Center-of-mass problem in nuclear structure calculations

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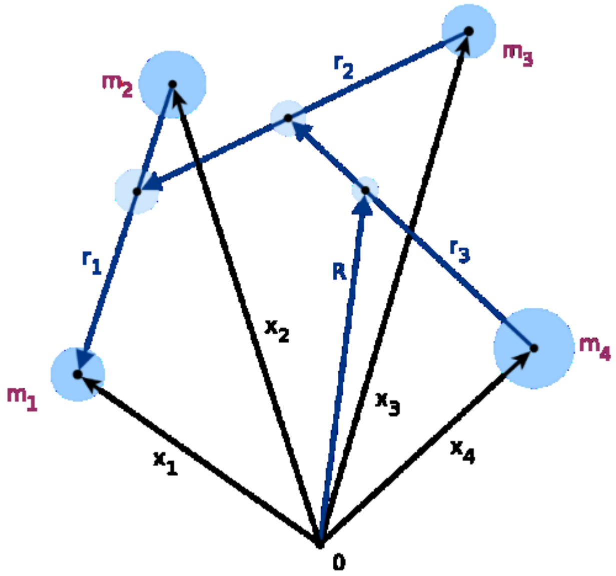
Outline

Center-of-mass (CM) problem in nuclear models (closed-shell nuclei)

- One-phonon models
- Multiphonon model
- Numerical examples

Center-of-mass problem in microscopic nuclear models

- translationally invariant nuclear Hamiltonian



$$\boldsymbol{H} = \sum_{i=1}^{A} \frac{\boldsymbol{p}_i^2}{2m} + \sum_{i<j}^{A} \boldsymbol{V}_{ij} = \boldsymbol{H}_{\boldsymbol{int}} + \frac{\boldsymbol{P}^2}{2Am}$$

factorization of eigenstates: $\psi(\boldsymbol{R}, \boldsymbol{r}) = \varphi_{\boldsymbol{CM}}(\boldsymbol{R})\chi_{\boldsymbol{int}}(\boldsymbol{r})$

- nuclear A-body problem:

→ central potential with fixed origin to which particle motion is referred → single-particle basis (Slater determinants)
→ *3A* coordinates, only *3A-3* describe intrinsic motion

- withinin most models **exact factorization is not possible** (finite model spaces)
  effective Hamiltonian is not translationally invariant → **appearance of CM spurious states in spectra**

  interacting shell model (excitations outside closed major shells)
  J. P. Elliot and T. H. Skyrme, Proc. Roy. Soc. London A232 561 (1955)

Center-of-mass (CM) problem is inherently present in all model based on the mean-field!

Center-of-mass problem in microscopic nuclear models

> APPENDIX C: THE CENTER-OF-MASS PROBLEM
>
> "What do you do about center of mass?" is probably the standard question most shell-model practitioners prefer to ignore or dismiss. Even if we may be tempted to do so, there is no excuse for ignoring what the problem is, and here we would like to explain it in sufficient detail to dispel some common misconceptions.
>
> *E. Caurier et at, Rev. Mod. Phys. 77, 2005*

Are there solutions of CM problem in nuclear physics?
Yes, many "solutions"! (…and some are wrong)
But in many cases we just hope that CM effects are small in our calculation!

Some approaches avoid the CM problem

- ***few body systems*** - Jacobi coordinates – feasible just for the lightest systems
- ***Ab-initio No-core shell model (NCSM)***
  exact factorization of intrinsic and center-of-mass wave function in **HO sp. basis only** (complete set of N_{max} basis states)

Plethora of ***approximative methods*** developed for more or less specific situations

some examples:

- **Shell model**: *G.H. Gloeckner, R.D. Lawson, Phys. Lett B **53**, 313 (1974)*
- **RPA**: *F. Dönau, Phys. Rev. Lett. **94**, 092503 (2005)*
- **Nuclear level densities**: *M. Horoi and V. Zelevinsky Phys. Rev. Lett. **98**, 262503 (2007)*
- **Coupled-cluster**: *G. Hagen, T. Papenbrock, and D.J. Dean Phys. Rev. Lett. **103**, 062503 (2009)*
- **QRPA**: *A. Repko, J. Kvasil, V. O. Nesterenko, Phys. Rev. C**99**,044307 (2019)*

Microscopic models of (collective) excitations

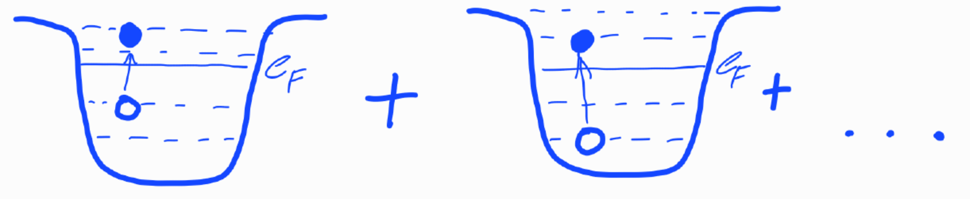
- mean-field → optimisation of single-particle basis → refference state (HF vacuum) $|HF\rangle$

$$\boldsymbol{H_{intr}} = \sum_i e_i \boldsymbol{a_i^\dagger a_i} + \frac{1}{4}\sum_{ijkl} V_{ijkl}\!:\boldsymbol{a_i^\dagger\, a_j^\dagger\, a_l\, a_k}\!: - \frac{1}{2}\sum_{ij\in h} V_{ijij}$$

- excited states → superpositions of elementary particle-hole (*1p-1h)* excitations $\boldsymbol{a_p^\dagger a_h}|0\rangle \rightarrow \boldsymbol{Q_\nu^+}|0\rangle$

collective excitations → phonons $[\boldsymbol{H_{intr}}, \boldsymbol{Q_\nu^\dagger}]|0\rangle \equiv \hbar\omega_\nu \boldsymbol{Q_\nu^\dagger}|0\rangle$

$$|\nu\rangle = \boldsymbol{Q_\nu^\dagger}|0\rangle, \quad \boldsymbol{Q_\nu}|0\rangle = 0$$



- **RPA (Random Phase Approximation):** *1p-1h* model with ground state correlations ($|0\rangle \neq |HF\rangle$)

$$\boldsymbol{Q_\nu^+} = \sum_{ph} X_{ph}\, \boldsymbol{a_p^\dagger a_h} - Y_{ph} \boldsymbol{a_h^\dagger a_p}$$

quasiboson approximation $[\boldsymbol{Q_\mu}, \boldsymbol{Q_\nu^\dagger}] \approx \delta_{\mu\nu}$ → $\boldsymbol{H_{intr}} \approx \sum_\nu \hbar\omega_\nu \boldsymbol{Q_\nu^\dagger Q_\nu} + E_{RPA}$

→ *harmonic oscillations around the mean-field minimum*

- **TDA (Tamm-Dancoff Approximation):** *1p-1h* model without ground state correlations ($|0\rangle = |HF\rangle$, $Y_{ph} = 0$)

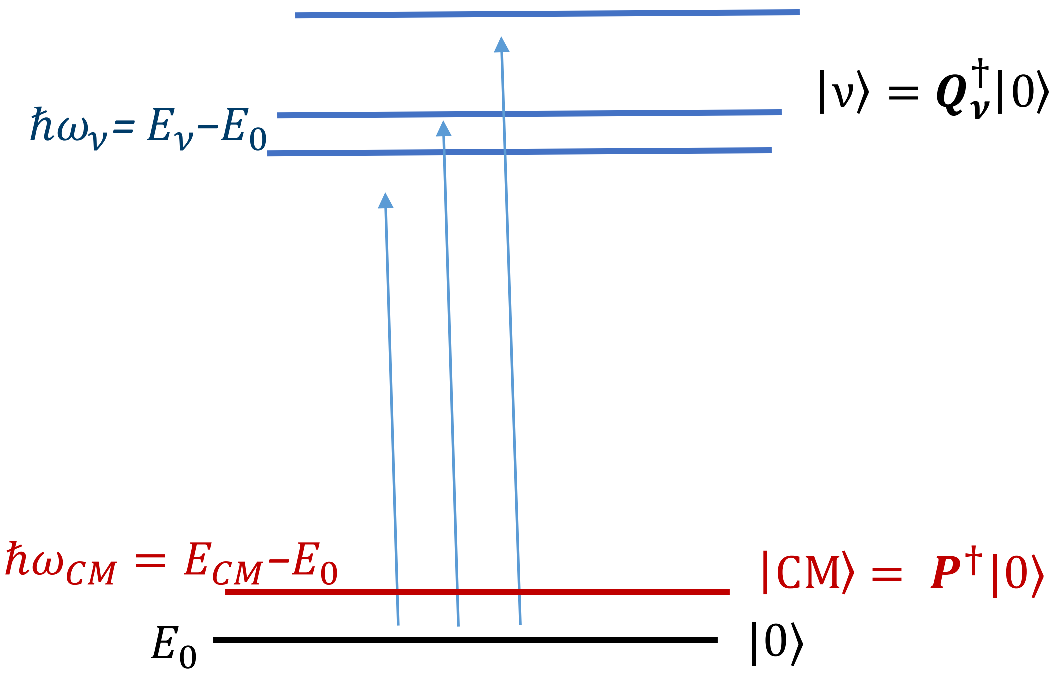
CM problem in phonon models (RPA/TDA)

- breaking of translational symmetry in the HF → **existence of spurious solution with $\hbar\omega_{CM} = 0$ in the RPA (not TDA)**

  → separation from physical states

  hard to achieve numerically (finiteness of the model space)

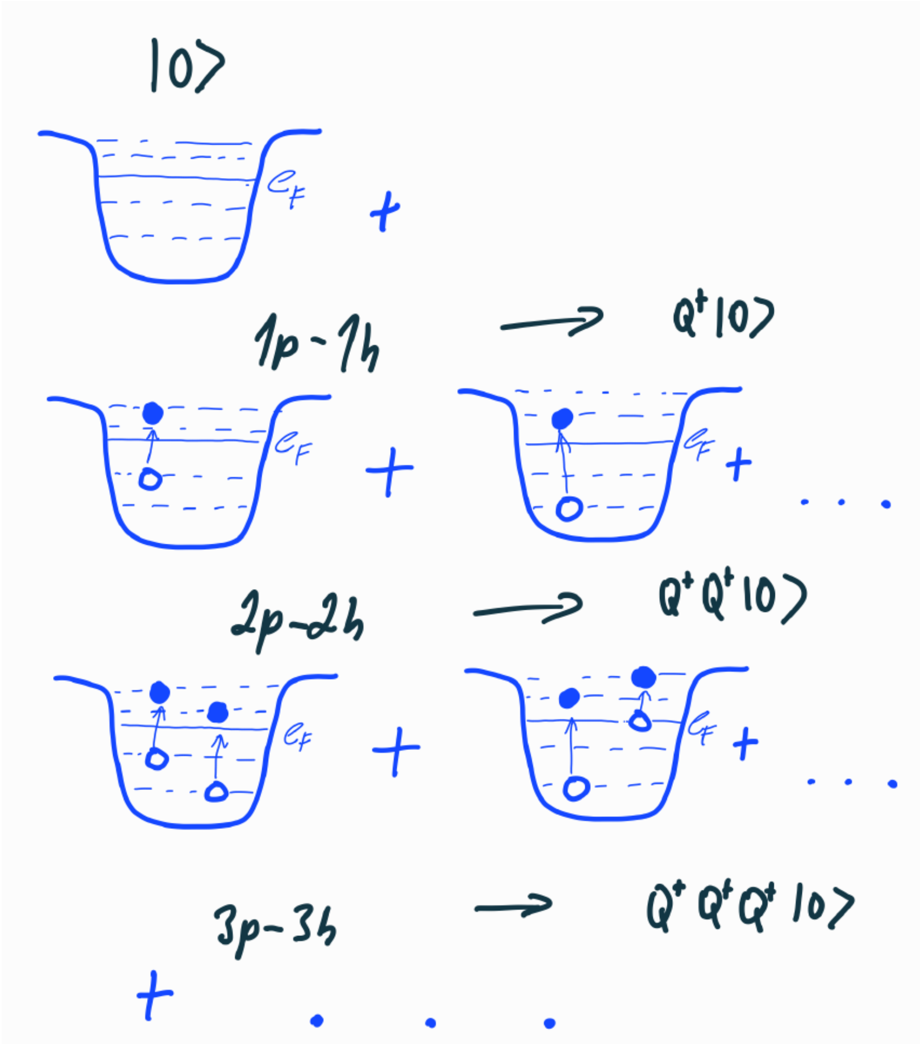
  → spurious CM mode with small energy (*isoscalar dipole mode* $J^\pi = 1^-, T = 0$) → mixing with physical states
- elimination of CM state → construction of basis $\{|\alpha\rangle\}$ orthogonal to the CM mode $\boldsymbol{P}^\dagger|0\rangle$ ↔ $\langle\alpha|\boldsymbol{P}^\dagger|0\rangle$=0



Multiphonon excitations

- nuclear states are more complicated than 1-phonon excitations
- expansion of many-body states into basis of TDA multiphonon states: $\{\,|HF\rangle, \boldsymbol{Q}_\nu^\dagger|HF\rangle\,, \boldsymbol{Q}_\nu^\dagger\boldsymbol{Q}_\mu^\dagger|HF\rangle, \boldsymbol{Q}_\nu^\dagger\boldsymbol{Q}_\mu^\dagger\boldsymbol{Q}_\lambda^\dagger|HF\rangle \ldots\,\}$
- Equation of motion Phonon Method (EMPM) → partitioning of the many-body space into phonon subspaces

G. De Gregorio, F. Knapp, N. Lo Iudice, and P. Veselý Phys. Rev. C ***101****, 024308 (2020)*



n=0 → **HF**

n=1 → **TDA**

n=2 → **STDA**

n=3

$$\boldsymbol{H}_{intr} = \sum_{n,\alpha} E_\alpha^n |n,\alpha\rangle\langle n,\alpha| + \sum_{nn',\alpha\alpha'} |n',\alpha'\rangle\langle n',\alpha'|\boldsymbol{H}_{intr}|n,\alpha\rangle\langle n,\alpha|$$

n-phonon subspace

- generalized eigenvalue problem in **redundant nonorthogonal basis**

$$H^n\, C = E^n\, D^n\, C$$

$$H_{\beta\alpha}^n = \langle n,\beta|\boldsymbol{H}_{intr}|n,\alpha\rangle \qquad D_{\beta\alpha}^n = \langle n,\beta|n,\alpha\rangle$$

- fermionic structure of phonons
- **removal of CM contamination**

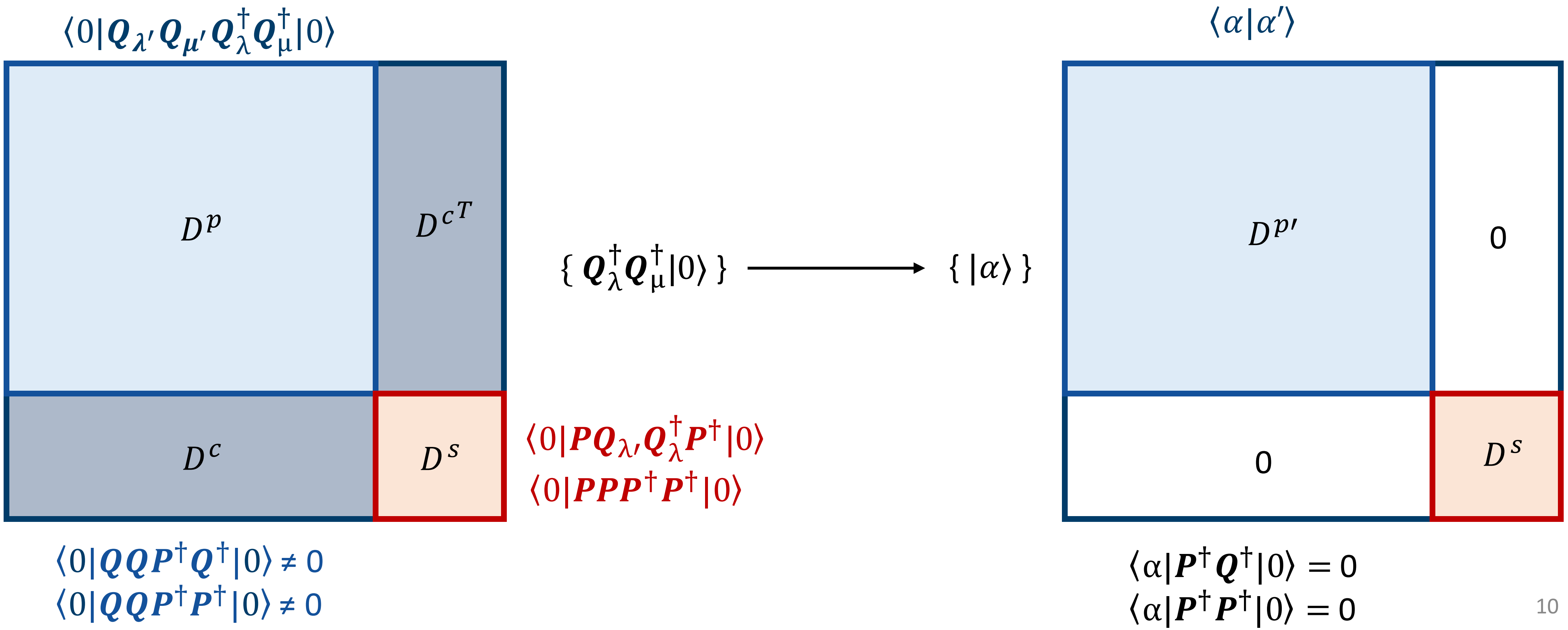
The most difficult task is to calculate matrices H and D without approximations for *n>2*

CM problem in EMPM

- construction of spurious-free phonon states and the CM state in the TDA (Gramm-Schmidt ort. in $J^{\pi}=1^{-}$ sector)
- decomposition of model space into spurious and physical subspaces (for *n>1*)
- construction of basis orthogonal to spurious subspace (for *n>1*)
- diagonalization of $\boldsymbol{H}_{intr}$ in transformed (and reduced) basis

  → singular value decomposition of the overlap submatrix D^{c}

  G. De Gregorio, F. Knapp, N. Lo Iudice, P. Veselý, Phys. Lett. B ***821****, 136636 (2021)*

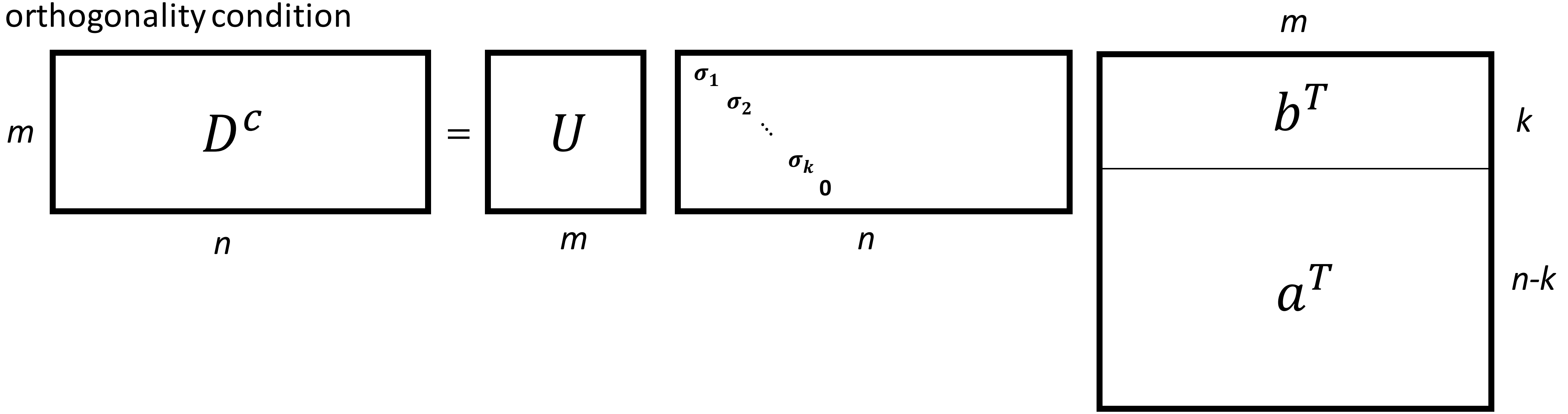


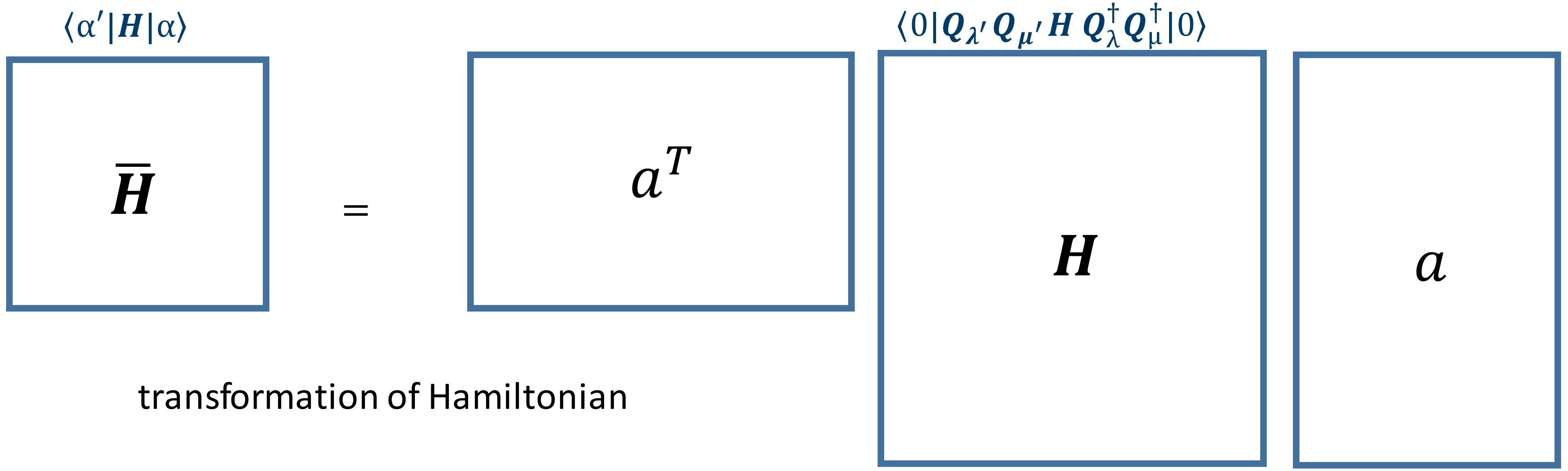
CM problem in EMPM

Singular value decomposition of real *m* x *n* matrix $\boldsymbol{D^c}$: $\boldsymbol{D^c = U\Sigma V^T}$, where (*m* x *m*) $\boldsymbol{U}$ and (*n* x *n*) $\boldsymbol{V}$ are orthogonal matrices

right singular vectors $\boldsymbol{V}$ corresponding to zero singular values span the null space(kernel) of $\boldsymbol{D^c}$

$\boldsymbol{D^c}a = 0 \leftrightarrow$ orthogonality condition





transformation of Hamiltonian

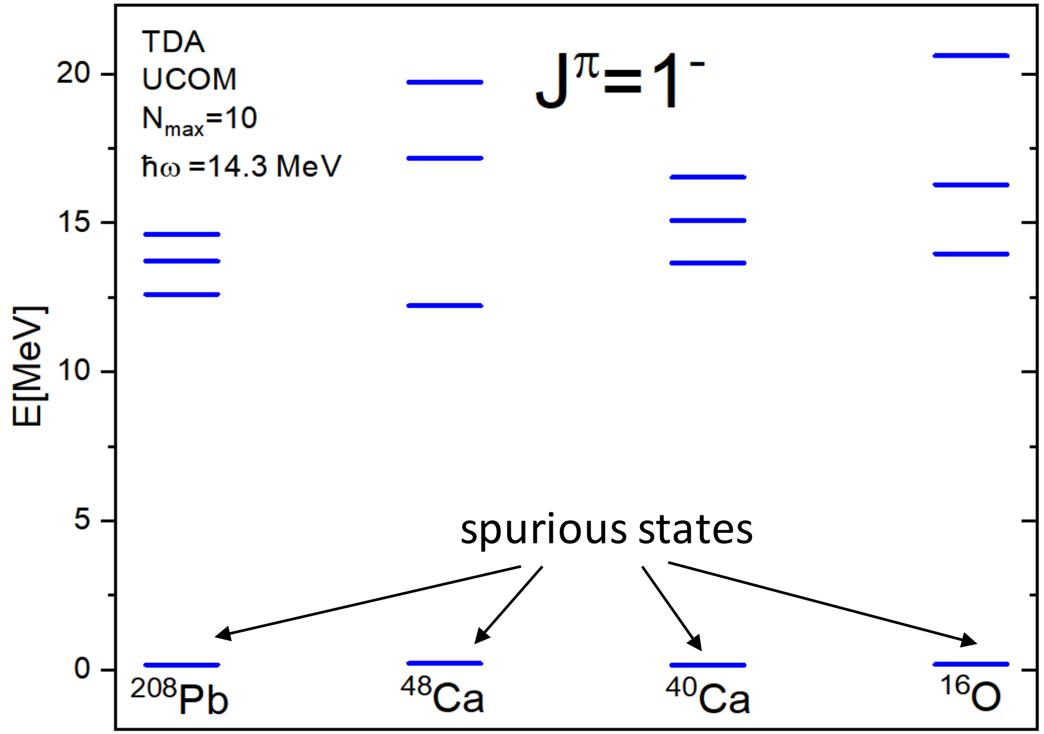
CM problem in phonon models (RPA/TDA)

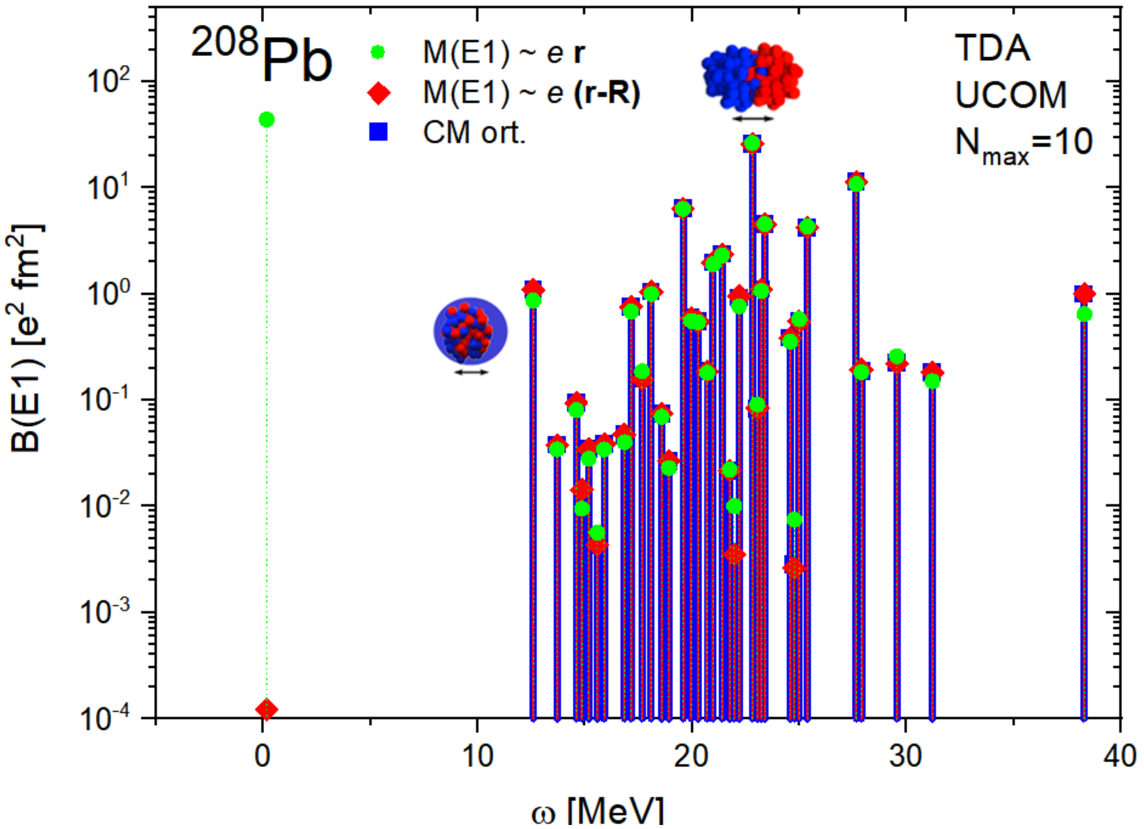
- closed-shell nuclei: CM mode contaminates $J^\pi=1^-$ excitation spectrum
- RPA/TDA: subtraction of CM contribution from transition operators only → wave functions contain CM admixture
  reasonable approximation if $\hbar\omega_{CM} << \hbar\omega_{\nu}$

electric dipole transition $B(E1) \sim |\langle i|\boldsymbol{M}(\boldsymbol{E1})|g.s.\rangle|^2$

$$\boldsymbol{M}(E1\ IS) \sim \boldsymbol{R}, \qquad \boldsymbol{R} = \frac{1}{A}\sum_{i=1}^{Z}\boldsymbol{r}_i + \frac{1}{A}\sum_{i=1}^{N}\boldsymbol{r}_i$$

$$\boldsymbol{M}(E1) \sim e\sum_{i=1}^{Z}\underbrace{(\boldsymbol{r}_i - \boldsymbol{R})}_{r_{intr}} = e\frac{N}{A}\sum_{i=1}^{Z}\boldsymbol{r}_i - e\frac{Z}{A}\sum_{i=1}^{N}\boldsymbol{r}_i$$

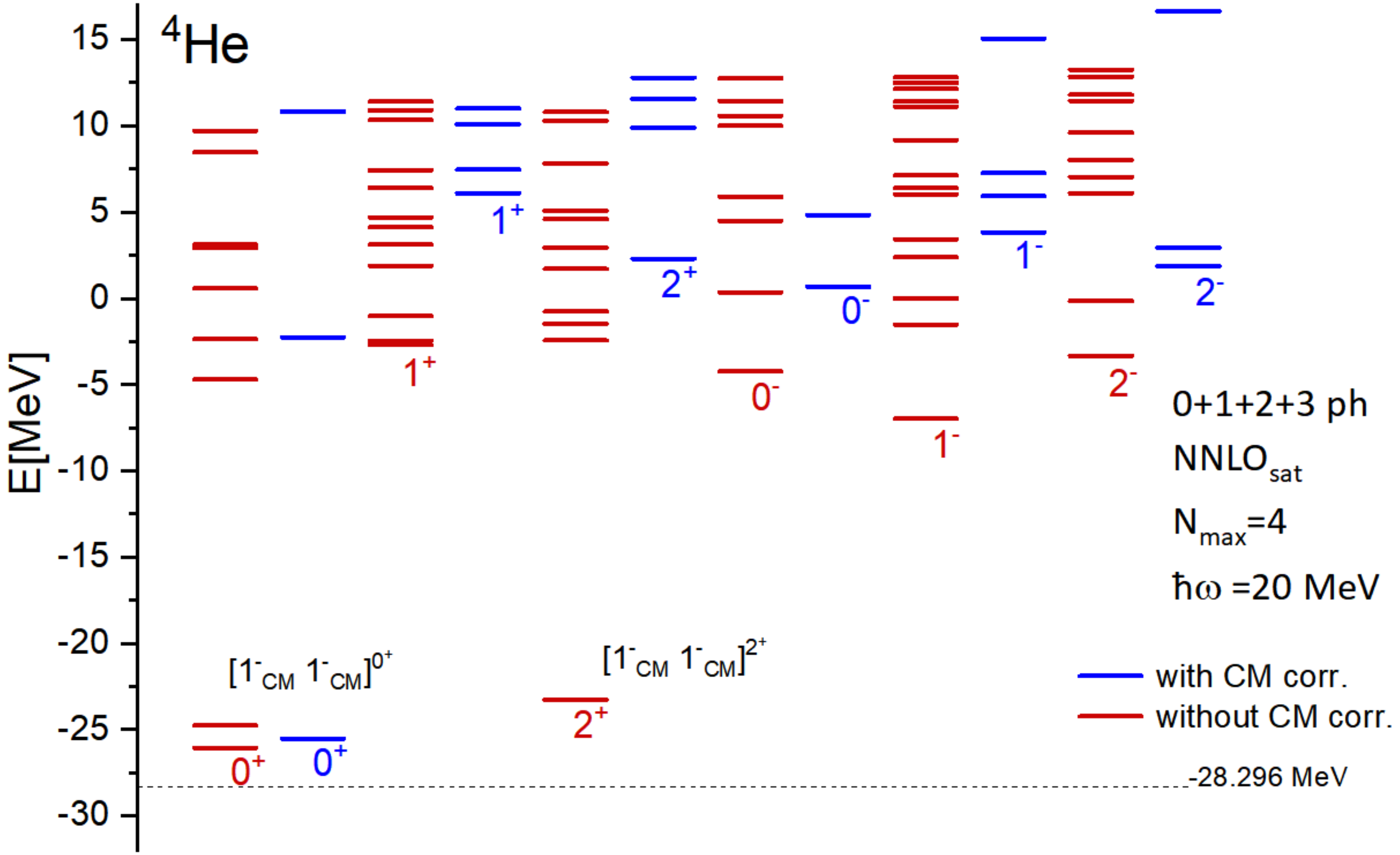




CM problem in EMPM

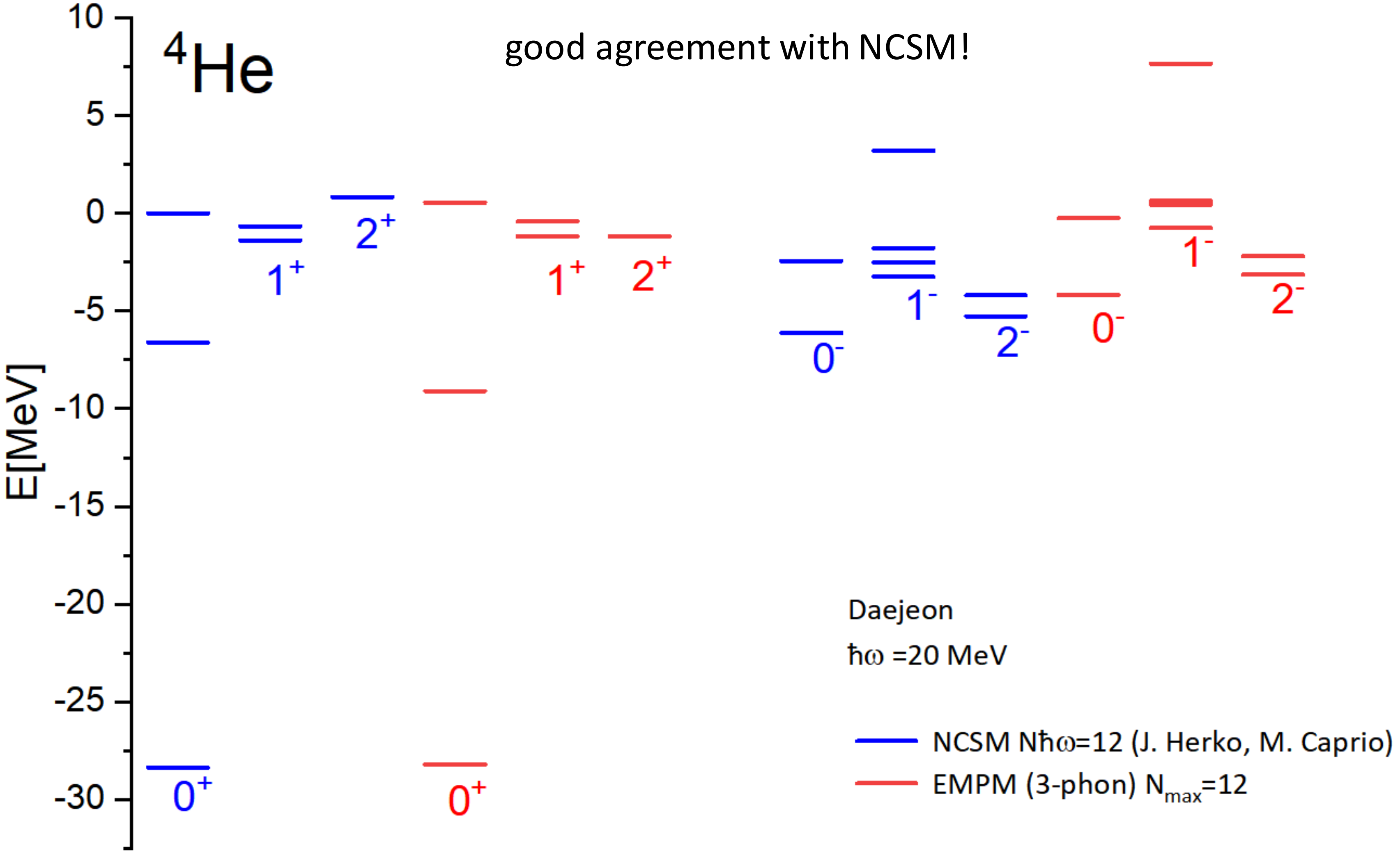
Test of the method: spectrum of ^{4}He calculated up to 3-phonons

- spurious states for all spins and both parities
- is the removal procedure correct and effective? → comparison with the exact approach (NCSM with Daejeon potential)
- is the CM contamination exaggerated in the EMPM? → comparison with other commonly used approaches (STDA, SRPA)



EMPM vs. NCSM

- NCSM and EMPM model spaces are different (HF vs HO sp. basis, phonon vs. $\mathbf{N}\hbar\omega$ truncation)
- large space calculation lengthy → approximative calculation of 3-phon. subspace (we omit interaction between 3-ph. states)
- heavier systems in near future (in collaboration with J. Herko and M. Caprio)

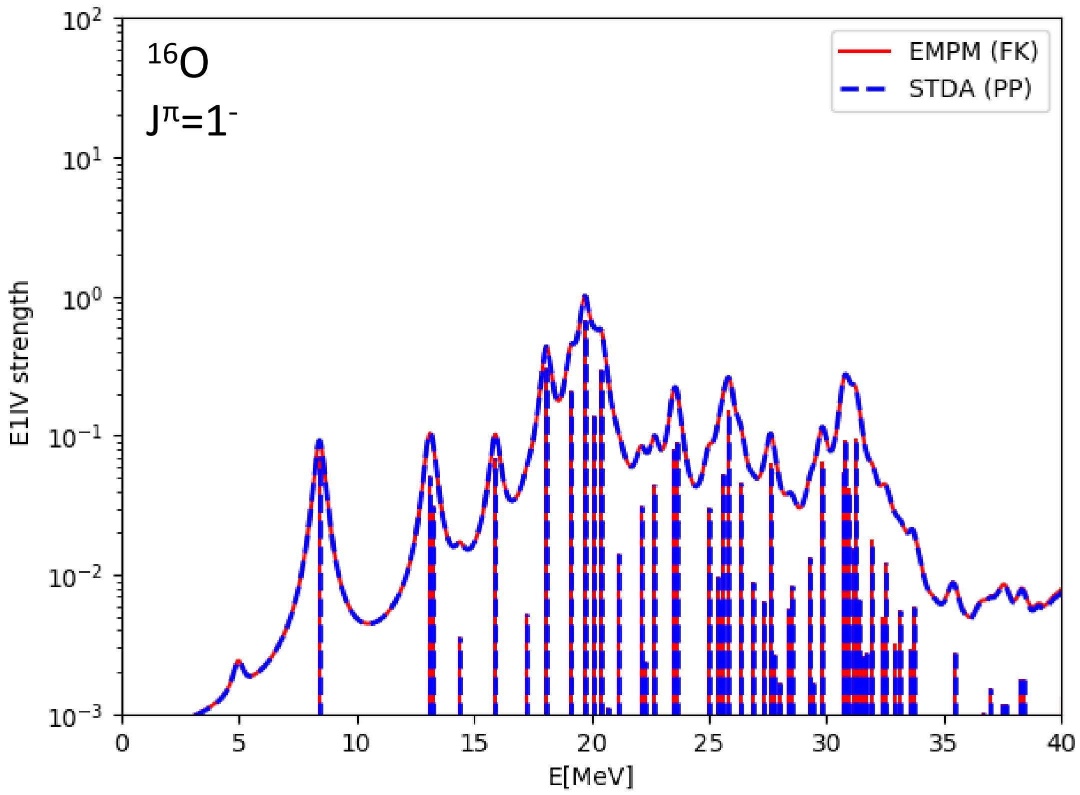


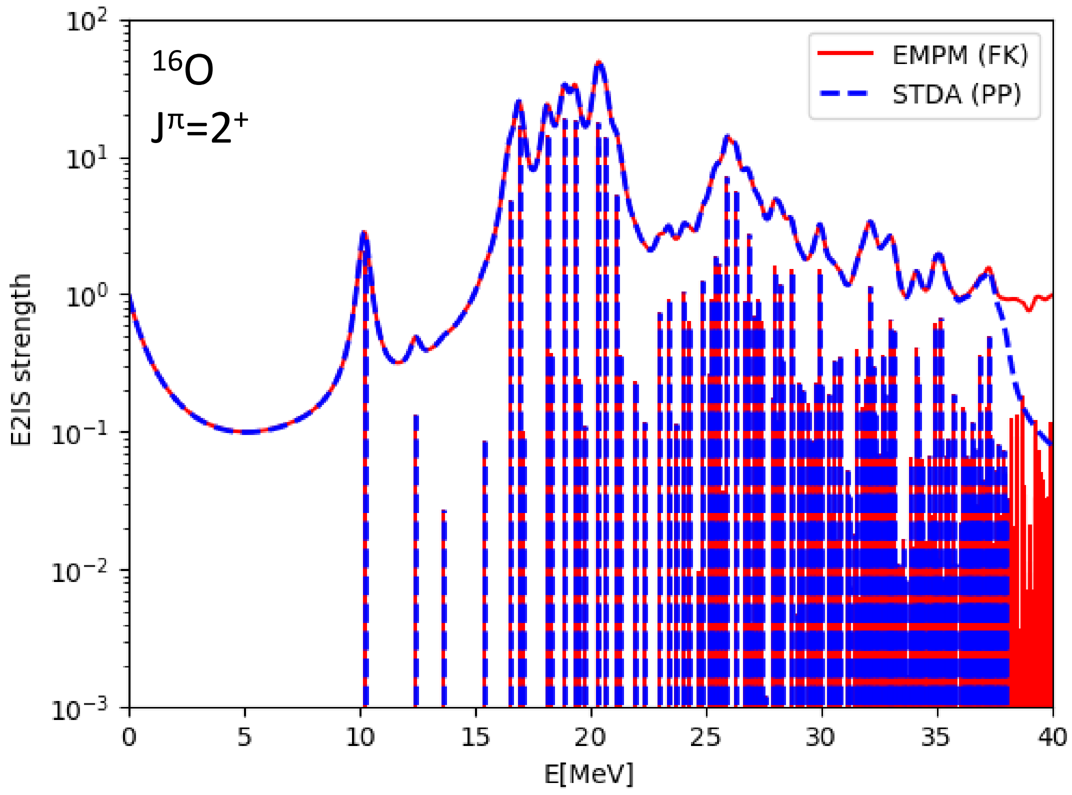
EMPM vs. STDA

- **Second-RPA/TDA**: extension of RPA/TDA which considers TDA/RPA phonon + *2p-2h* configurations

→ benchmark with large-scale SRPA/STDA calculations
P. Papakonstantinou and R. Roth, Phys. Rev C 81, 024317 (2010)

→ **EMPM (up to 2-ph. without CM ort.) and STDA are equivalent** in complete model space for all multipolarities
→ **the same spurious states in STDA and EMPM**



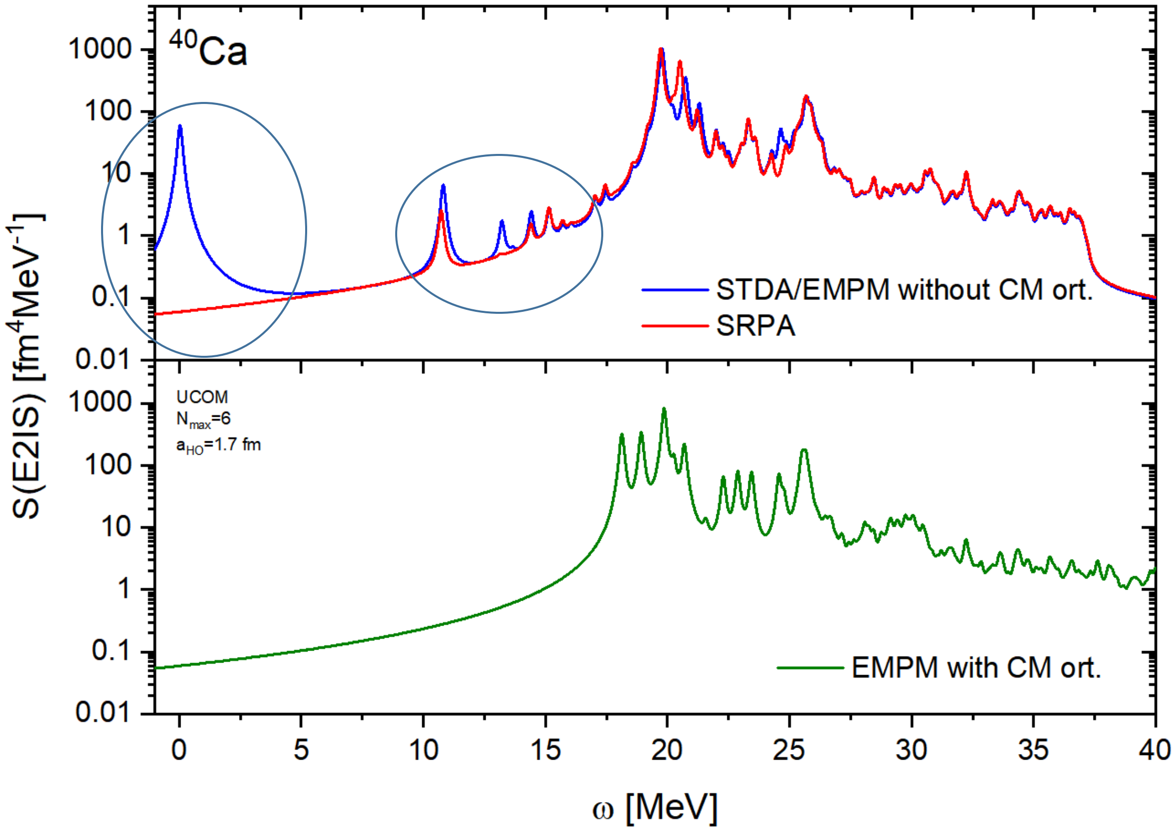


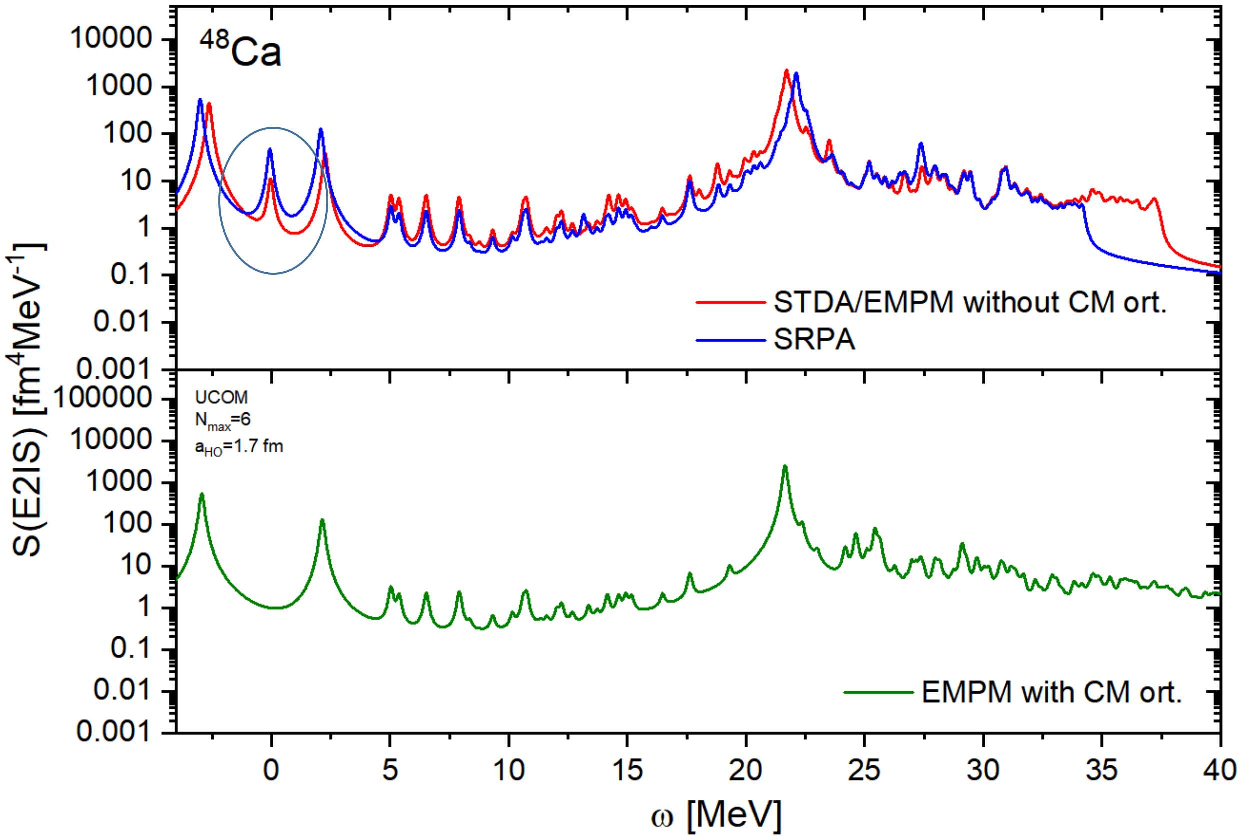
EMPM vs. STDA/SRPA

- comparison with large-scale STDA/SRPA calculations with UCOM potential
  *P. Papakonstantinou and R. Roth, Phys. Rev C **81**, 024317 (2010)*

→ **spurious states appear also in SRPA!**

$$S(E\lambda,\omega) = \sum B(E\lambda, i \to f)\delta(\omega - \omega_f) \approx \sum B(E\lambda, i \to f)\rho_\Delta(\omega - \omega_f)$$





F. Knapp, P. Papakonstantinou, P. Veselý, in preparation

Conclusions & Prospects

CM problem studied within microscopic phonon model

- effective procedure for elimination of CM contamination from nuclear spectra developed

  G. De Gregorio, F. Knapp, N. Lo Iudice, P. Veselý, Phys. Lett. B ***821****, 136636 (2021)*

  G. De Gregorio, F. Knapp, N. Lo Iudice, P. Veselý, submitted to Phys. Rev. C

- EMPM and NCSM results for ^{4}He are in good agreement
- small effect on ground-state (energy radius), but huge for excited states (spectra, EM transitions)
- equivalence of EMPM and STDA
- commonly used selfconsistent SRPA generates spurious solutions

Prospects:

- CM effect in particle-phonon model (odd nuclei with one valence particle)
- CM contamination of low-lying dipole strength in heavy systems (Pygmy resonance)
- spurious modes connected with particle number violation (quasiparticle SRPA/STDA/EMPM)

Collaborators

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