# Spurious states in „beyond“ RPA and multiphonon calculations

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11.-16.6. 2023, Catania

7th International Conference on Collective Motion in Nuclei under Extreme Conditions

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# Outline

- Spurious states in RPA
- Second RPA(TDA)
- Equation of motion phonon method (EMPM)
- Spurious states in SRPA and EMPM
- Conclusions

# Reminder: spurious states in RPA

- mean-field Hamiltonian → breaking of symmetries → **solutions with zero energy in (Q)RPA**

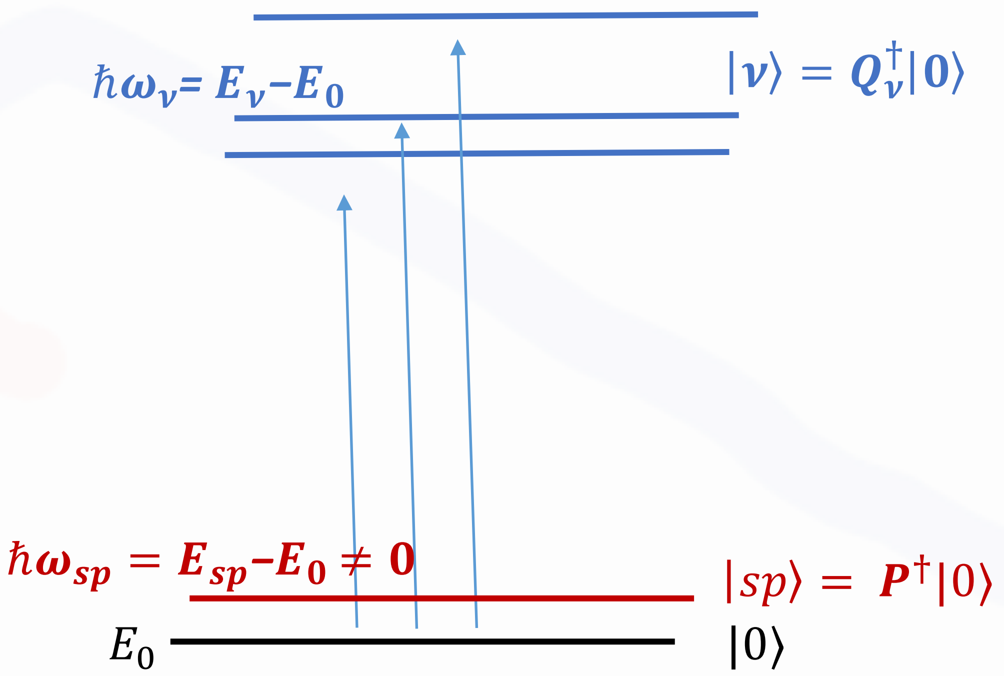
$$\hbar\omega_{sp} = 0$$

**inherent symmetries treated consistently**

✓ translational invariance → $J^{\pi}=1^{-}$ (spurious CM motion)

✓ particle number violation → $J^{\pi}=0^{+}$ (quasiparticles, BCS/HFB)

✓ rotational invariance → $K^{\pi}=1^{+}$ (axial deformation)




- **separation is not perfect in practical (Q)RPA calculations**

  finiteness of the model space, numerical precision

  → mixing with physical states

# Reminder: spurious states in RPA

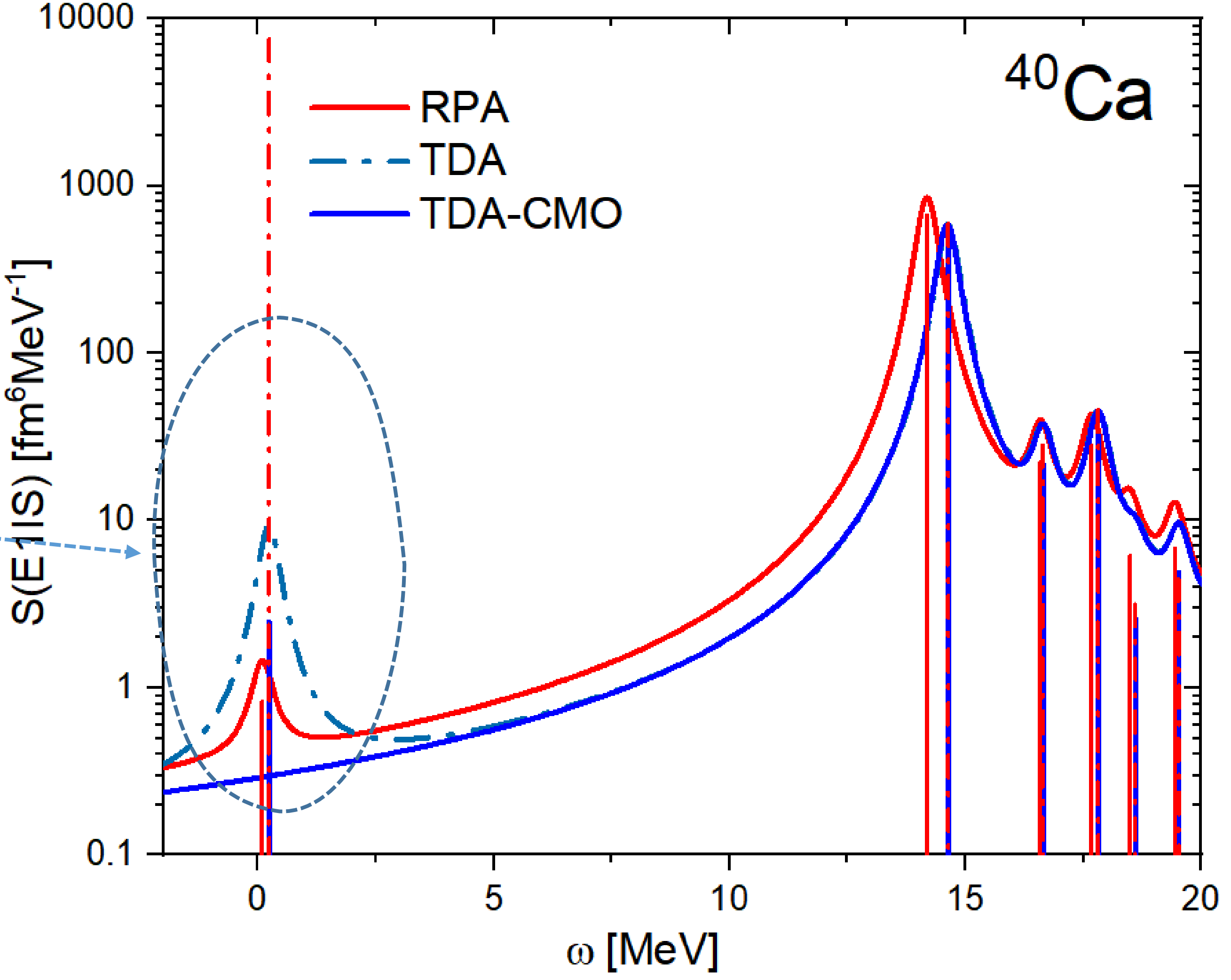
In real life, $\hbar\omega_{sp} \neq 0$

→ wave functions contain spurious admixtures, which are expected to be small **if** $\hbar\omega_{sp} \ll \hbar\omega_{\nu}$

→ „effective solution“: spurious strength subtraction

**but it does not cure wave functions!**

$$M(\mathrm{E1IS}) \sim \sum_{i=1}^{A} \left(r_i^3 - \frac{5}{3}\langle r_i^2\rangle r_i\right) Y_{1M}$$




→ **more general approach:** construction of basis $\{|\alpha\rangle\}$

orthogonal to spurious mode $P^\dagger|0\rangle \leftrightarrow \langle\alpha|P^\dagger|0\rangle = 0$

→ diagonalisation in **spurious-free basis**

*A. Repko et al, Phys. Rev. C 99, 044 307 (2019)*

# „Complex“ configurations

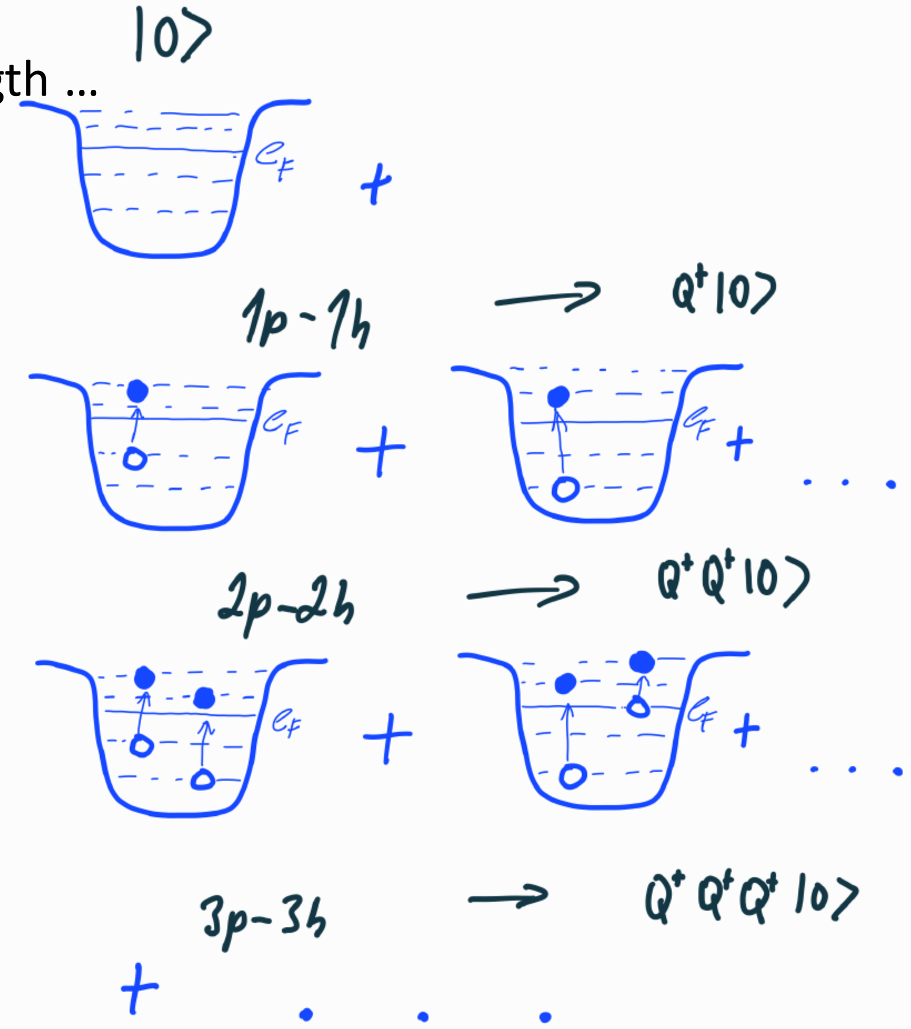
- **Why are „complex“ configurations important?**
  energies can be comparable to „simple“ (1p-1h,2qp) excitations
  fine structure of giant resonances (spreading widths), low lying strength …

- **(R)QTBA**: relativistic DFT: (*1p-1h) x RPA phonon, 2qp x QRPA phonon*
  **EOM**: 2qp x 2-phonon: **E. Litvinova**

- **QPM** : *1+2+3 Q(RPA) phonons*
- **PVC : G. Coló, Y. F. Niu, G. Potel** …

- **SRPA**: RPA + *2p-2h*
  SSRPA: **D. Gambacurta, H. Sagawa**

- **Equation of motion phonon method (EMPM)**



# Second RPA (SRPA)

Straightforward extension of RPA → $\boldsymbol{Q^\dagger} \sim \boldsymbol{a_p^\dagger a_h} + \boldsymbol{a_{p_1}^\dagger a_{p_2}^\dagger a_{h_2} a_{h_1}}$ + h.c.

Matrix form

$$\left(\begin{array}{cc|cc} \boldsymbol{A} & \boldsymbol{A_{12}} & \boldsymbol{B} & \boldsymbol{B_{12}} \\ \boldsymbol{A_{21}} & \boldsymbol{A_{22}} & \boldsymbol{B_{21}} & \boldsymbol{B_{22}} \\ \hline -\boldsymbol{B^*} & -\boldsymbol{B_{12}^*} & -\boldsymbol{A^*} & -\boldsymbol{A_{12}^*} \\ -\boldsymbol{B_{21}^*} & -\boldsymbol{B_{22}^*} & -\boldsymbol{A_{21}^*} & -\boldsymbol{A_{22}^*} \end{array}\right) \left(\begin{array}{c} \boldsymbol{X^{\nu\,(1)}} \\ \boldsymbol{X^{\nu\,(2)}} \\ \hline \boldsymbol{Y^{\nu\,(1)}} \\ \boldsymbol{Y^{\nu\,(2)}} \end{array}\right) = \hbar\omega_{\boldsymbol{\nu}}^{SRPA} \left(\begin{array}{c} \boldsymbol{X^{\nu\,(1)}} \\ \boldsymbol{X^{\nu\,(2)}} \\ \hline \boldsymbol{Y^{\nu\,(1)}} \\ \boldsymbol{Y^{\nu\,(2)}} \end{array}\right)$$

← 1p-1h

← 2p-2h

amplitudes

**Quasiboson approximation**

$$(\boldsymbol{A_{12}})_{ph,\ p_1p_2h_1h_2} \approx \langle HF| \left[\boldsymbol{a_h^\dagger a_p}, \left[\boldsymbol{H_{intr}}, \boldsymbol{a_{p_1}^\dagger a_{p_2}^\dagger a_{h_2} a_{h_1}}\right]\right] |HF\rangle$$

$$(\boldsymbol{A_{22}})_{p_1h_1p_2h_2\ ,p_1'h_1'p_2'h_2'} \approx \langle HF| \left[\boldsymbol{a_{h_1}^\dagger a_{h_2}^\dagger a_{p_1} a_{p_2}}, \left[\boldsymbol{H_{intr}}, \boldsymbol{a_{p_2'}^\dagger a_{p_1'}^\dagger a_{h_2'} a_{h_1'}}\right]\right] |HF\rangle$$

For 2-body Hamiltonian and HF reference state → QBA → $\boldsymbol{B_{12}, B_{21}, B_{22}}$ =0
No explicit mixing between $|HF\rangle$ and $|2p2h\rangle$, g.s. correlations induced via $\boldsymbol{B}$

*C. Yannouleas, Phys. Rev. C* ***35****, 1159 (1987)*

$\boldsymbol{B} = 0 \rightarrow Y_{ph}^{\boldsymbol{\nu}\,(1)}, Y_{p_1p_2h_1h_2}^{\boldsymbol{\nu}\,(2)} = 0$

STDA → diagonalisation in *1p-1h + 2p-2h* model space

# Equation-of-motion Phonon method (EMPM)

- partitioning of the model space into *n*-(TDA)phonon (n=0,1,2,3..) subspaces spanned by

$$|0\rangle,\ Q^\dagger\ |HF\rangle,\ Q^\dagger Q^\dagger|HF\rangle,\ Q^\dagger Q^\dagger Q^\dagger|HF\rangle\ \ldots$$

- iterative construction of basis → pre-diagonalisation in each subspace → diagonalisation in full space (0+1+2+3..)

$$\langle n,\beta|\boldsymbol{H_{intr}}|n,\alpha\rangle = E^n_\alpha \delta_{\alpha\beta}$$

$$\boldsymbol{H_{intr}} = \sum_{n,\alpha} E^n_\alpha |n,\alpha\rangle\langle n,\alpha| + \sum_{nn',\alpha\alpha'} |n',\alpha'\rangle\langle n',\alpha'|\boldsymbol{H_{intr}}|n,\alpha\rangle\langle n,\alpha|$$

| | | | |
|---|---|---|---|
| $E^0_0$ | 0 | $H_{02}$ | 0 |
| 0 | $E^1_1$ $E^1_2$ $\ddots$ | $H_{12}$ | 0 |
| $H_{20}$ | $H_{21}$ | $E^2_1$ $E^2_2$ $\ddots$ | $H_{23}$ |
| 0 | 0 | $H_{32}$ | $E^3_1$ $E^3_2$ $E^3_3$ $\ddots$ |

$$|\mathrm{n}=0\rangle = |\mathrm{HF}\rangle$$

$$\boldsymbol{Q}^\dagger_\alpha|\mathrm{HF}\rangle \dashrightarrow |\mathrm{n}=1,\alpha\rangle$$

$$\boldsymbol{Q}^\dagger_\nu|\mathrm{n}=1,\alpha\rangle = \boldsymbol{Q}^\dagger_\nu\boldsymbol{Q}^\dagger_\alpha|\mathrm{HF}\rangle \dashrightarrow |\mathrm{n}=2,\beta\rangle$$

$$\boldsymbol{Q}^\dagger_\nu|\mathrm{n}=2,\beta\rangle \dashrightarrow |\mathrm{n}=3,\mu\rangle$$

# Equation-of-motion Phonon method (EMPM)

- expansion of many-body states into a basis of multiphonon states
- fermionic structure fully taken into account
- J-coupled scheme
- quasiparticle version
- odd-particle(hole) version

$$\langle n-1,\alpha|\boldsymbol{H_{intr}}|n-1,\alpha'\rangle = E_{\alpha}^{n-1}\delta_{\alpha\alpha'}$$

$$\downarrow$$

$$\langle n,\beta|[\boldsymbol{H_{intr}},\boldsymbol{Q}_{\nu}^{\dagger}]|n-1,\alpha\rangle = (E_{\beta}^{n}-E_{\alpha}^{n-1})\langle n,\beta|\boldsymbol{Q}_{\nu}^{\dagger}|n-1,\alpha\rangle$$

$$\downarrow$$

$$\langle n,\beta|\boldsymbol{H_{intr}}|n,\beta'\rangle = E_{\beta}^{n}\delta_{\beta\beta'} \qquad |n,\beta\rangle = \sum_{\nu\alpha} C_{\nu\alpha}^{\beta(n)*}\boldsymbol{Q}_{\nu}^{\dagger}|n-1,\alpha\rangle$$

generalized eigenvalue problem in an **overcomplete nonorthogonal basis**

*D. Bianco, F.K. et al., Phys. Rev. C* ***85****, 014313 (2012)*

# Equation-of-motion Phonon method (EMPM)

- generalized eigenvalue problem in the redundant nonorthogonal basis

$$\boldsymbol{A}^{(n)}\ \boldsymbol{D}^{(n)}\ C = E\ \boldsymbol{D}^{(n)}\ C$$

$$(A^{(n)}D^{(n)})_{\nu\alpha,\nu'\alpha'} = \langle n-1,\alpha|\boldsymbol{Q}_\nu \boldsymbol{H}_{intr}\ \boldsymbol{Q}^\dagger_{\nu'}|n-1,\alpha'\rangle \qquad D^{(n)}_{\nu\alpha,\nu'\alpha'} = \langle n-1,\alpha|\boldsymbol{Q}_\nu\ \boldsymbol{Q}^\dagger_{\nu'}|n-1,\alpha'\rangle$$

Generalization of TDA matrix $A^{(n)}_{\nu\alpha,\nu'\alpha'} = (E^{n-1}_\alpha + E^1_\nu) + \mathcal{V}^{(n)}_{\nu\alpha,\nu'\alpha'}$

Overlap matrix $D^{(n)}_{\nu\alpha,\nu'\alpha'} = \delta_{\alpha\alpha'}\delta_{\nu\nu'} + \sum_\beta X^{\alpha\,(n-1)}_{\nu'\beta} X^{\alpha'(n-1)}_{\nu\beta} - \sum_{\substack{(ij)=(p_1p_2)\\(h_1h_2)}} \rho^{(n-1)}_{\alpha\alpha'}(ij)\rho^{(1)}_{\nu\nu'}(ij)$

phonon amplitudes

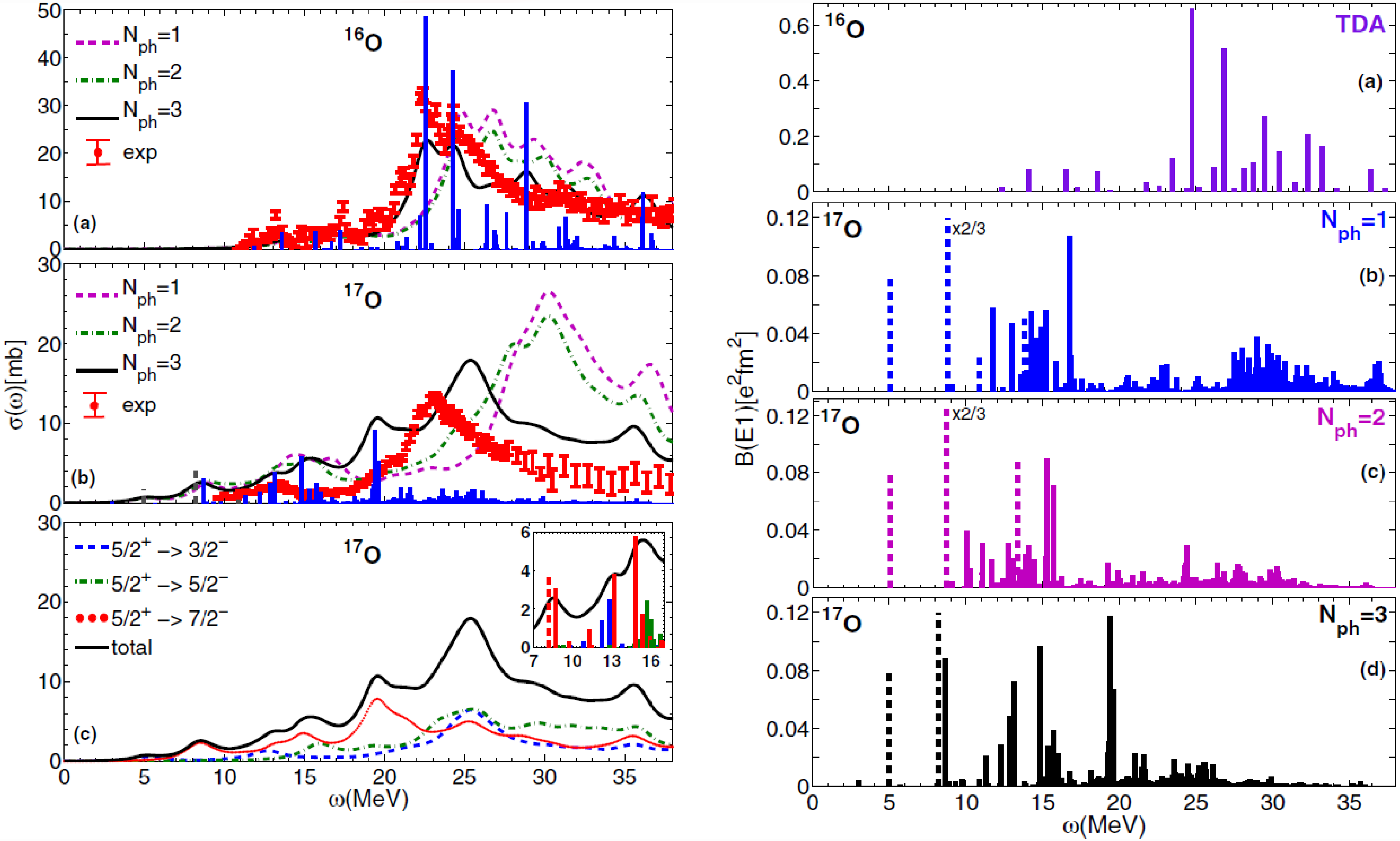
$$X^{\alpha\,(n-1)}_{\nu\beta} = \langle n-1,\alpha|\ \boldsymbol{Q}^\dagger_\nu|n-2,\beta\rangle = \sum_{\nu'\beta'} D^{(n-1)}_{\nu\beta,\nu'\alpha'} C^{\alpha(n-1)}_{\nu'\beta'}$$

*pp,hh* phonon densities

$$\rho^{(n-1)}_{\alpha\alpha'}(pp') = \langle n-1,\alpha|\ \boldsymbol{a}^\dagger_p \boldsymbol{a}_{p'}|n-1,\alpha'\rangle$$
$$\rho^{(n-1)}_{\alpha\alpha'}(hh') = \langle n-1,\alpha|\ \boldsymbol{a}^\dagger_h\ \boldsymbol{a}_{h'}|n-1,\alpha'\rangle$$

# EMPM: illustrative example

- EMPM (1+2+3) phonon calculation
- exact treatment computationally demanding → 3-phonon subspace → diagonal approximation

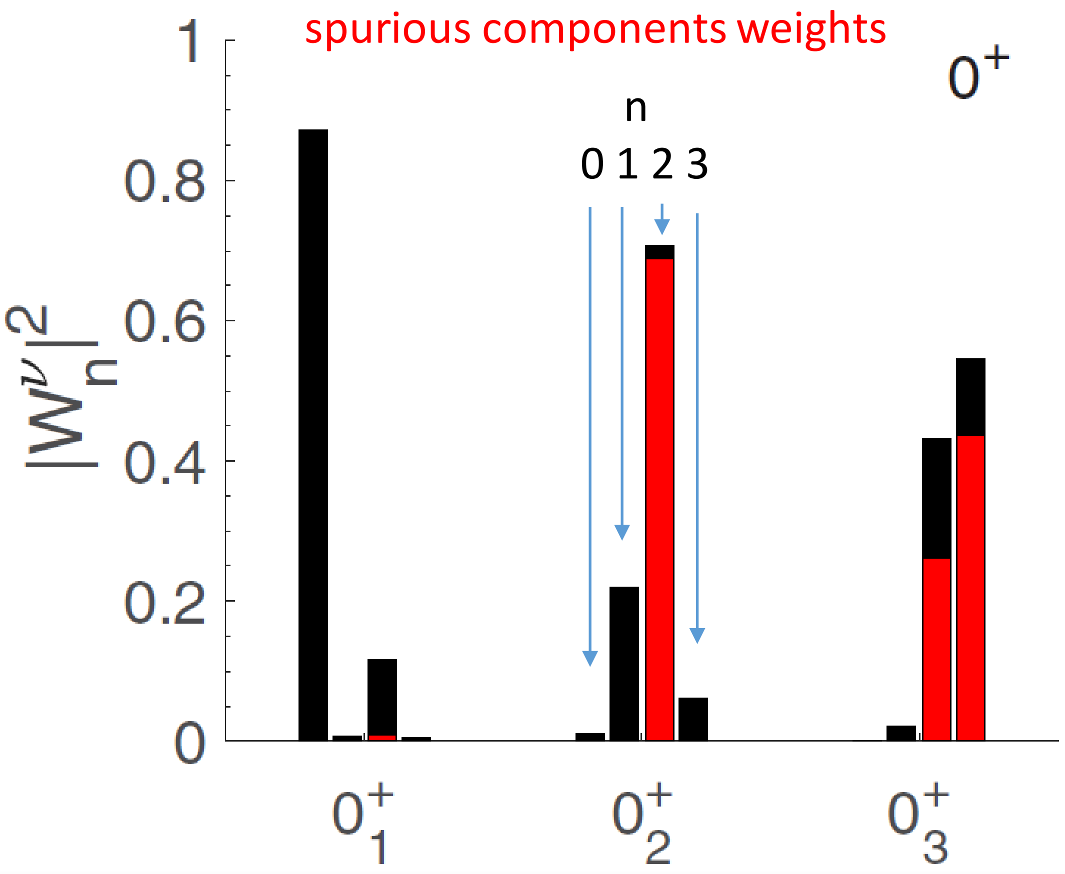


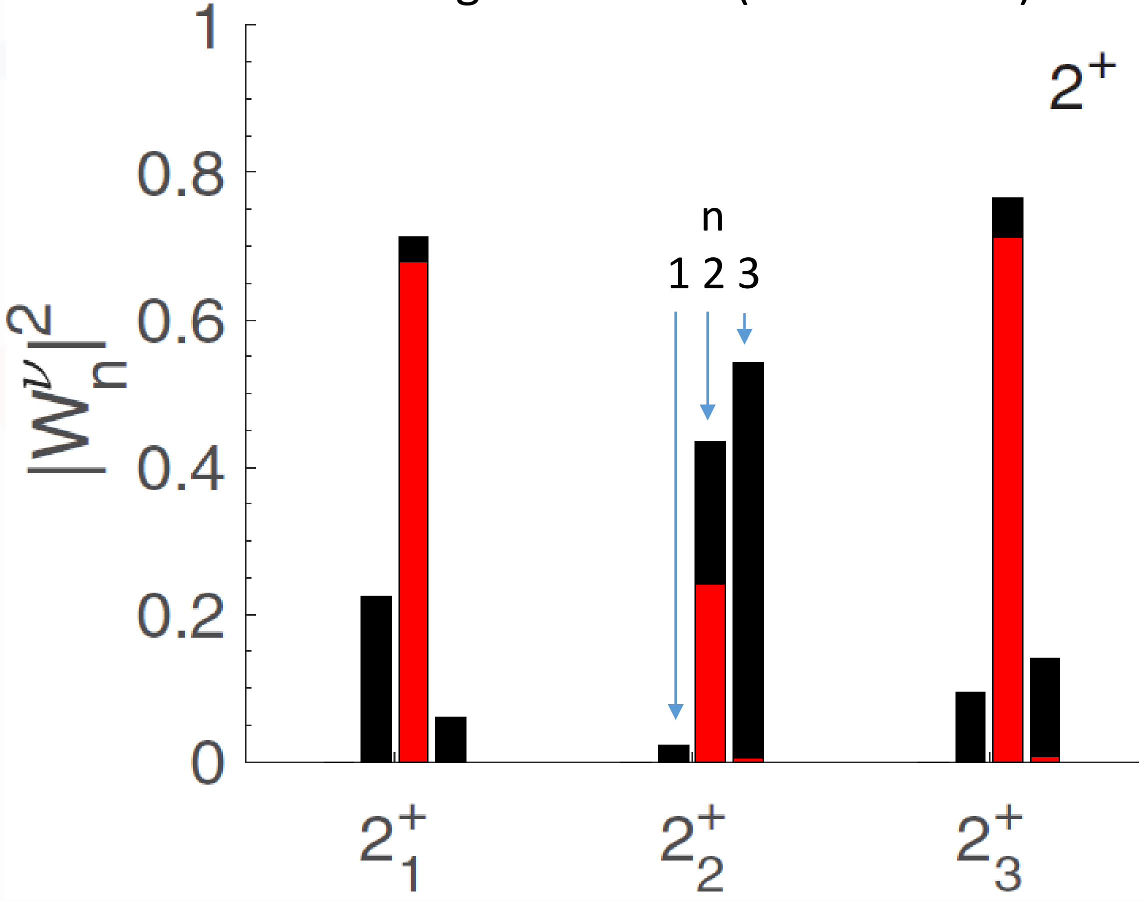

*G. De Gregorio, F.K.,N. Lo Iudice and P. Veselý, Phys. Rev. C 95, 034327 (2017), Phys. Rev. C 97, 034311 (2018)*

# Spurious states in EMPM

- test case: $^4$He, 0+1+2+3 phonon calculation
- How spurious is spectrum obtained within EMPM if n>1?

→ wave functions are contaminated, but we know how to fix it → CM orthogonalisation (EMPM-CMO)



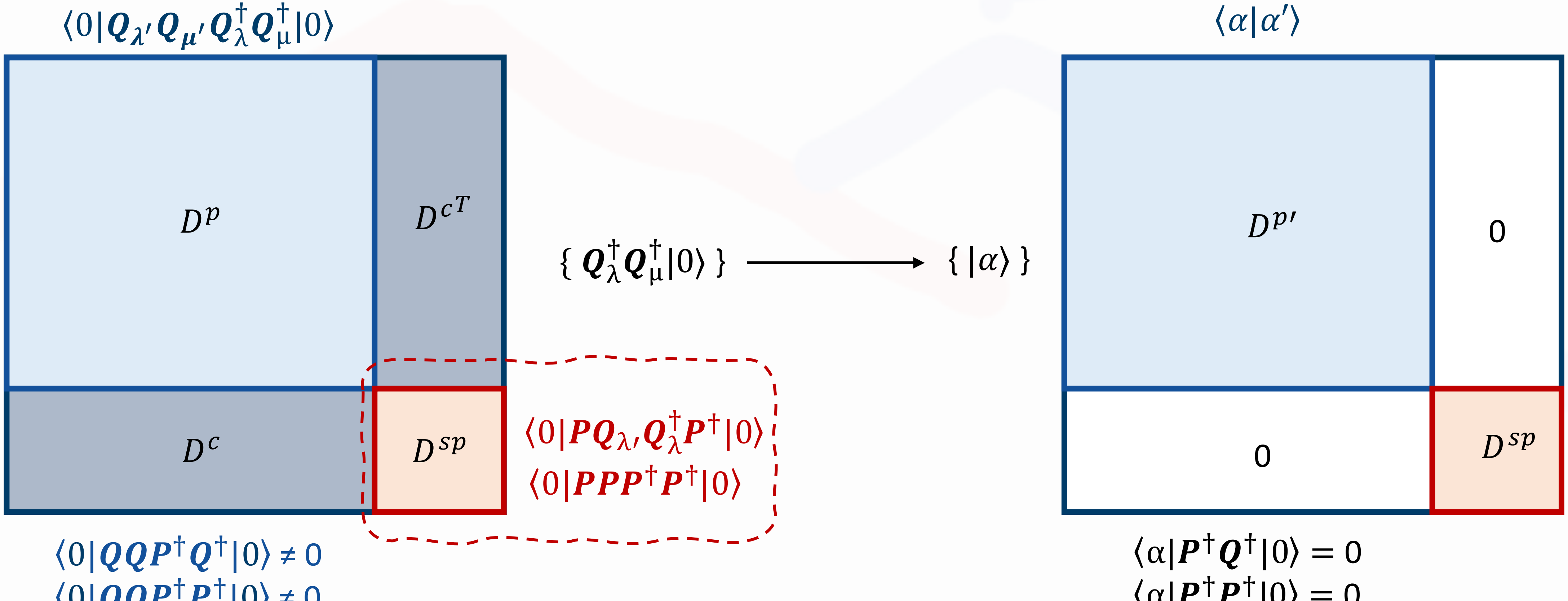

*G. De Gregorio, F.K., N. Lo Iudice and P. Veselý, Phys. Rev. C 105, 024326 (2022)*

# Elimination of spurious states in (2-phonon) EMPM

- advantage of the phonon basis → we know which basis states generate a spuriosity
- construction of spurious-free basis decoupled from the spurious subspace (for *n>1*)

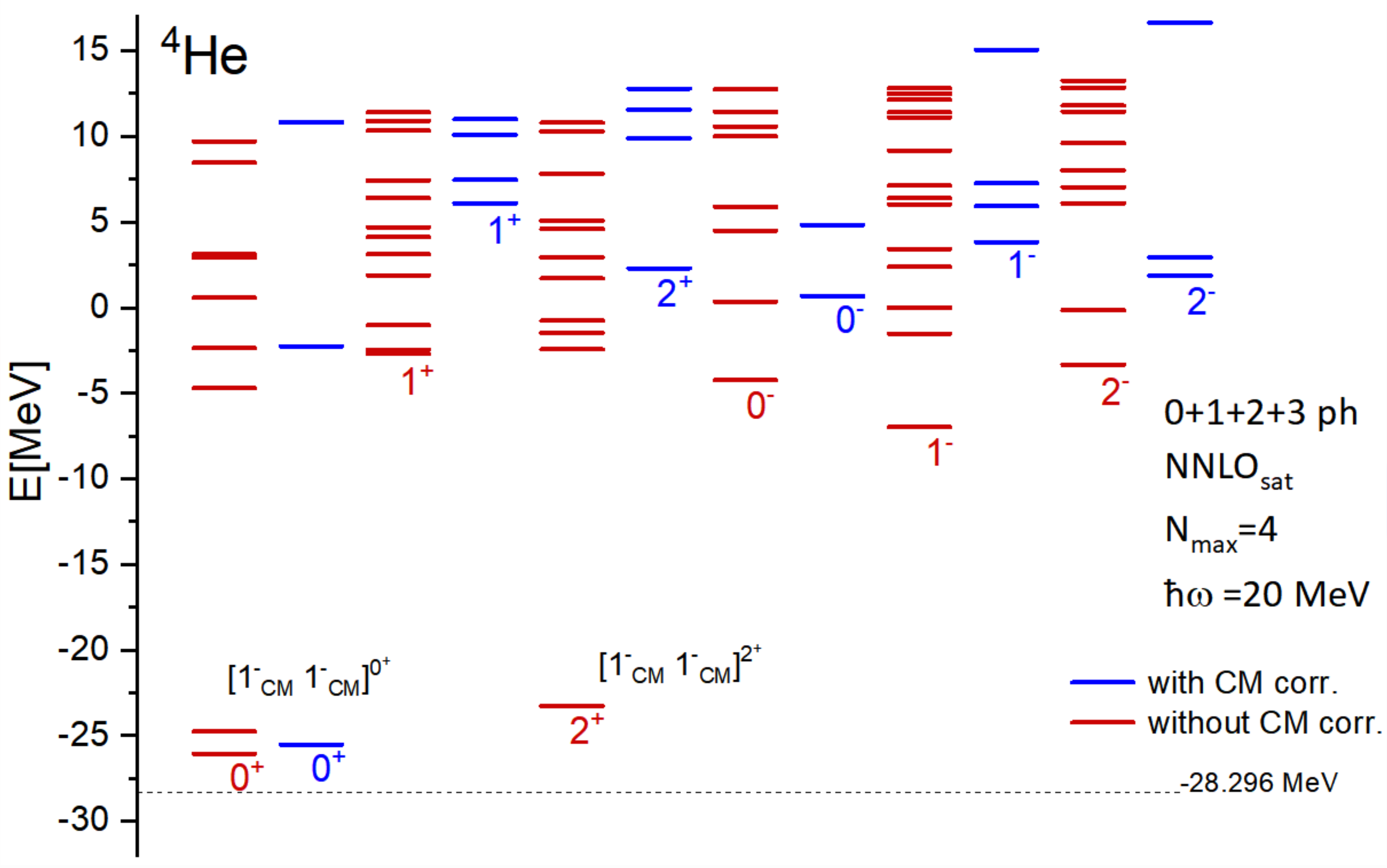
✓ singular value decomposition (SVD) of the overlap submatrix $D^c$

✓ **diagonalization of $H_{intr}$ in spurious-free basis**



# Spurious states in EMPM for n>1

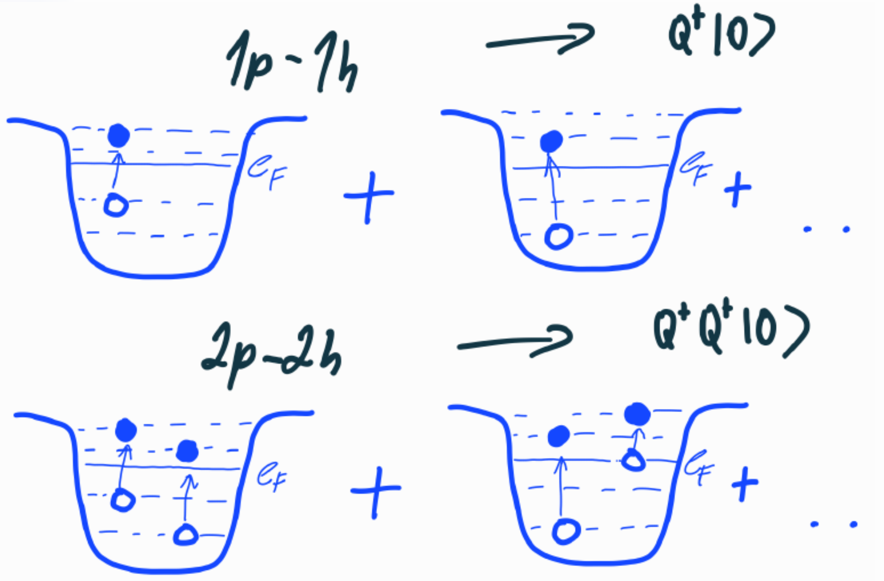
- Test case: $^4$He, n=0+1+2+3 phonon calculation



# EMPM-CMO vs. SRPA

- **Elimination of spuriosity is more tricky if „complex“ (multi-phonon) configurations are taken into account**

spurious dipole mode in extended RPA theories studied by
*V. Tselyaev, Phys. Rev C 106, 064327 (2022)*



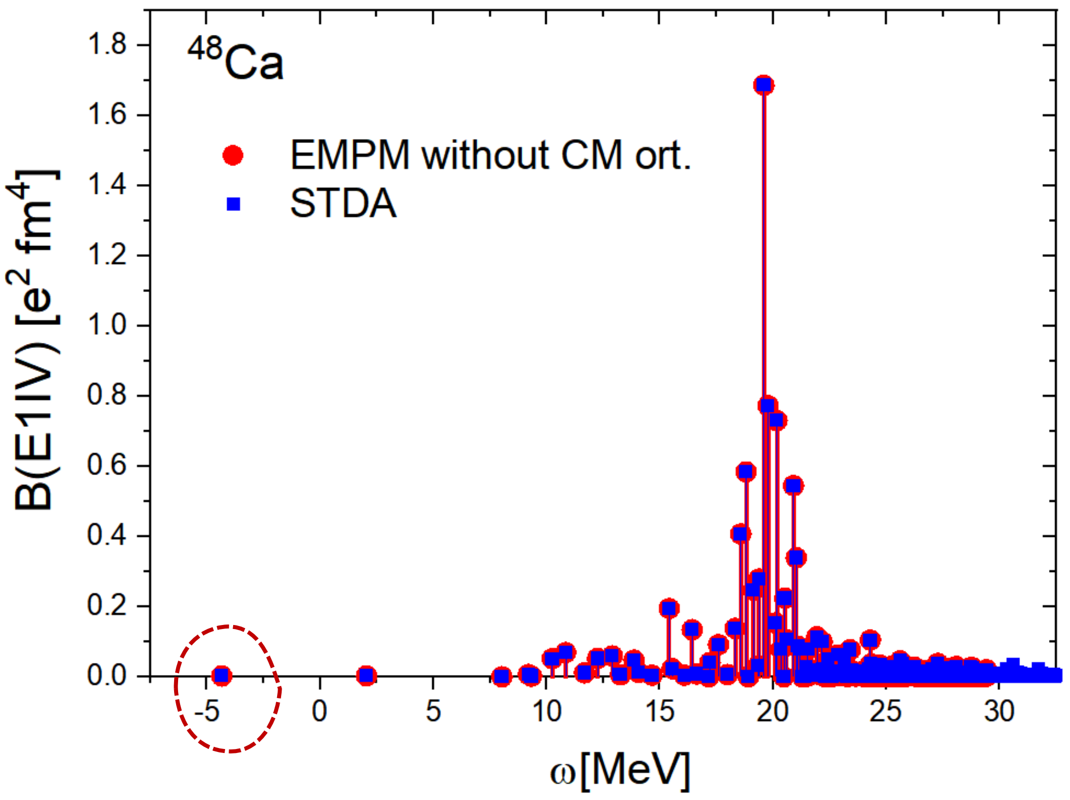

- **Is spurious CM contamination specific for EMPM**?
- **What about other methods?**
  → benchmark with large-scale SRPA calculations

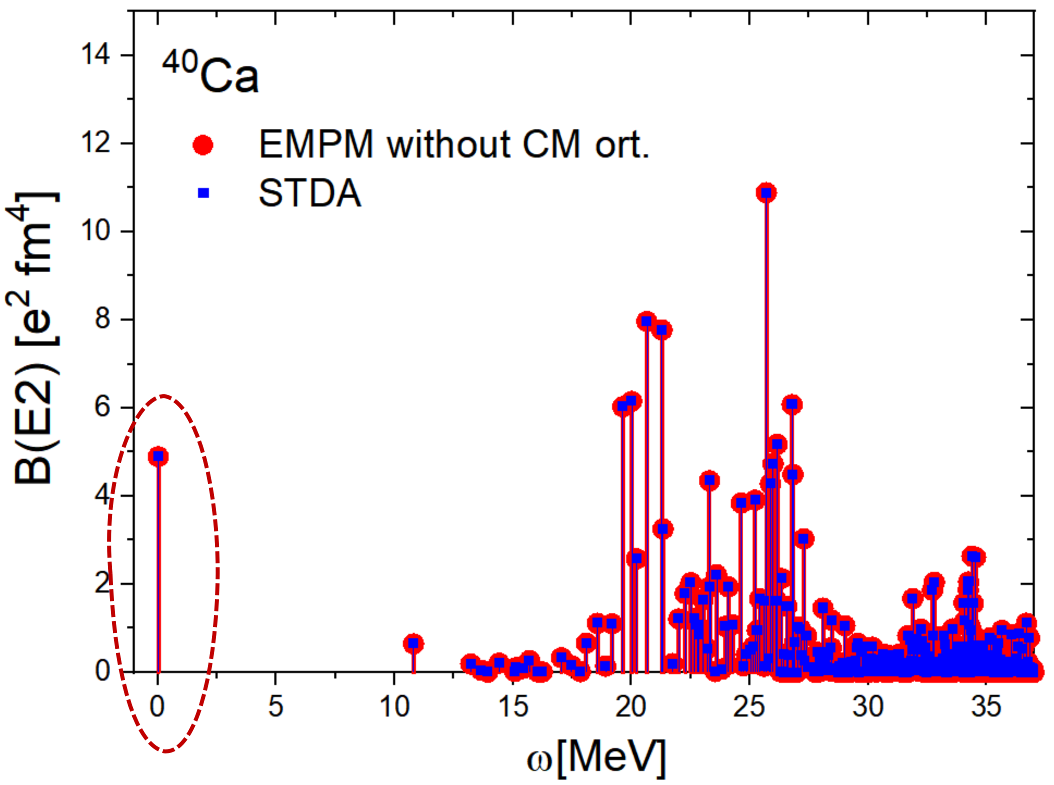
independent numerical check (HF, RPA/TDA, SRPA/STDA/EMPM),
only interaction m.e. were shared.

✓ EMPM (1+2-phonon) vs. SRPA, similarities/differences
✓ EMPM-CMO → impact on strength distributions?

# EMPM vs. STDA

- benchmark with large-scale SRPA/STDA calculations with UCOM potential (P. Papakonstantinou)
- electric responses in $^{16}$O,$^{40}$Ca,$^{48}$Ca




→ **EMPM** (1+2 phonon without CMO) **and STDA are equivalent in complete model space** (no truncation of *2p-2h* or 2-phonon basis) for all multipolarities **(„numerical proof“)**

→ **the same spurious states appear in STDA and EMPM** → so what about SRPA?

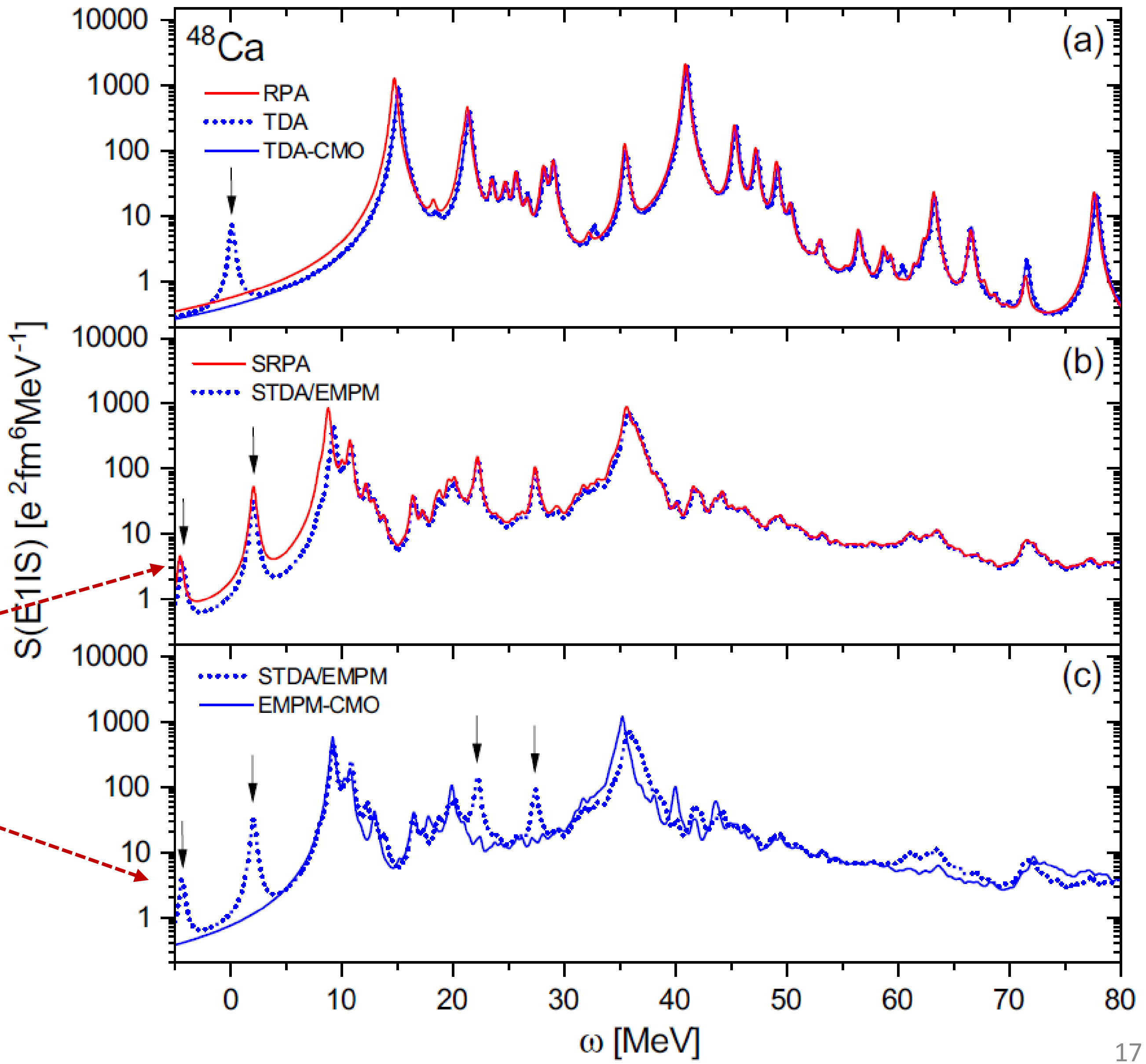
# EMPM-CMO vs. STDA/SRPA

- Isoscalar E1 sensitive to CM spurious states

$$M(\mathbf{E1IS}) \sim \sum_{i=1}^{A} \left(r_i^3 - \frac{5}{3}\langle r_i^2 \rangle r_i\right) Y_{1M}$$

- contribution from CM correction of the transition operator is 0 (by construction) in EMPM-CMO

✓ STDA/SRPA states with negative energy disappears in EMPM-CMO! (dominantly 1-phonon ≈ 95%)




*F.K., P. Papakonstatinou, P. Veselý, G. De Gregorio, J. Herko and N. Lo Iudice, Phys. Rev. C 107, 014305 (2023)*

# EMPM-CMO vs. STDA/SRPA

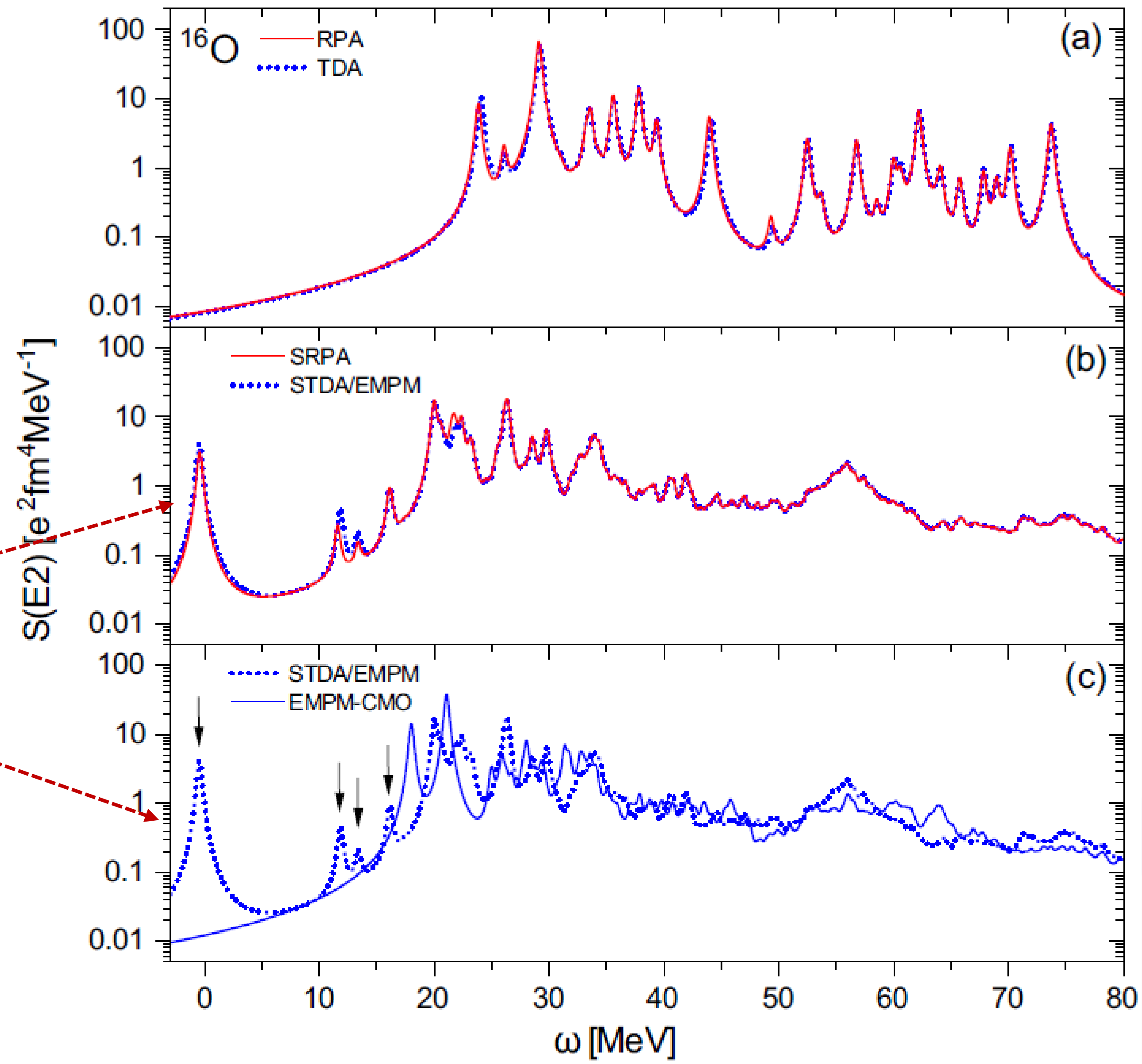
What about quadruple response?

$$M(\mathrm{E2}) \sim \sum_{i=1}^{A} r_i^2\, Y_{2M}$$

✓ several low-energy $2^+$ states dissapear after CMO

dominant 2-phonon componnent (≈ 88 %)

$$[1^-_{CM}\ \ 1^-_{CM}]^{2+}$$




*F.K., P. Papakonstatinou, P. Veselý, G. De Gregorio, J. Herko and N. Lo Iudice, Phys. Rev. C 107, 014305 (2023)*

# EMPM-CMO vs. STDA/SRPA

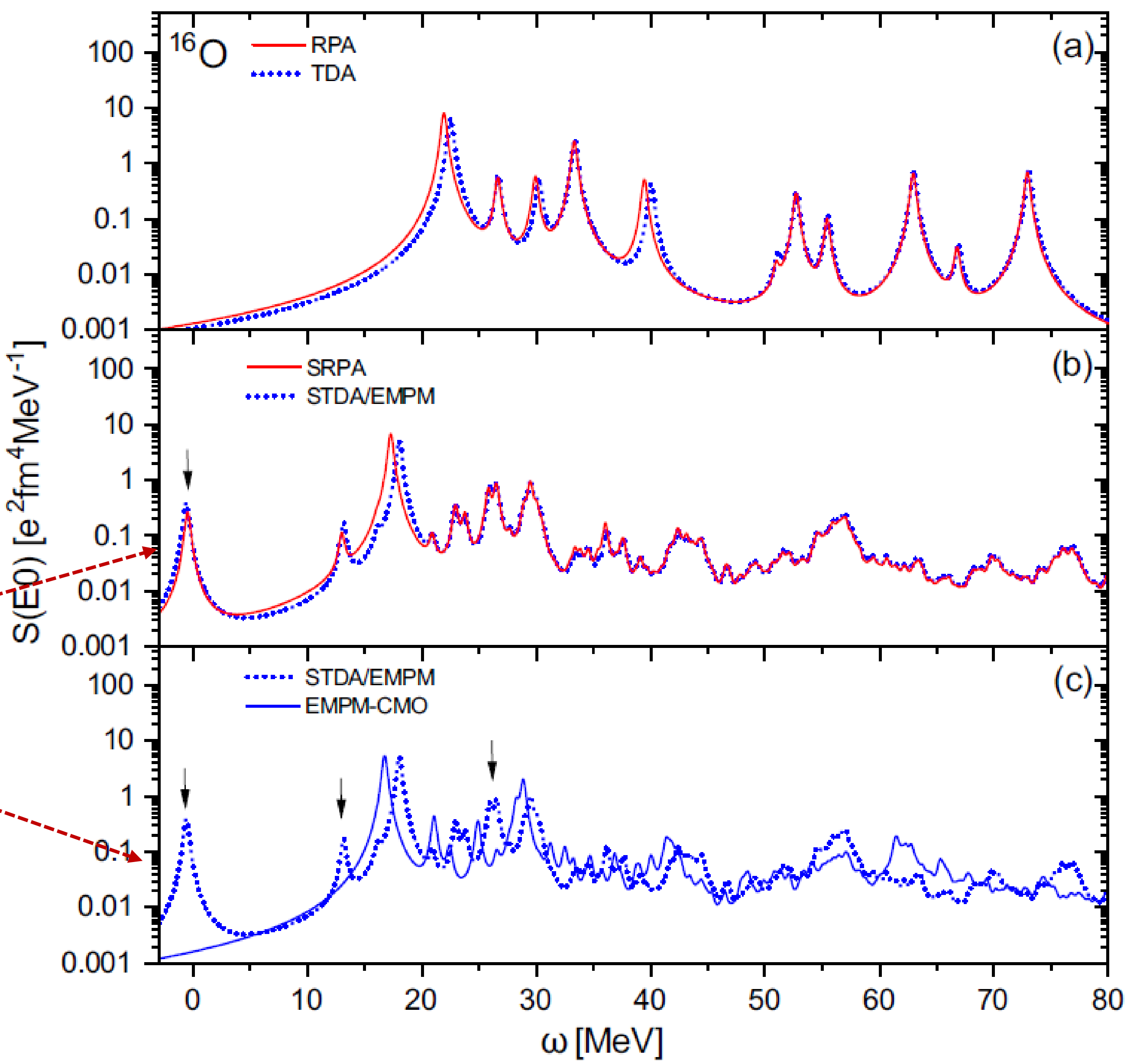
A similar behavior for monopole …

$$M(\mathrm{E0}) \sim \sum_{i=1}^{A} r_i^2\, Y_{00}$$

✓ several low-energy $0^+$ states disapear after CMO

dominant 2-phonon componnent (≈ 88%)

$$[1^-_{CM}\ 1^-_{CM}]^{0+}$$




*F.K., P. Papakonstatinou, P. Veselý, G. De Gregorio, J. Herko and N. Lo Iudice, Phys. Rev. C 107, 014305 (2023)*

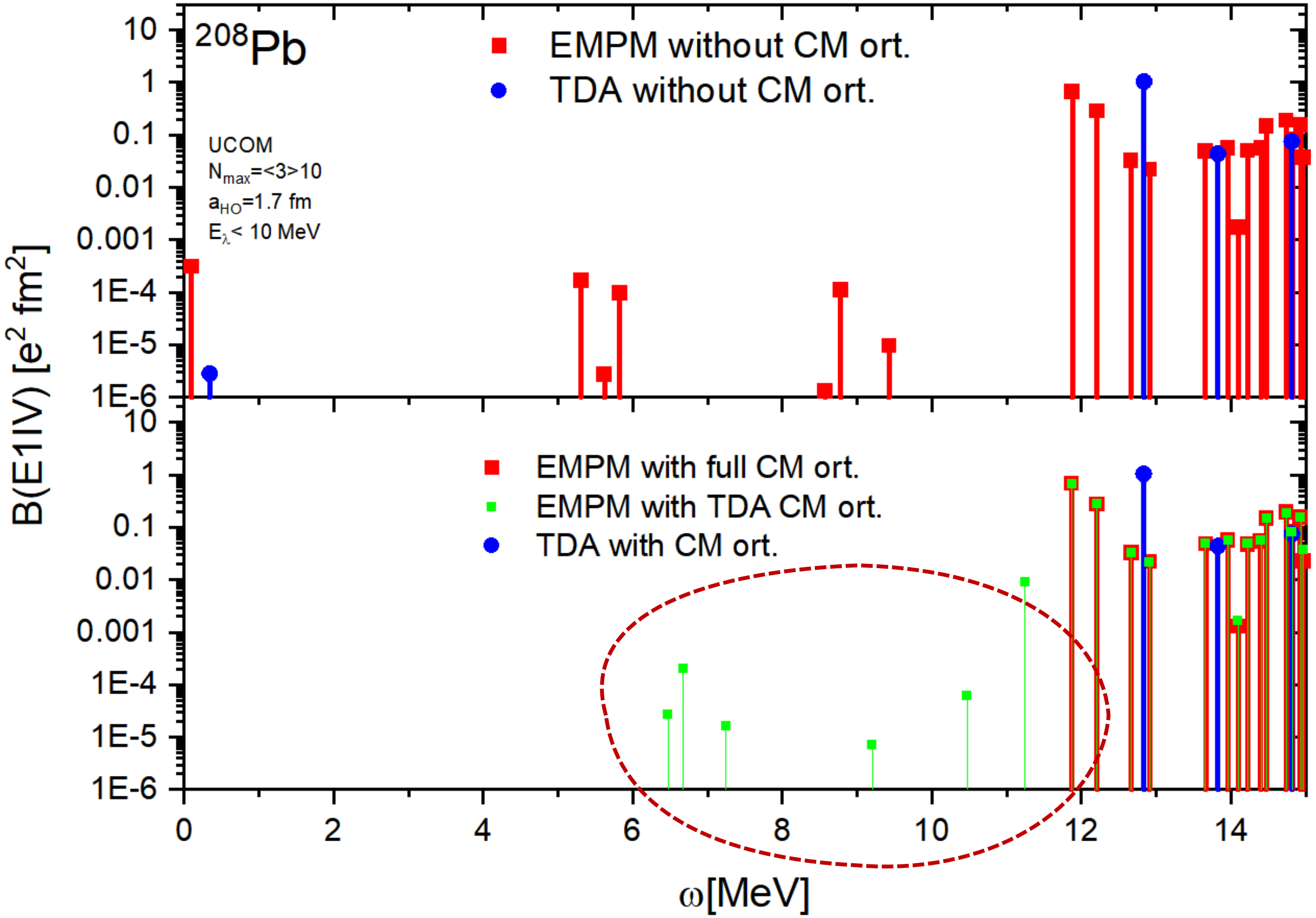
# EMPM-CMO vs. STDA/SRPA

- does it have an impact on low-lying dipole strength?

→ preliminary calculation in restricted model space → peaks are too high in energy

✓ we can effectively eliminate CM in TDA only, and no significant spurious strength appears in E1IV response

✓ **fake states in the low-lying dipole spectrum** which disappear if we apply CMO



# Conclusions & Prospects

- problem of spurious states studied within microscopic approaches SRPA/STDA and EMPM
- effective procedure for elimination of spurious contamination within EMPM from nuclear spectra and responses was developed
- **existence of fake states in SRPA/STDA , especially in the low-energy part of spectra**

**Prospects:**

- effect of CMO in odd systems (one particle/hole-phonon coupling)
- CM contamination of low-lying dipole strength in heavy systems
- spurious modes connected with particle number violation