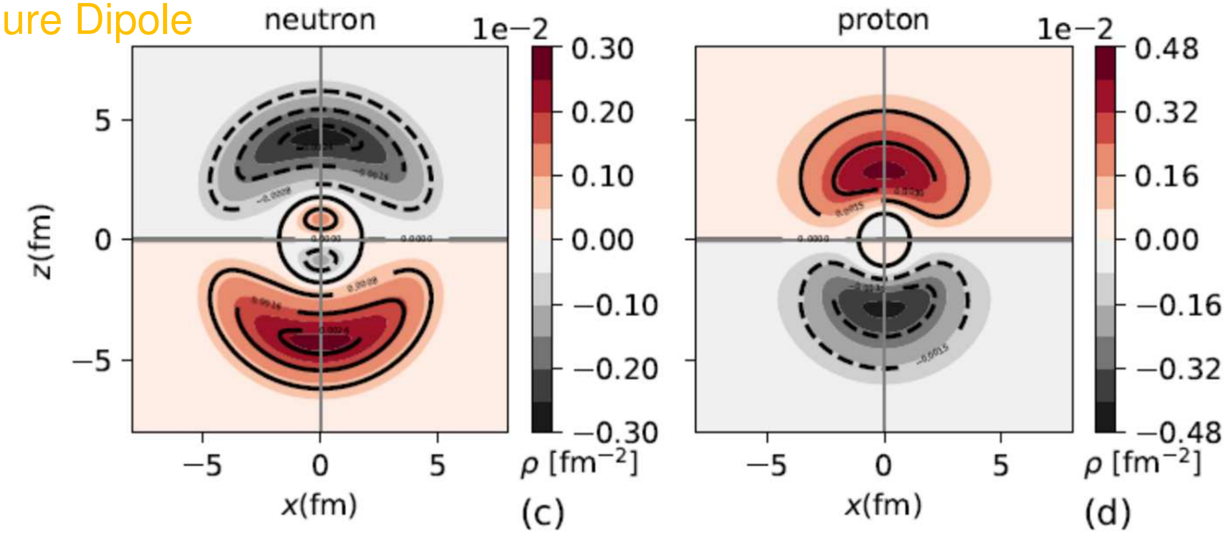


Spherical isotope ^{96}Zr.



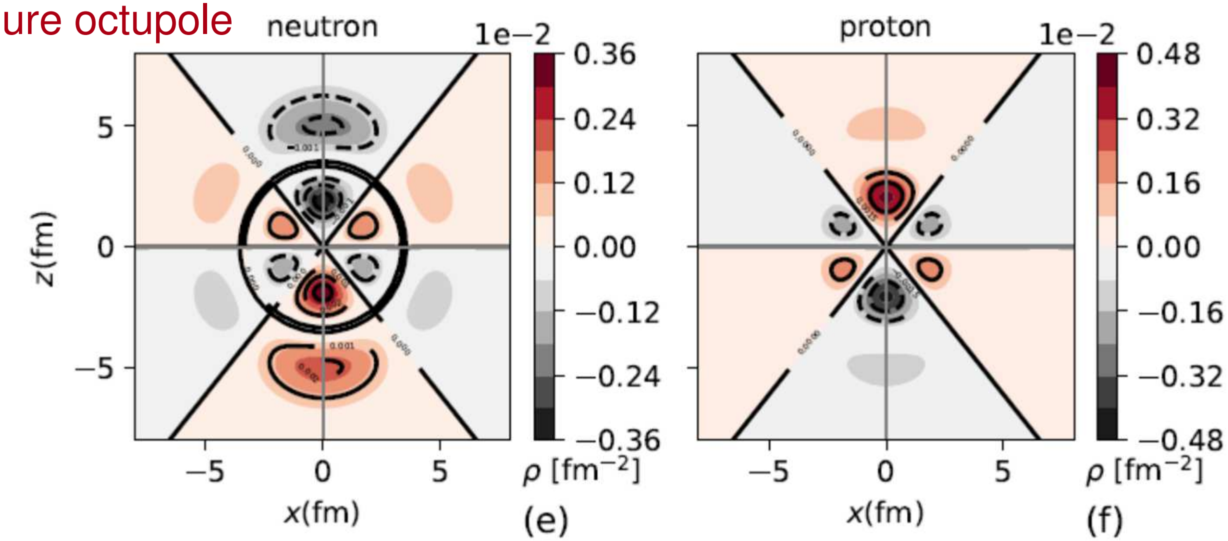
K=0,J=1, E_{QRPA} = 17.22 MeV

Pure Dipole

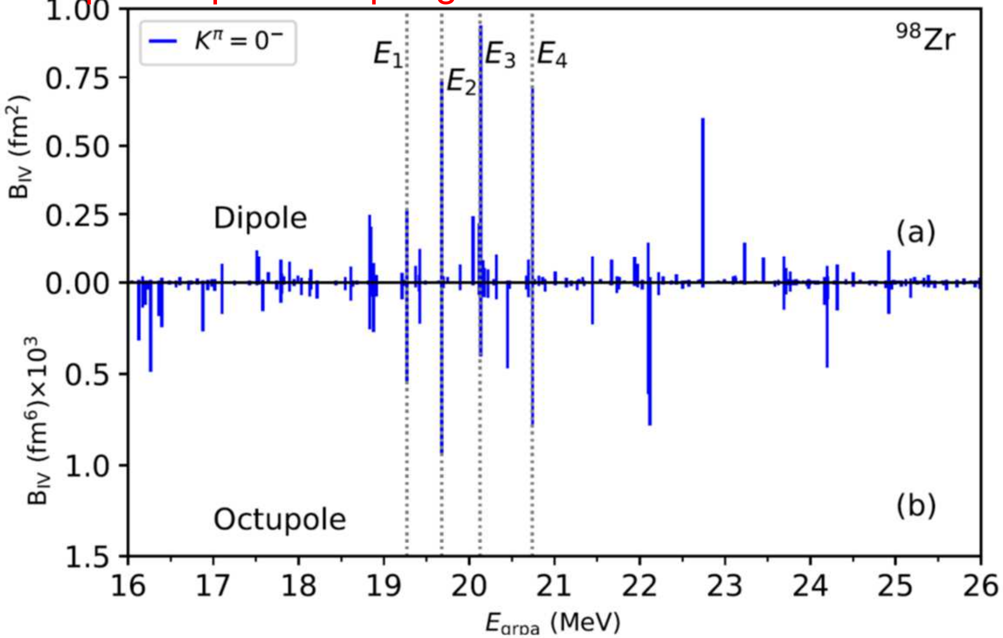


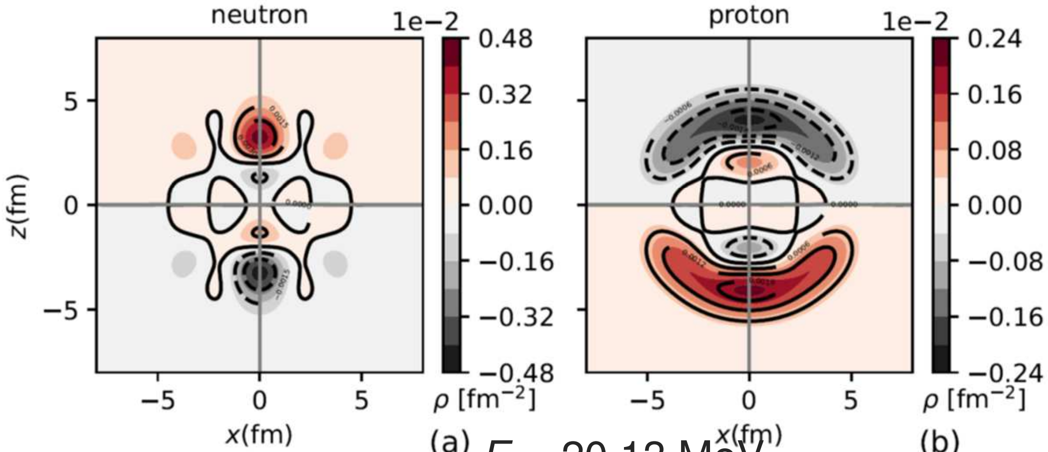
K=0,J=3, E_{QRPA} = 15.12 MeV

Pure octupole

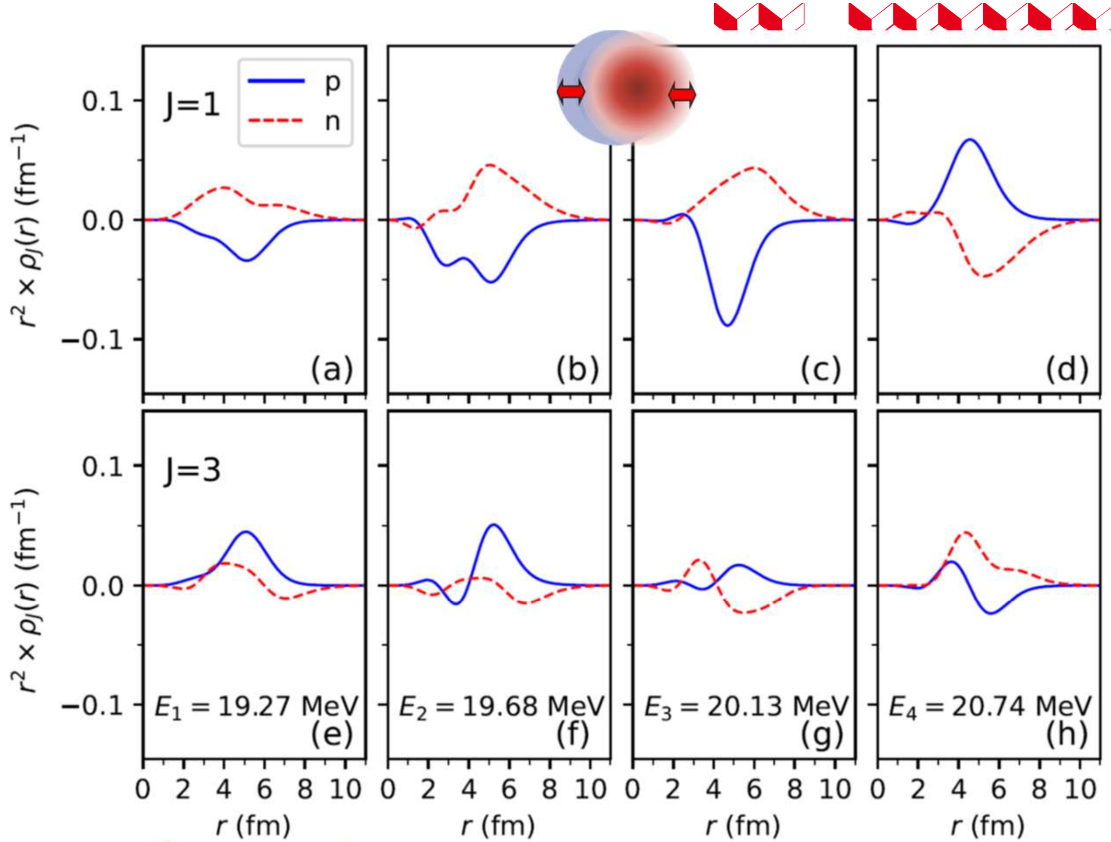


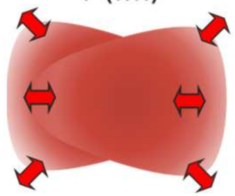
Octupole-dipole coupling in deformed nuclei





E_3 =20.13 MeV

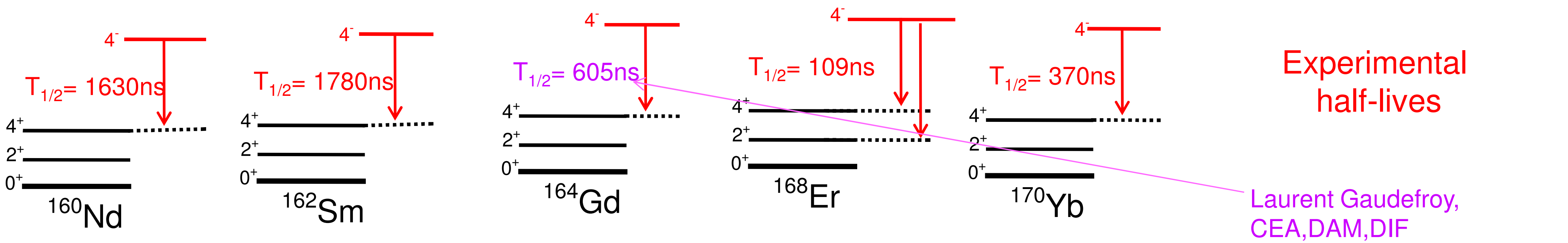




E.V. Chimanski et al,
Phys. Rev. C 111, 054314 (2025)

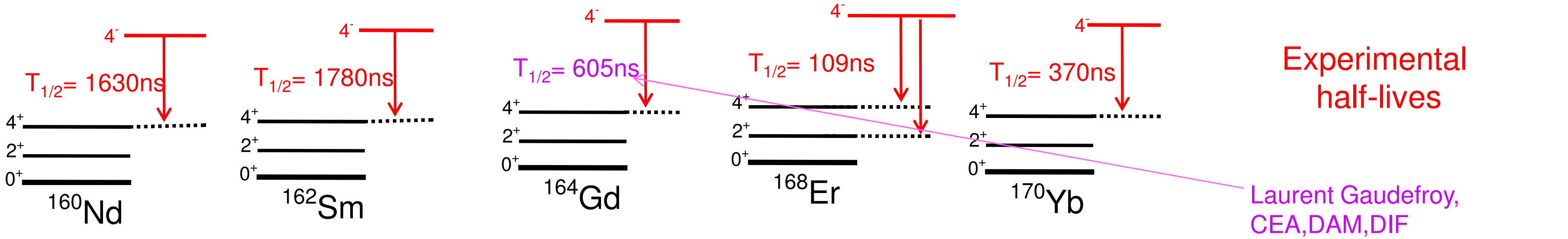
2 QRPA and its unusual application

Unusual application: 4^- isomers in N=100 isotones

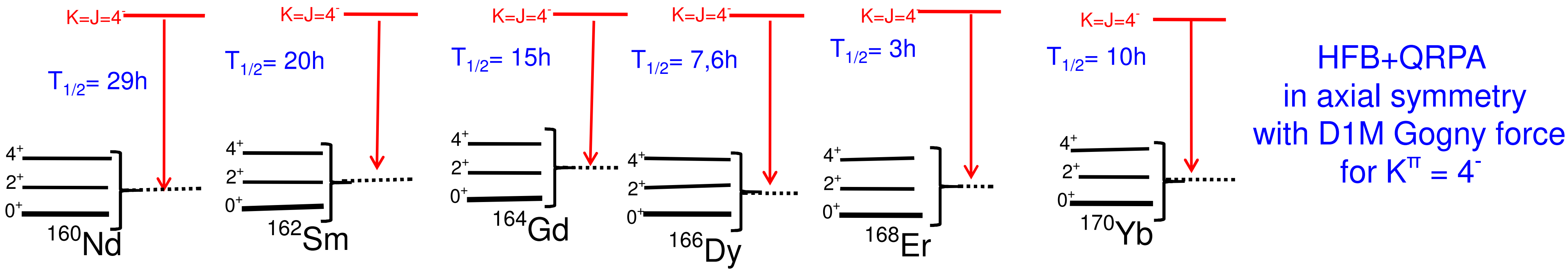


The $4^- \rightarrow 4^+$ transition is expected to be E1

Unusual application: 4⁻ isomers in N=100 isotones



The $4^- \rightarrow 4^+$ transition is expected to be E1



Only M4 and E5 transitions are allowed ← $\lambda \geq K=4$

L. Gaudefroy, S. Péru, et al, PRC97, 064317 (2018)

What is the nature of these J=4 isomers?

Example : ^{162}Sm

$T_{1/2}$= 1780ns

J=4, K^{π}=0^{-}	J=4, K=1	J=4, K=2	J=4, K=3	J=4, K=4
B(E1) B(M2)	B(E1) B(M2)	B(E3) B(M2)	B(E3) B(M4)	B(E5) B(M4)
$T_{1/2} \approx$ 0,5 ps	$T_{1/2} \approx$ 300 ps	$T_{1/2} \approx$ 20 ns	$T_{1/2} \approx$ 700 µs	$T_{1/2} \approx$ 20 h

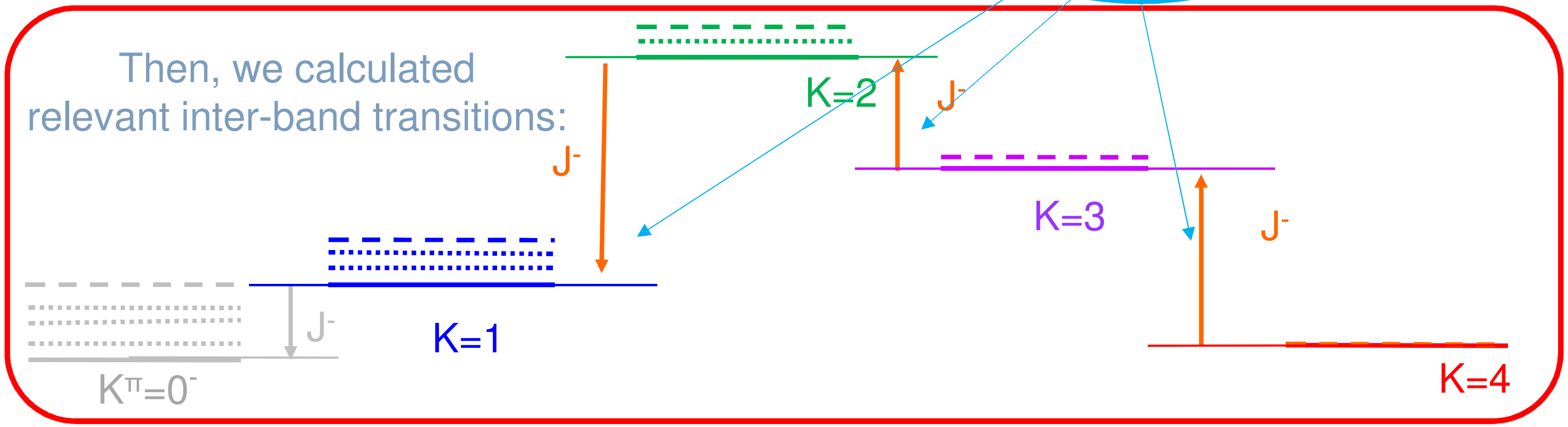
No calculated half-live reproduces the experimental one.
A very small K=1 component in the wave function would explain the observations.

There are 3 main mechanisms for K admixture :
F. G. Kondev, G.D. Dracoulis and T. Kibedi, ADNDT 103, 50 (2015)

- High level density
- Triaxial shape
- $\boxed{\text{Mixing with Coriolis interaction}}$

to fix it:

$$< K \mid Hc \mid K{+}1 > = -\frac{\hbar}{2I}\sqrt{(J-K)(J+K+1)}\,< K \mid j^- \mid K{+}1 >$$

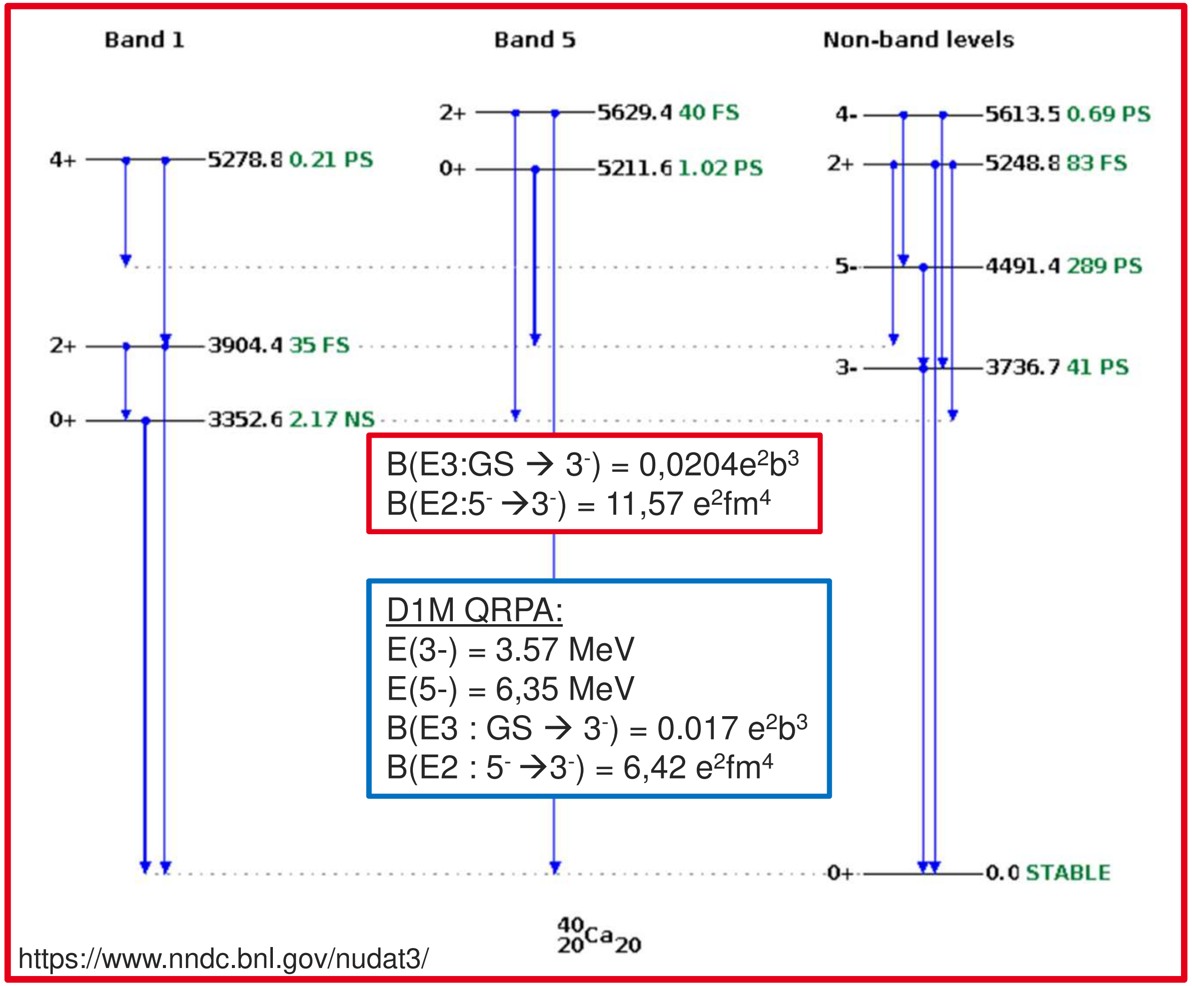


T ½ ns	^{160}Nd	^{162}Sm	^{164}Gd	^{166}Dy	^{168}Er	^{170}Yb	^{172}Hf
Exp.	1670(210)	1780(70)	605(30)	?	109(7)	370(15)	~1
QRPA	6970	11105	3980	285	365	260	1,5
QRPA/Exp.	4,17	6,24	6,57	?	3,35	0,703	1,5

L. Gaudefroy, S. Péru, et al, PRC97, 064317 (2018)

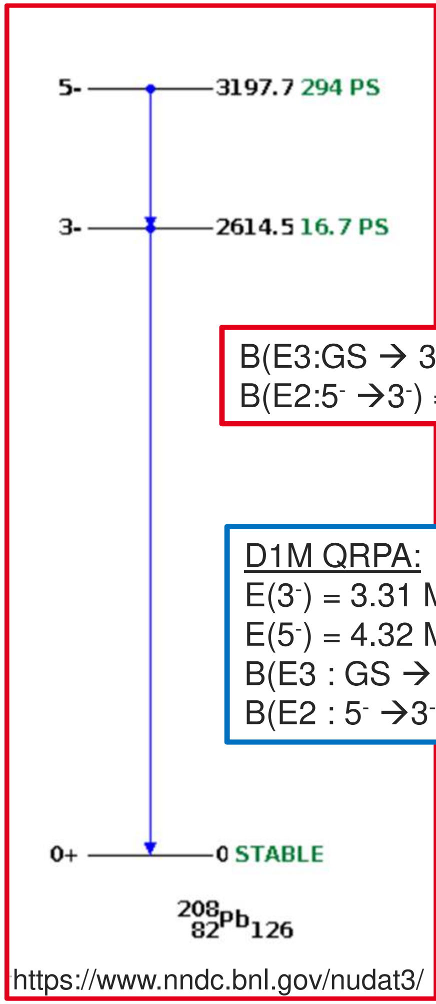
More transition probabilities are now available

Low energy spectroscopy in spherical nuclei :



B(E3:GS → 3⁻) = $0,0204 e^2b^3$
B(E2:5⁻ →3⁻) = $11,57\ e^2fm^4$

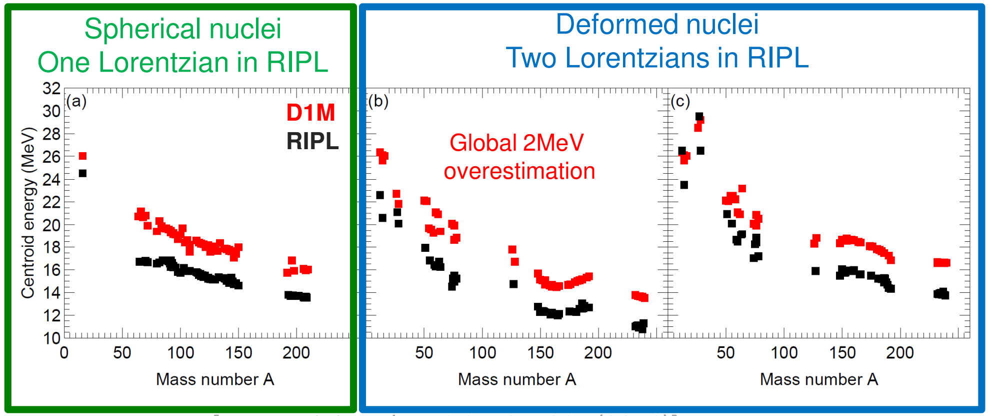
D1M QRPA:
E(3-) = 3.57 MeV
E(5-) = 6,35 MeV
B(E3 : GS → 3⁻) = $0.017\ e^2b^3$
B(E2 : 5⁻ →3⁻) = $6,42\ e^2fm^4$



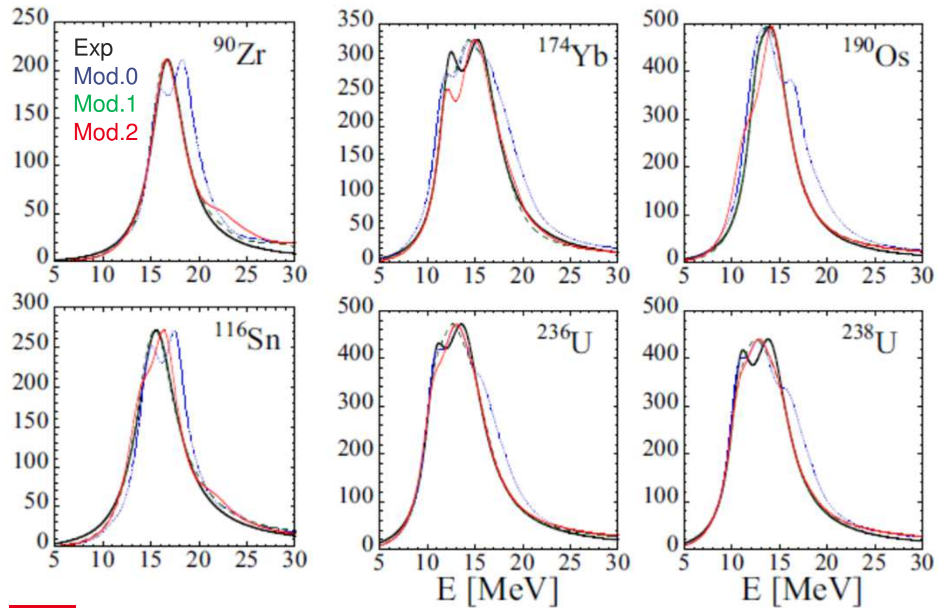
B(E3:GS → 3⁻) = $0.611\ e^2b^3$
B(E2:5⁻ →3⁻) = $0,00413\ e^2b^2$

D1M QRPA:
E(3⁻) = 3.31 MeV
E(5⁻) = 4.32 MeV
B(E3 : GS → 3⁻) = $0.702\ e^2b^3$
B(E2 : 5⁻ →3⁻) = $0,00723\ e^2b^2$

D1M HFB+QRPA for γ strength function



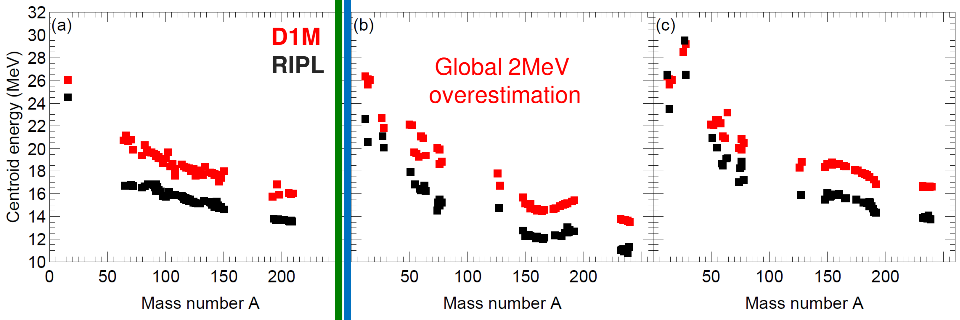
[M. Martini et al, PRC 94, 014304 (2016)]



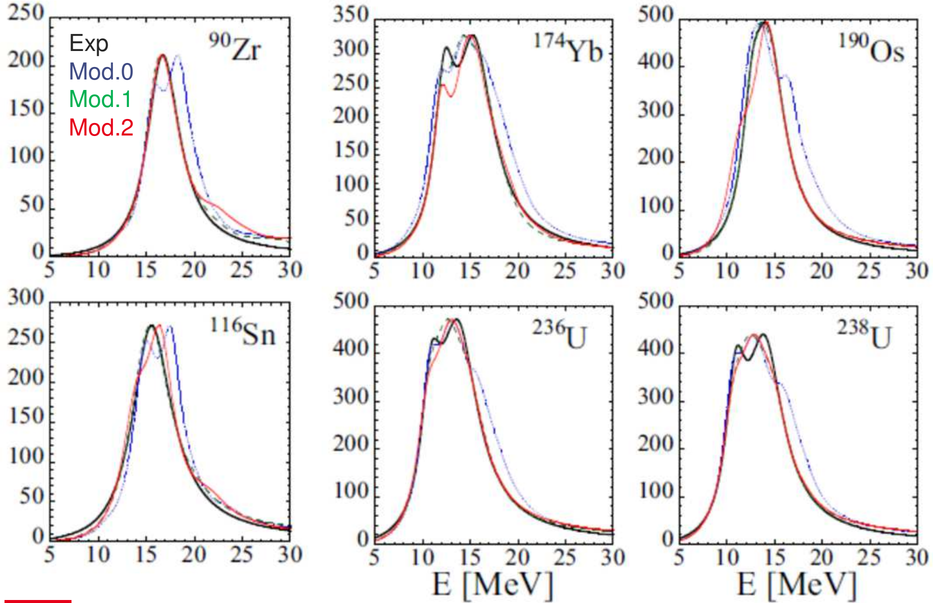
D1M HFB+QRPA for γ strength function

Spherical nuclei
One Lorentzian in RIPL

Deformed nuclei
Two Lorentzians in RIPL

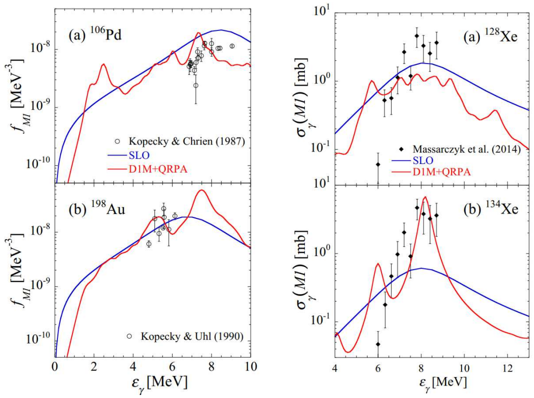


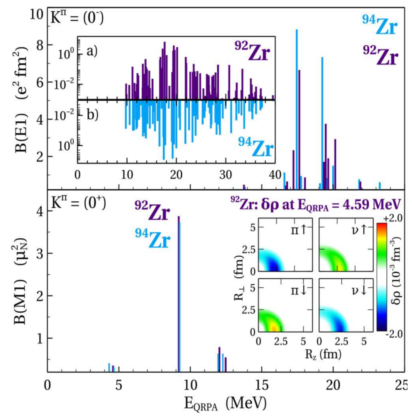
[M. Martini et al, PRC 94, 014304 (2016)]



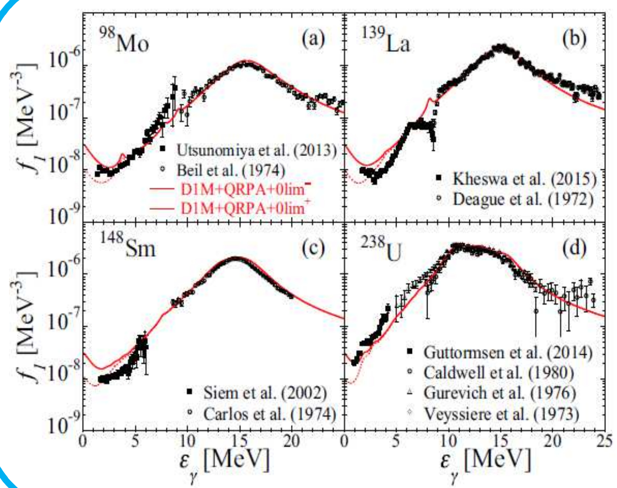
Magnetic and electric modes on the same footing

S. Goriely et al, PRC 94, 044306 (2016)





I.Deloncle et al, EPJA 53:170(2017)



Gogny-HFB + QRPA

[S. Goriely et al, PRC98,014327 (2018)]

QRPA B(E1) and B(M1)

- Lorentzian folding
- shift in energy to fit data

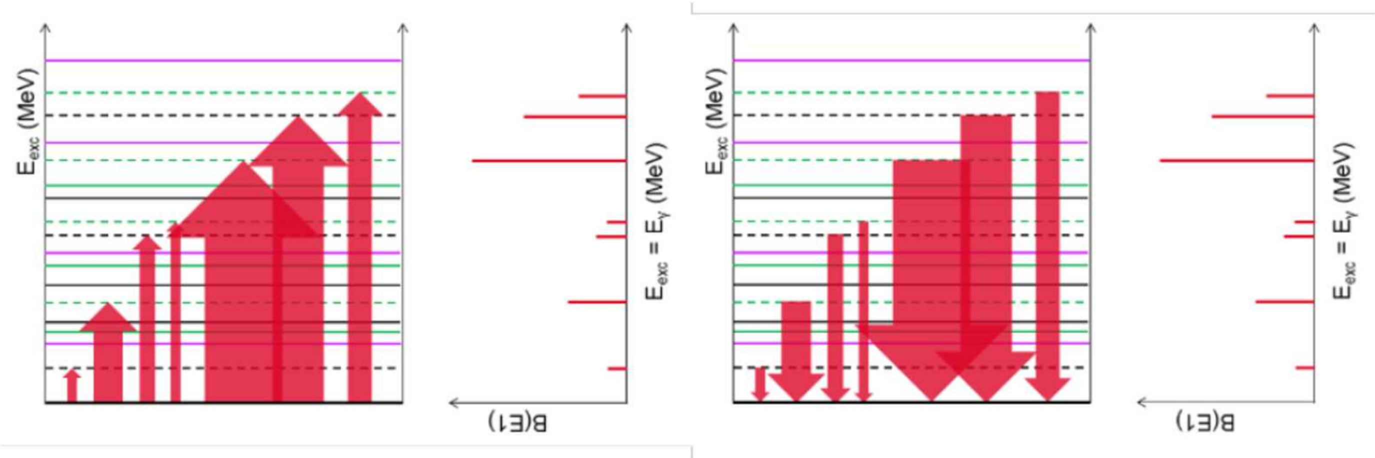
Phenomenological upbend inspired by shell model for the decay strength

Photon strength function modelling, status and perspectives

Sophie Péru, Stephane Goriely and Stéphane Hilaire

EPJ Web of Conferences **322**, 06003 (2025) *CNR*24*

PSF



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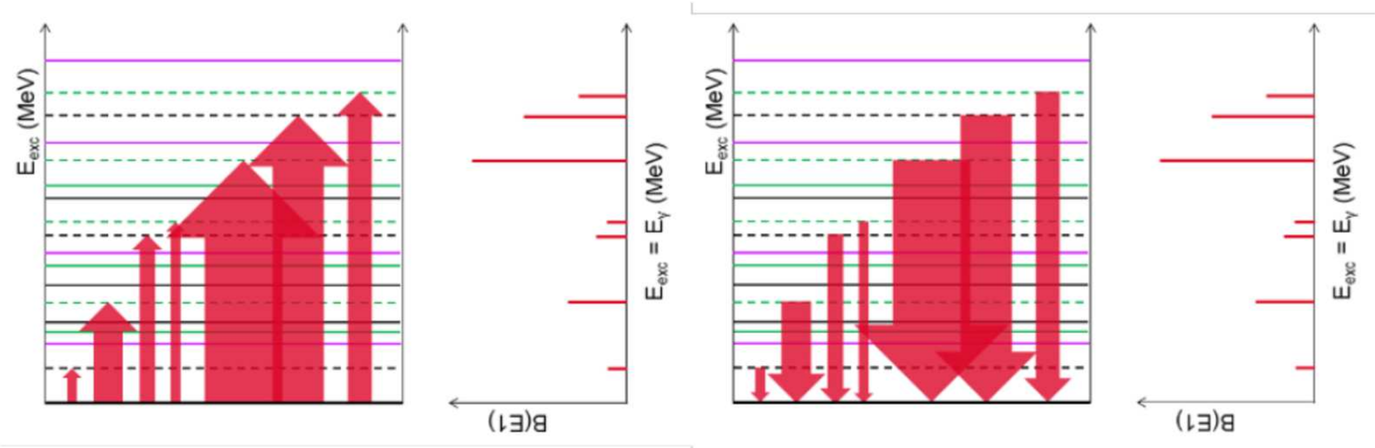

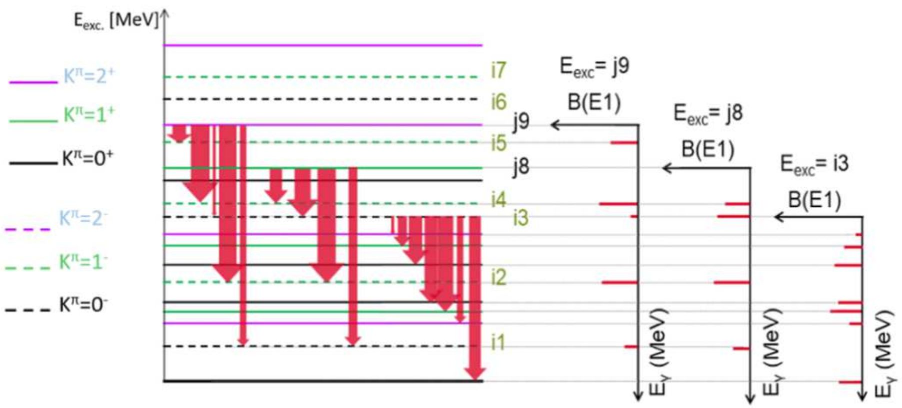

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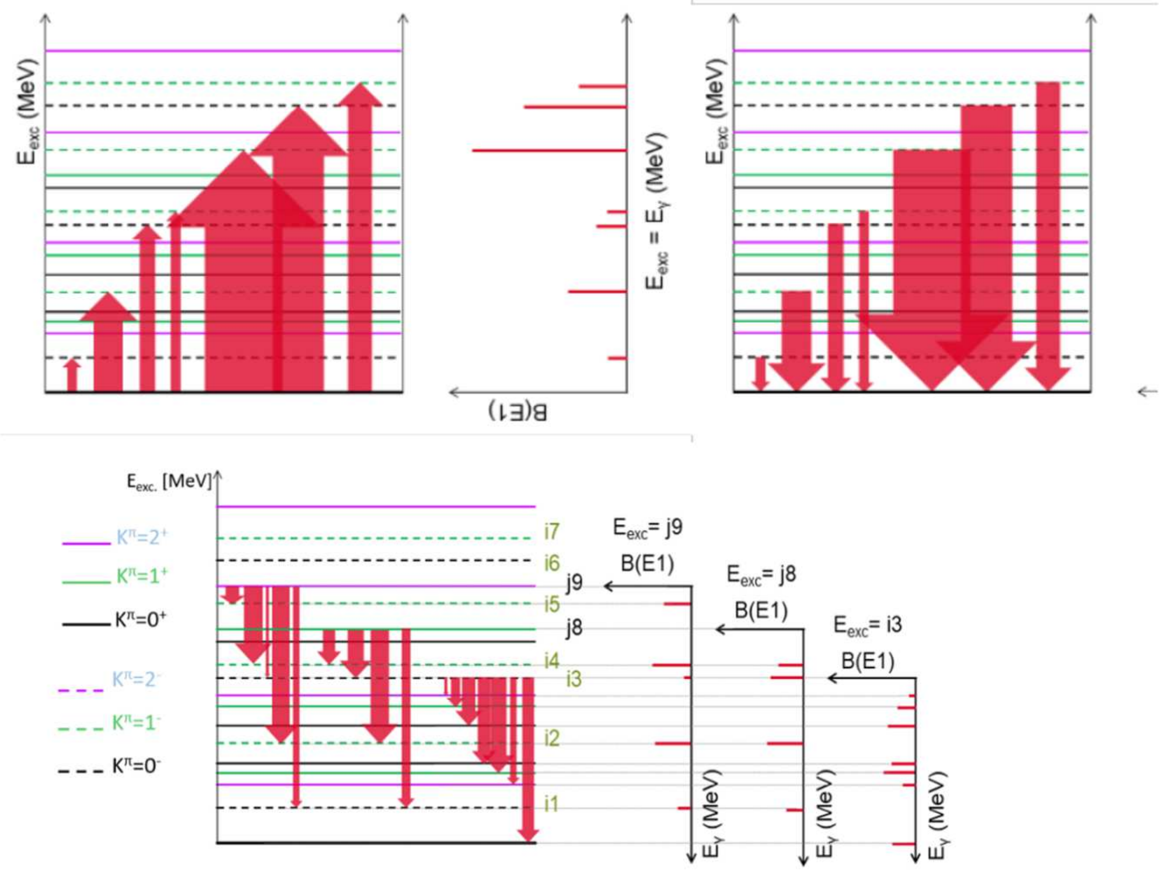
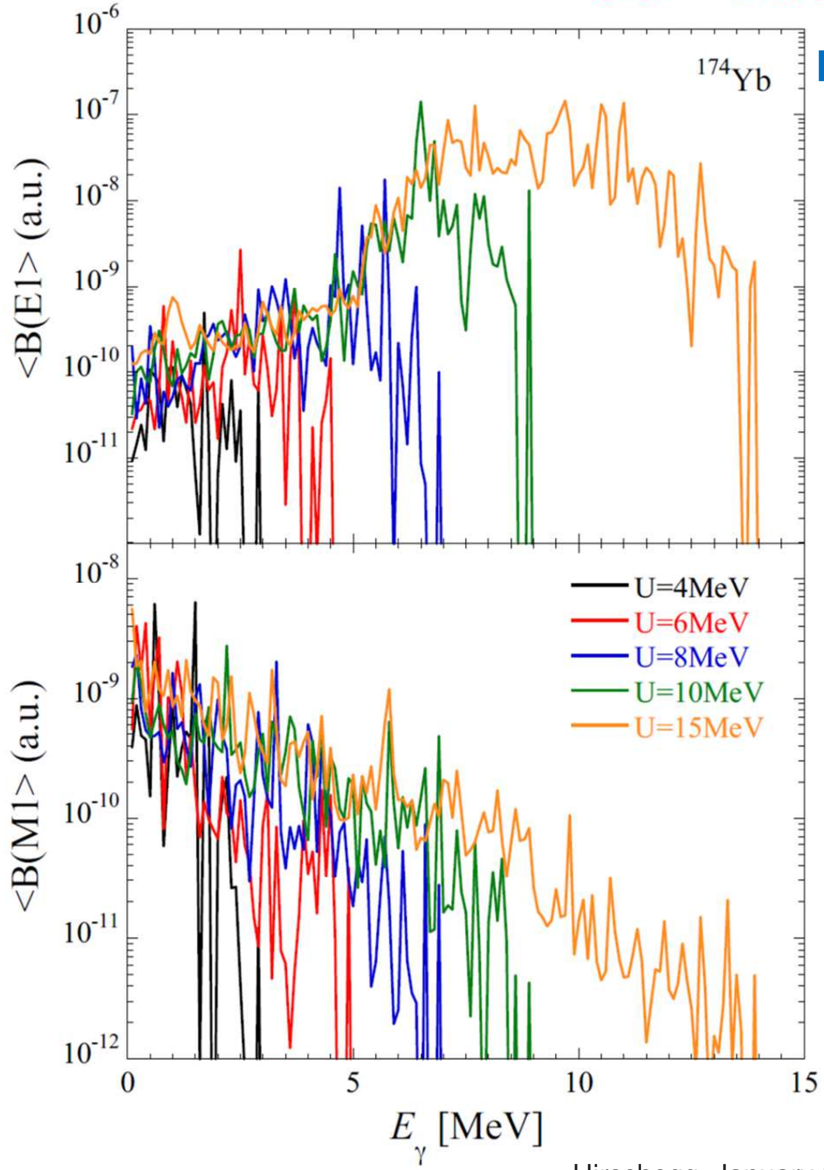
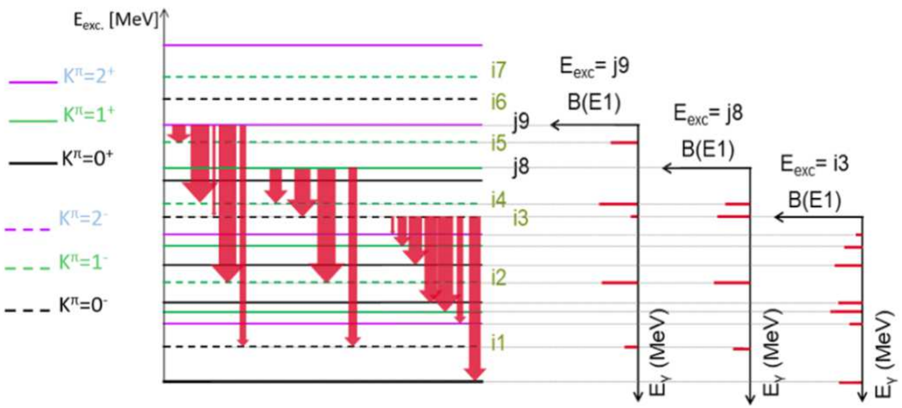


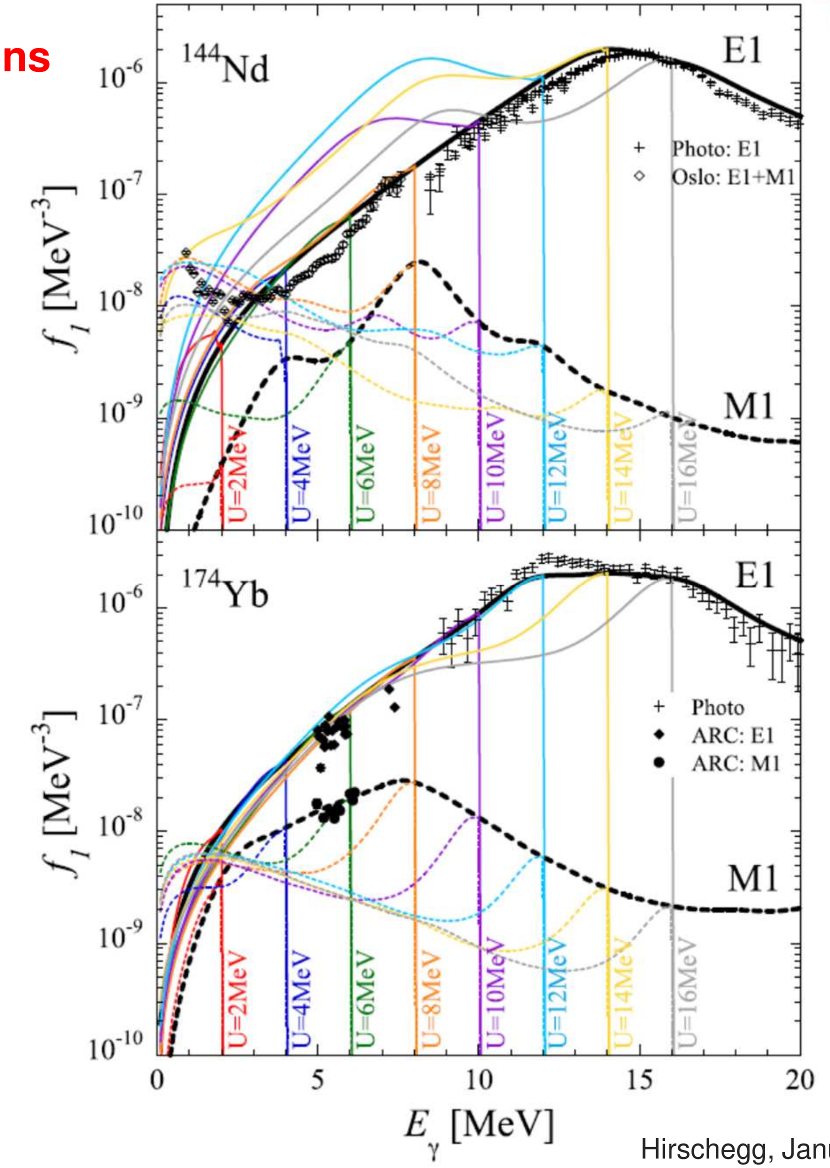


QRPA prediction of de-excitation photon strength functions

S. Goriely, S. Péru, S. Hilaire

Physics Letters B 868 (2025) 139677





Other problems remain open
Other challenges to address

- Projected QRPA for restoration of J in deformed nuclei: beyond the rotational approximation…
- Shape coexistence versus shape mixing, for instance the Hg isotopic chain
- Impact of “second” QRPA: 4qp states, particle vibration coupling
- ….

Thanks for you attention