# Microscopic effective interactions for the nuclear Shell Model

## (I) OLS transformation of No-Core Shell Model solution
## (II) Many-body perturbation theory (in Brillouin-Wigner form)

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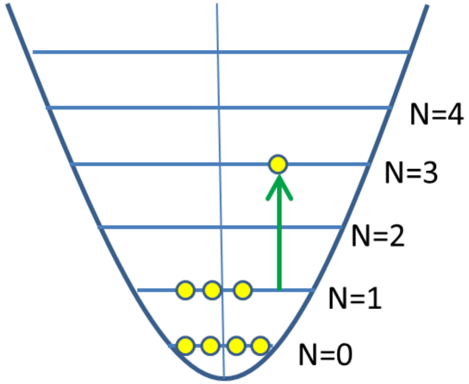
*Symposium in Honor of the 75th Anniversary of the Nuclear Shell Model and Maria Göppert-Mayer, Argonne National Laboratory, USA, 19-21 July 2024*

# No-core shell model - (full) configuration-interaction approach

$$H = T - T_{CM} + V = \underbrace{(T+U)}_{H_0} + \underbrace{(V - U - T_{CM})}_{H_1} = H_0 + H_1$$

$$\boxed{H_0|\Phi_k\rangle = E_k^0|\Phi_k\rangle}$$

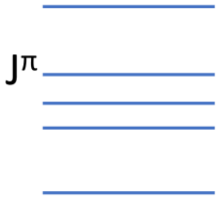
$$\boxed{|\Psi_n\rangle = \sum c_{kn}\,|\Phi_k\rangle}$$



$$\boxed{H|\Psi_n\rangle = E_n|\Psi_n\rangle}$$

$$\boxed{\sum_{k=1}^{d}\langle\Phi_l|H|\Phi_k\rangle\, c_{kn} = E_n c_{ln}}$$

$$\begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1d} \\ H_{21} & H_{22} & \cdots & H_{2d} \\ \vdots & & \ddots & \\ H_{d1} & H_{d2} & \cdots & H_{dd} \end{pmatrix}$$



***Ab-initio* No-Core Shell Model : sufficiently large model space so that the results for A nucleons do not depend on the basis parameters (hw and $N_{max}$)**

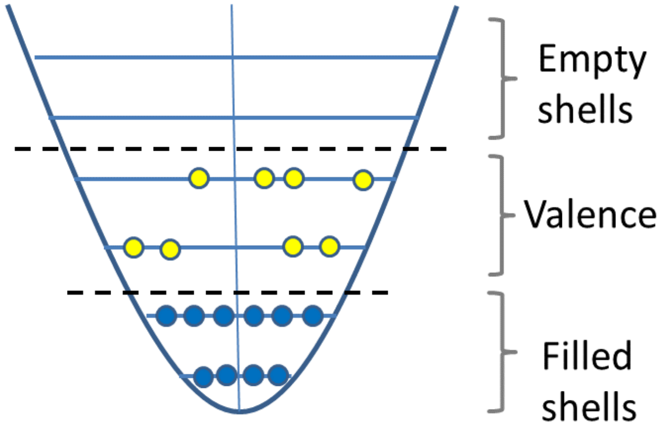
***Review by** Barrett, Navratil, Vary, **PPNP 69**, 131 (2013)*

**Basis dimension grows fast ! Heavier nuclei ?**

# Valence-space shell model for heavier nuclei

## Restricted model space

(P-space)



## *Effective operators*

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

$$\langle\Psi_f|O|\Psi_i\rangle = O_{if}$$

*Full model space*

$$\Rightarrow$$

$$H_{eff}|\Psi_n^P\rangle = E_n|\Psi_n^P\rangle$$

$$\langle\Psi_f^P|\, O_{eff}|\Psi_i^P\rangle = O_{if}$$

*P-space*

*Projectors :* $P \equiv \sum_{k\in P}|\Phi_k\rangle\langle\Phi_k|,\ \mathrm{Q} = 1 - \mathrm{P} = \sum_{k\in Q}|\Phi_k\rangle\langle\Phi_k|$

Removing the core, we get the Hamiltonian for valence nucleons :

$$H_{eff} = \sum_\alpha \varepsilon_\alpha a_\alpha^\dagger a_\alpha + \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V_{eff}|\delta\gamma\rangle\, a_\alpha^\dagger a_\beta^\dagger\, a_\gamma\, a_\delta$$

*Empirical or Microscopic*

*Microscopic*

*Empirical / Constrained by data*

**Current status :**

- Excellent description with experimentally constrained interactions (Cohen-Kurath, Wildenthal-Brown,..)
- Microscopic interactions -> recent progress and challenges

# Effective Interactions : multipole decomposition

**Particle-particle form :**

$$H = \sum \varepsilon_i a_i^\dagger a_i \;+ \tfrac{1}{4}\sum_{ijkl,\lambda} w_{ijkl,\lambda} \left[\, a_i^\dagger \tilde{a}_j \;\right]^{(\lambda)} \left[\, a_k^\dagger \tilde{a}_l \;\right]^{(\lambda)} + \cdots$$

**Multipole form :**

$$H = \underbrace{\sum_i \varepsilon_i n_i \;+\; \sum_{i<j} \bar{V}_{ij} \frac{n_i(n_j-\delta_{ij})}{1+\delta_{ij}}} \;+\; \underbrace{V_{pair} + V_{quad} + \cdots}$$

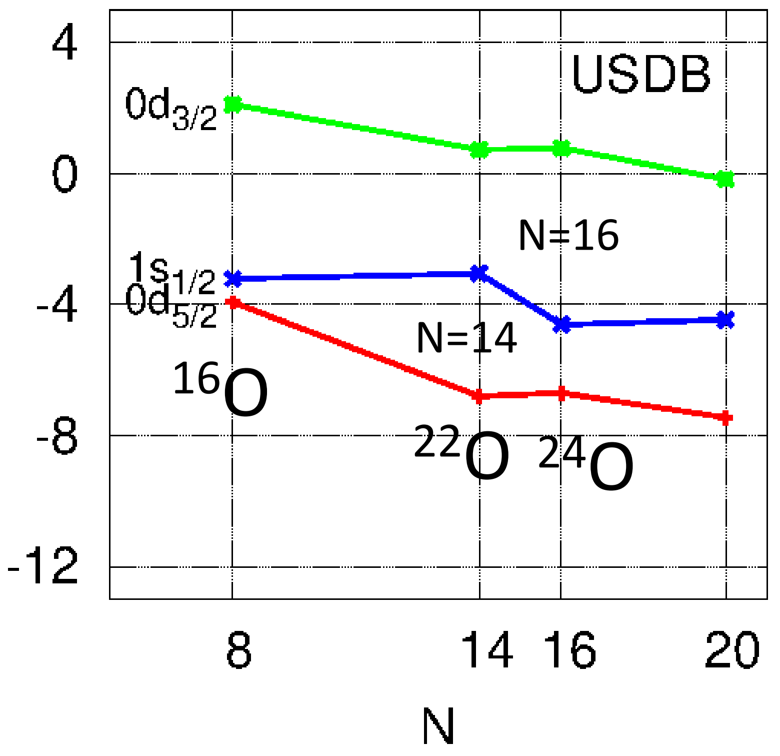
*Monopole part*
*(spherical mean-field)*

*Higher Multipole part*
*(correlations)*

- **Only a physically meaningful combination of these ingredients will results in a successful description !**

- **Important to understand the nature of nuclear excitations (competition between sphericity and deformation)**

Neutron ESPEs in O-isotopes
(from monopole part)



*USDB – universal sd interaction:*
*Richter, Brown, PRC74 (2006)*

*Caurier, Martinez-Pinedo, Nowacki, Poves, Zuker, RMP77,427 (2005)*

# Microscopic approaches to valence-space interactions

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

$$\langle\Psi_f|O|\Psi_i\rangle = O_{if}$$

Effective operators

$$H_{eff}|\Psi_n^P\rangle = E_n|\Psi_n^P\rangle$$

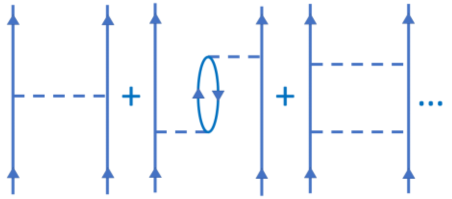
$$\langle\Psi_f^P|\,O_{eff}|\Psi_i^P\rangle = O_{if}$$

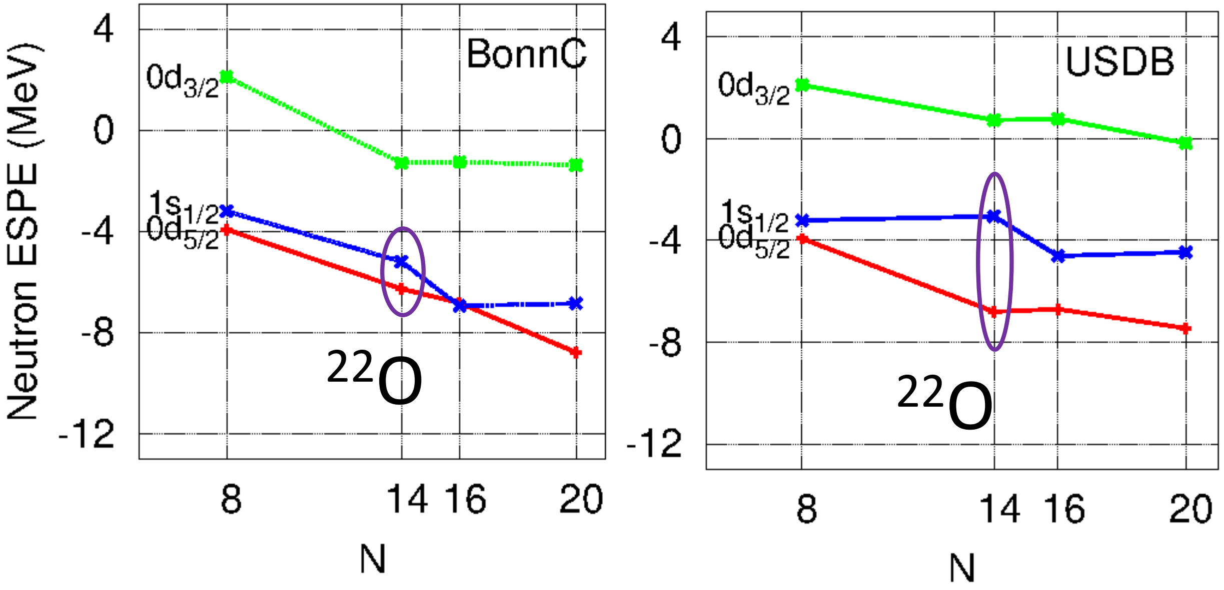
## Many-body perturbation theory (in Rayleigh-Schrödinger formalism up to 3rd order)

*Bethe, Brueckner, Goldstone (from 50's ..) ; Bertsch, Kuo, Brown, Barrett, Kirson, …. (from 60's)*

*Hjorth-Jensen, Kuo, Osnes, PR261, 126 (1995); Coraggio et al, Ann. Phys. (2009) PPNP(2012),…*

*Veff =*





Poor description of the monopole term (spherical mean-field)

Missing 3N forces

*Poves, Zuker, PR70, 71 (1981), …*

*NN+3N : Otsuka et al (2010), Holt et al (2013),Fukui et al,(2018); …*

Formal issue of the order-by-order convergence are not solved ! *(Roth, Langhammer, PLB (2010, 2016) – iterative approach) => converging in HF basis, but not in HO one!*

# Microscopic approaches to valence-space interactions

## Non-perturbative approaches

- **Valence-space In-Medium Similarity Renormalization Group – IMSRG** (NN + 3N)

  *Stroberg et al, PRC93, 051301 (2016); PRL118, 032502 (2017), etc.*

$$\boxed{H(s) = U(s)H(0)U^{\dagger}(s),}$$

$$\boxed{dH(s)/ds = [\eta(s), H(s)]}$$

- **OLS transformation applied to NCSM results**

$$H_{\text{eff}} = P\mathcal{H}P = \frac{U_p^{\dagger}}{\sqrt{U_p^{\dagger}U_p}} H_p^{\text{d}} \frac{U_p}{\sqrt{U_p^{\dagger}U_p}}$$

  *Dikmen, Lisetskiy, Barrett, Maris, Shirokov, Vary, PRC91, 064301 (2015)*
  *Vary, Basili, Weiji Du et al, PRC98, 065502 (2018)*
  *Smirnova, Barrett, Shin, Kim, Shirokov, Dikmen, Maris, Vary, PRC100, 054329 (2019)*
  *Shin, Smirnova, Shirokov, Yang, Barrett, Li, Kim, Maris, Vary, arXiv:2306.17289*

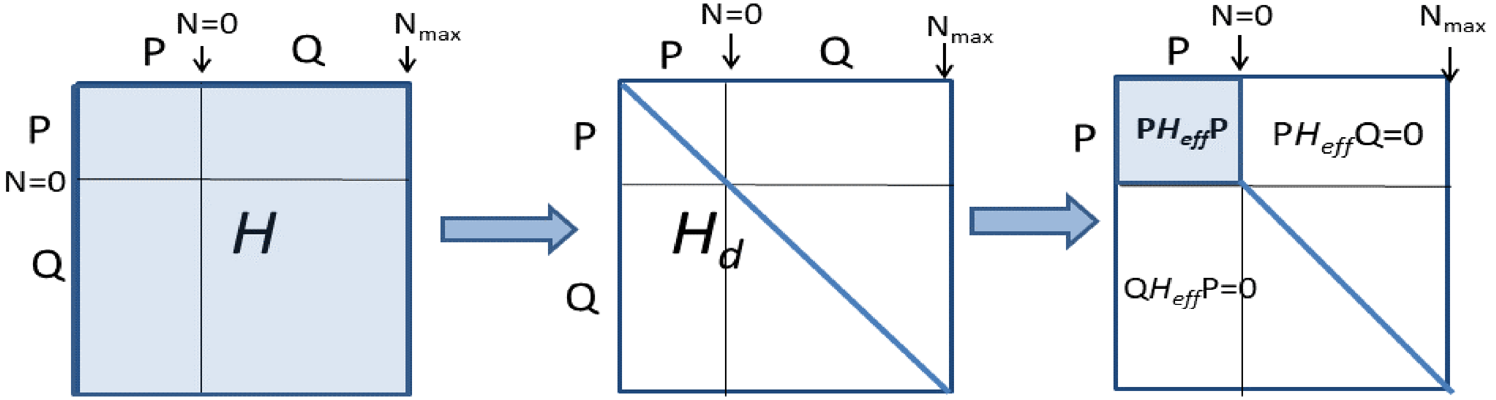
- **Coupled-cluster theory** (NN + 3N)

  *Jansen et al, PRC94, 011301 (2016);*
  *Sun, Morris, Hagen et al, PRC98, 054320 (2018)*

*For review see Stroberg, Heigert, Bogner, Holt, Ann. Rev. Nucl. Part. Science **69,** 307 (2019).*

# Ab-initio effective Hamiltonian from NCSM

Okubo-Lee-Suzuki (OLS) similarity transformation
of the NCSM solution



$$H_d = UHU^\dagger \qquad H_{eff} = \frac{U_P^\dagger}{\sqrt{U_P U_P^\dagger}} H_d \frac{U_P}{\sqrt{U_P U_P^\dagger}}$$

**FLOW**

☐ $^{18}$F from NCSM at $N_{max}$

☐ $H_{eff}$ for $^{18}$F at N=0

☐ $^{16}$O from the NCSM at $N_{max}$

→ Core energy

☐ $^{17}$O, $^{17}$F from the NCSM at $N_{max}$

→ One-body terms

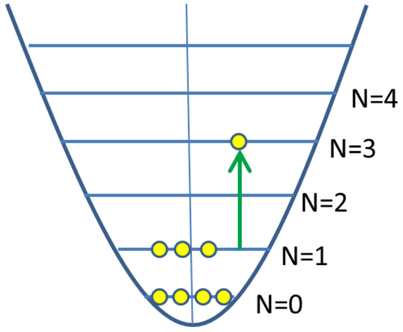
☐ Single-particle energies $\varepsilon_i$

two-body matrix elements $V_{ijkl}$

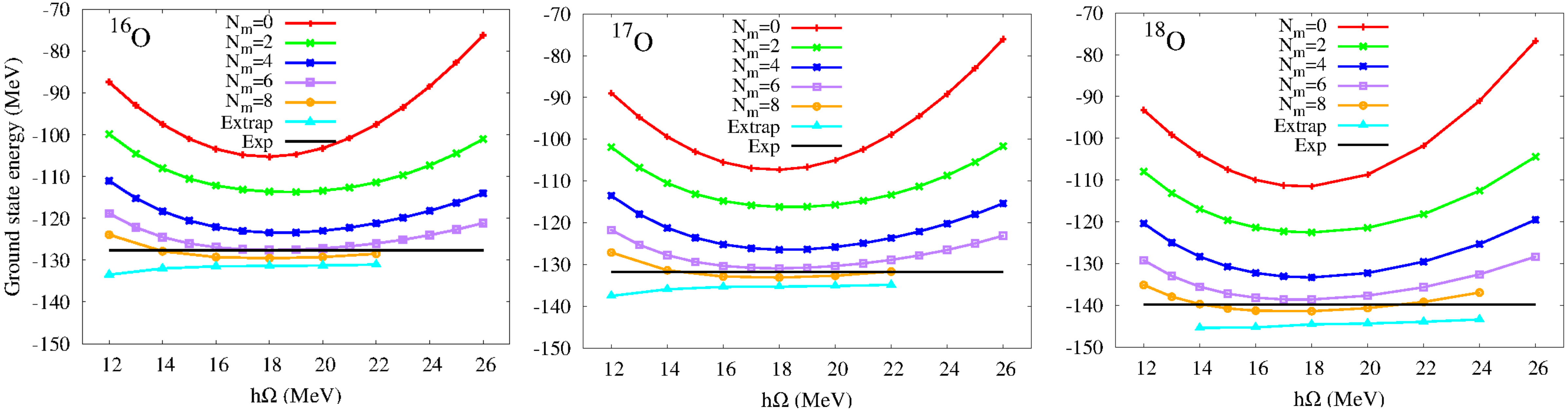
*Okubo, Prog. Theor. Phys. 12 (1954); Suzuki, Lee, Prog. Theor. Phys. 68 (1980)*
*Dikmen, Lisetskiy, Barrett, Maris, Shirokov, Vary, PRC91, 064301 (2015)*
*Vary, Basili, Weiji Du et al, PRC98, 065502 (2018)*
*Smirnova, Barrett, Shin, Kim, Shirokov, Dikmen, Maris, Vary, PRC100 (2019)*
*Shin, Smirnova, Shirokov et al, arXiv:2306.17289*

# No-Core Shell Model

$$H = \sum_{i<j} \frac{\left(\vec{p_i} - \vec{p_j}\right)^2}{2mA} + \sum_{i<j}^{A} V_{ij} + \left( \sum_{i<j<k}^{A} V_{ijk} \right)$$



Daejeon16 *NN* potential (*EM-N3LO + SRG evolved + PETs*)

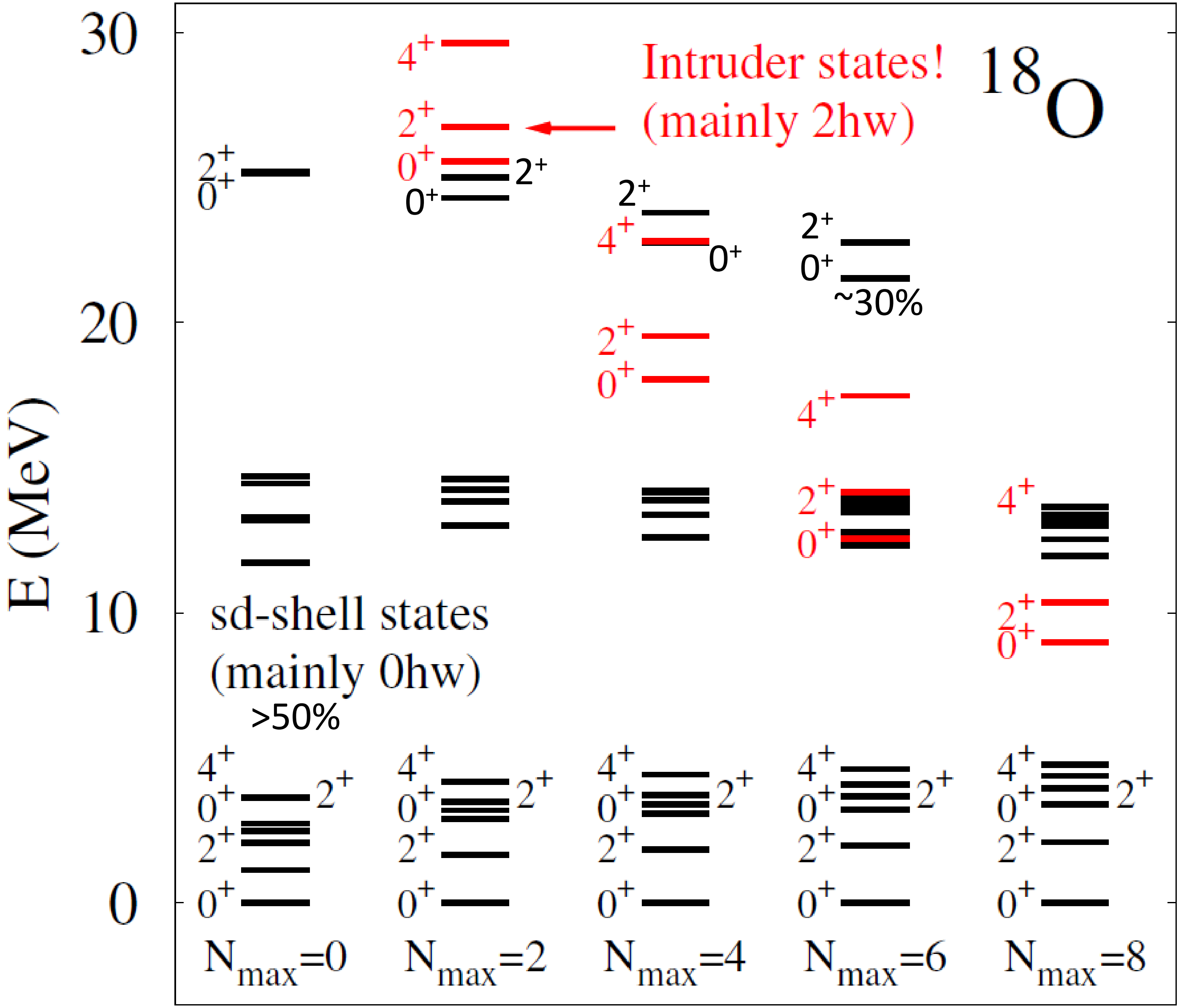


**Daejeon16**: *Shirokov, Shin, Kim, Sosonkina, Maris, Vary, PLB761, 87 (2016)*

***NCSM*** *: Barrett, Navratil, Vary,* ***PPNP 69****, 131 (2013).*

*MFDn code: Vary, Maris et al,*
*Iowa State University*

# Low-energy spectrum of $^{18}$O from the NCSM with Daejeon16

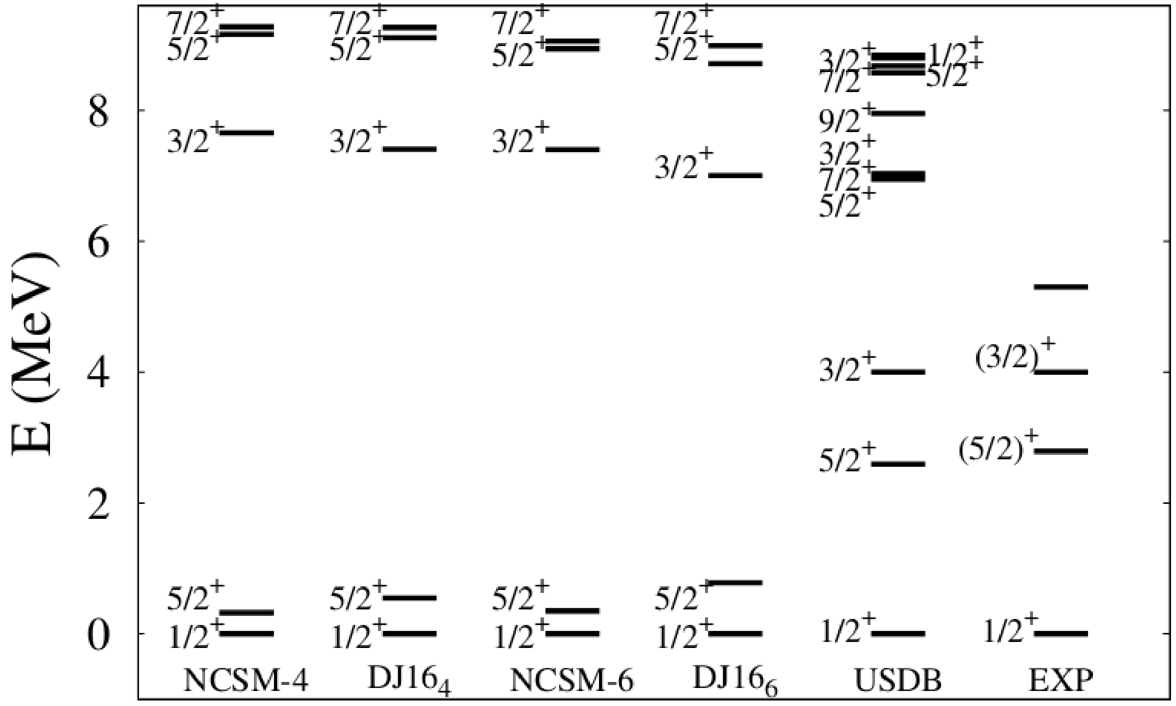


- The states dominated by sd-shell components are quickly converged!
- Intruder states (identified experimentally by large E2 matrix elements) are not converged yet!
- Such general structure of the spectrum is also typical for heavier sd-shell nuclei

# Ab-initio effective Hamiltonian from the NCSM : A>18 nuclei

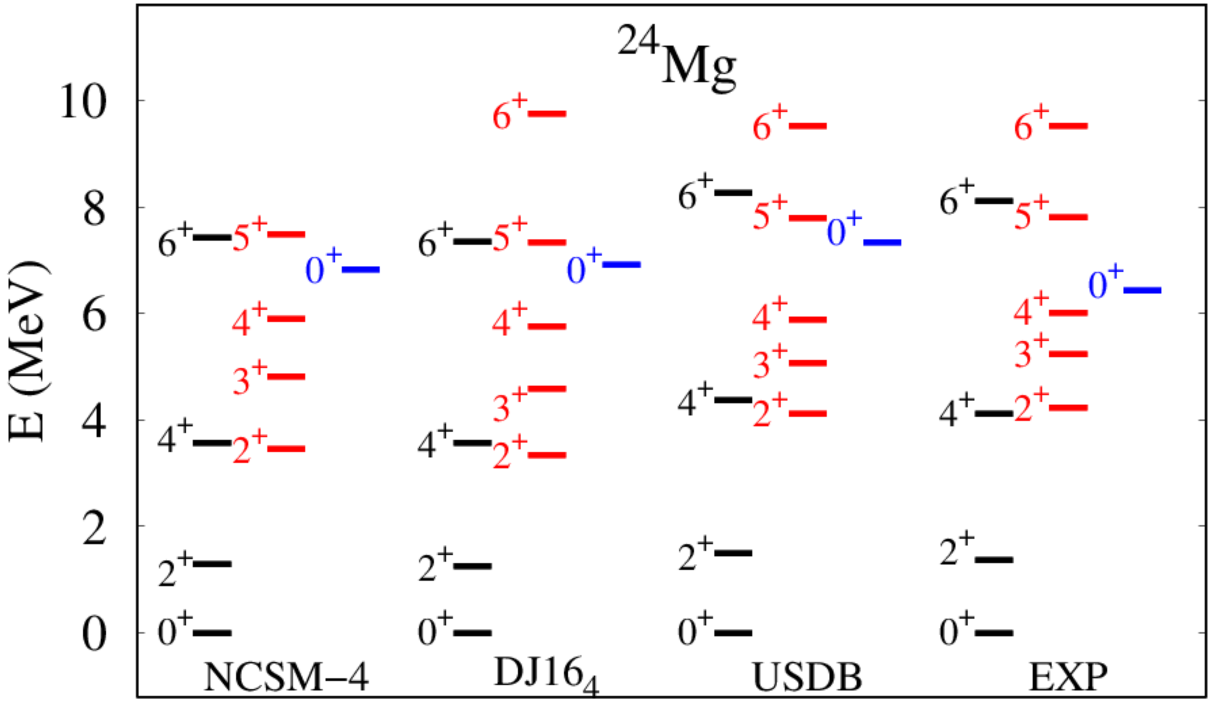
$^{23}$O

*14 states : rms error  63 keV*



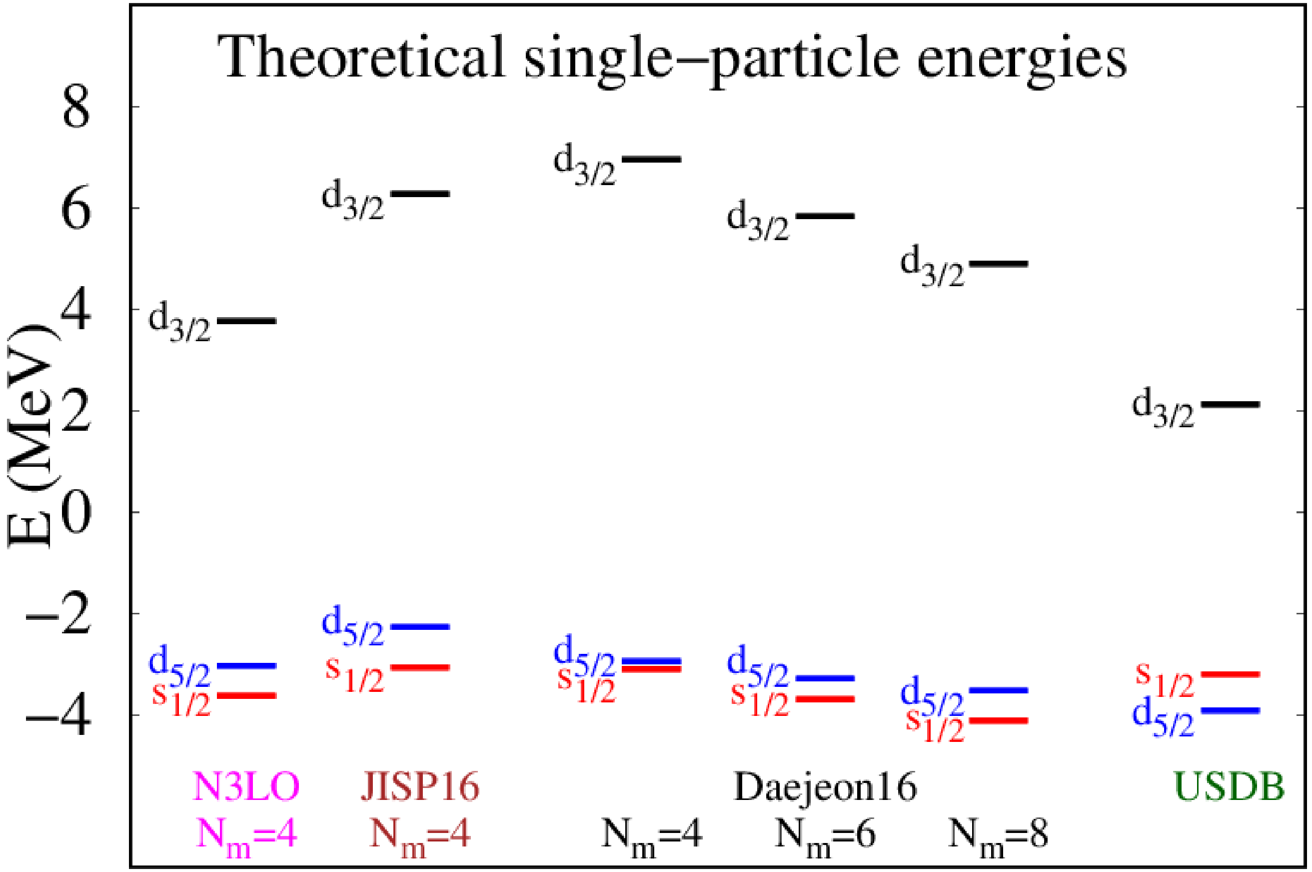
- Sometimes poor agreement with experiment -> wrong theo s.p. energies

- Theoretical valence-space TBMEs and s.p.e.'s (without any A-dependence) robustly reproduce the NCSM results !



*9 states : rms error 225 keV*

# Ab-initio effective Hamiltonian from the NCSM : Theory & Experiment



**Drawbacks (hw=14 MeV):**

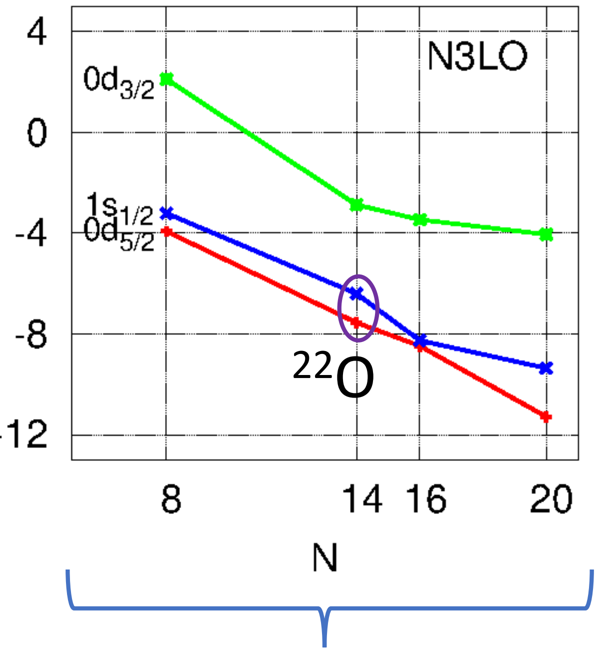
- ☐ *Inversion of s1/2 and d5/2 orbitals*
- ☐ *Too large d3/2 – d5/2 spin-orbit splitting*

We adopt USDB single-particle energies and impose an $A^{-0.3}$ mass dependence on TBMEs

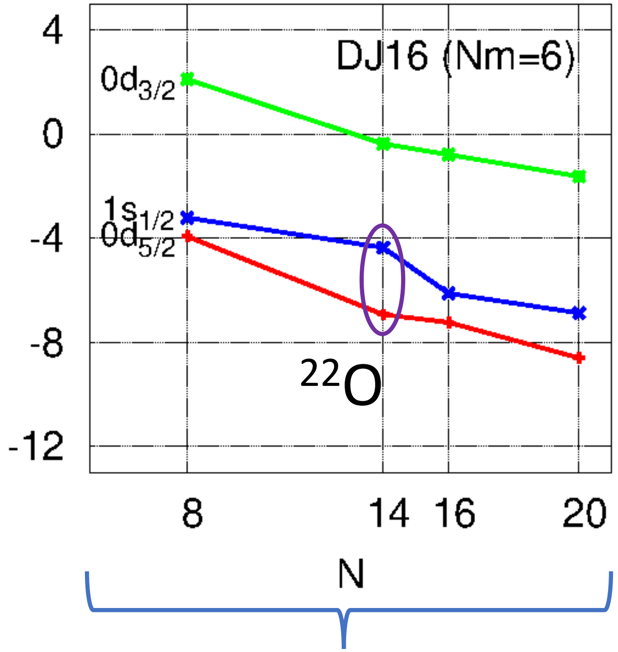
***N3LO*** *: from chiral EFT by Entem, Machleidt, PRC68 (2003)*
***JISP16*** *: Shirokov et al, PRC70, 044005 (2004)*
***Daejeon16*** *: Shirokov et al, PLB761, 87 (2016) – based on N3LO*
*+ SRG evolved + phase-equivalently transformed*

# Comparison of monopole properties valence-space interactions

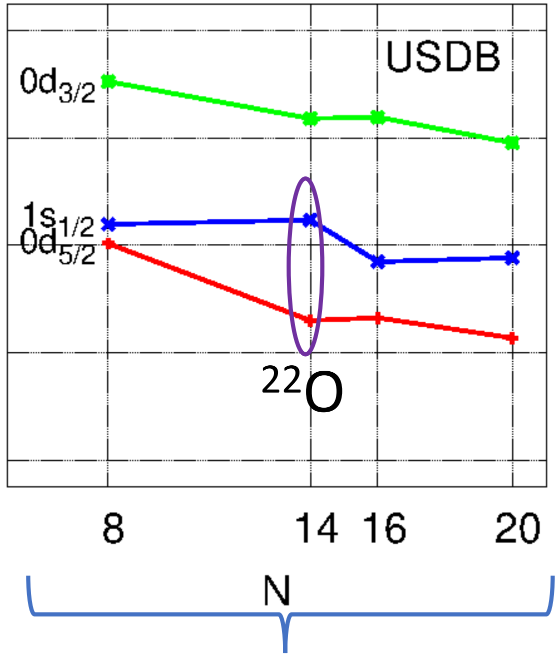
Neutron ESPEs in O-isotopes



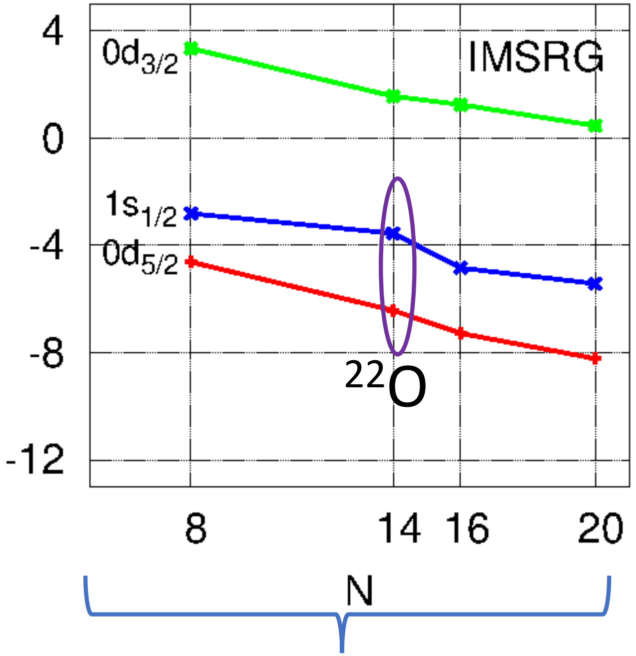
*From NN interaction*



*From Daejeon16 NN interaction*



*Empirical (=governed by experimental data)*

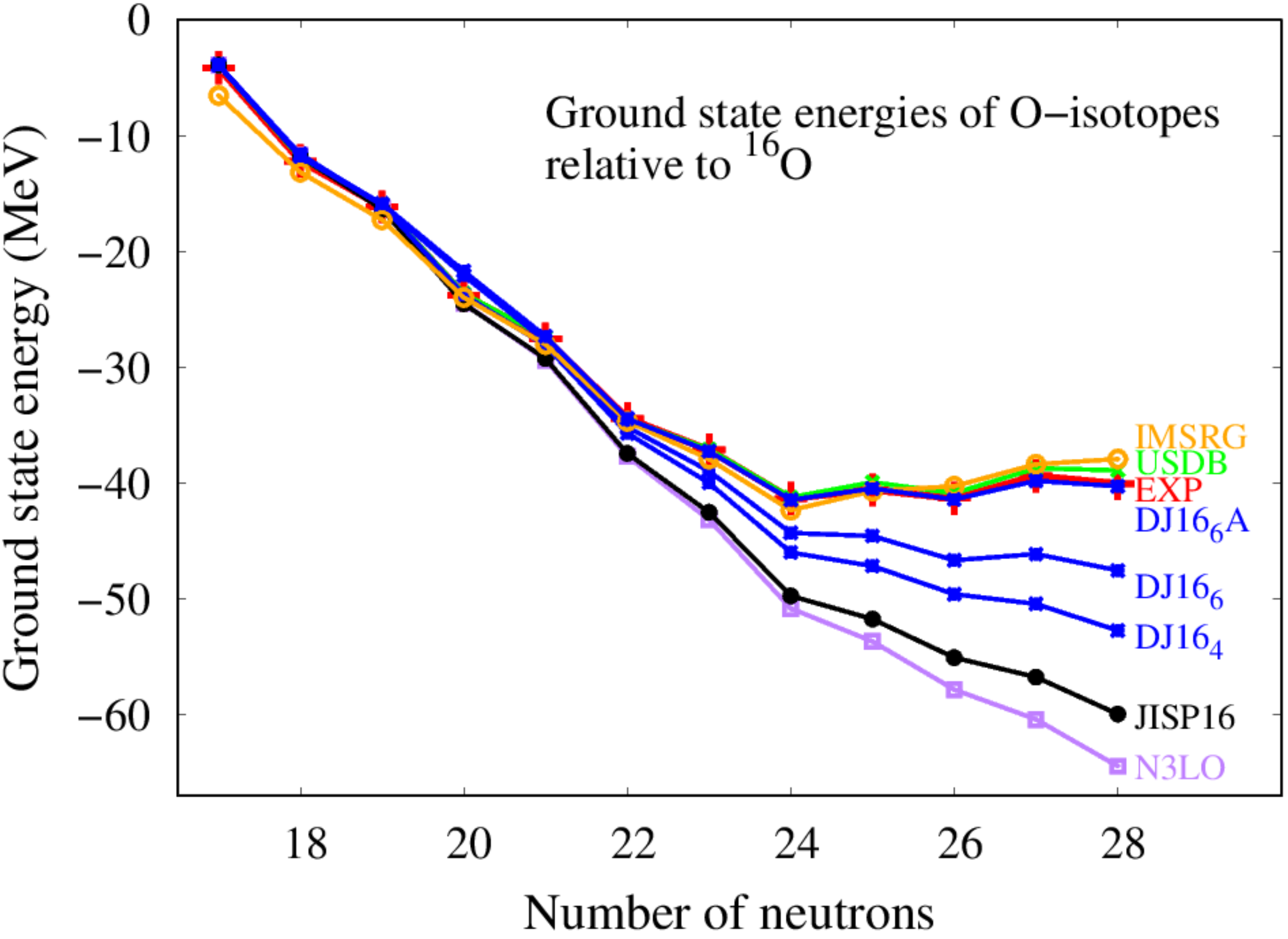


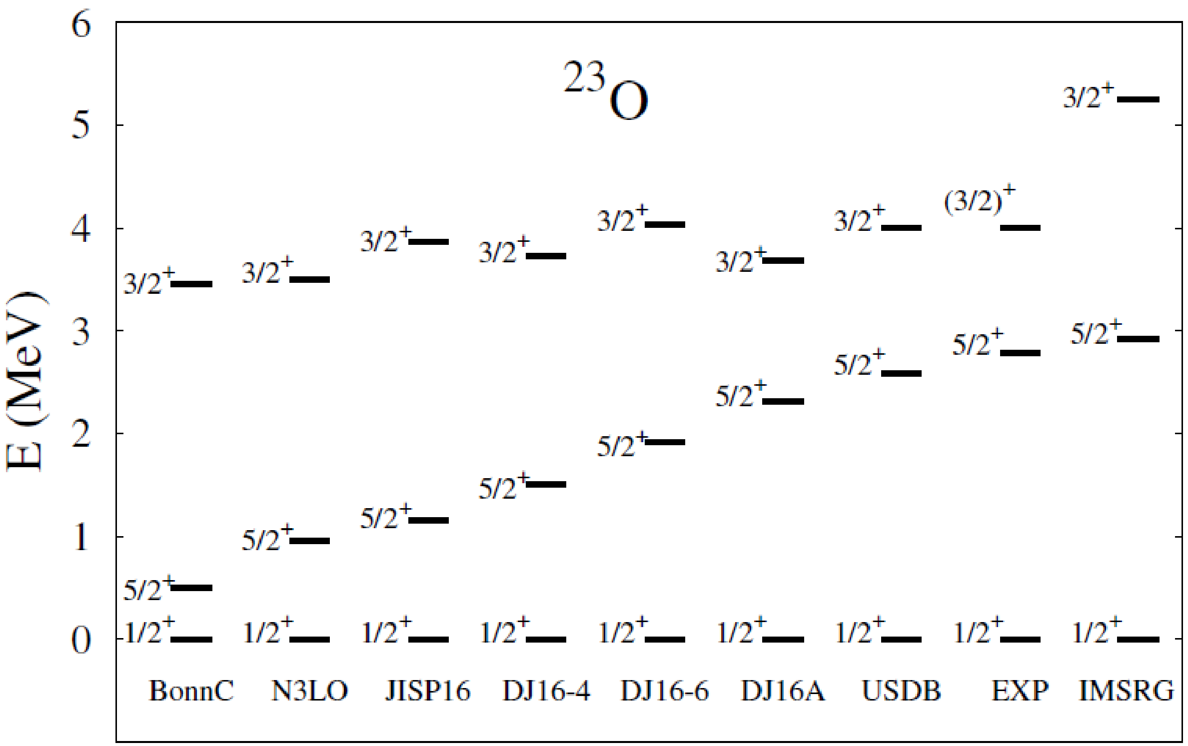
*From NN+3N interaction*

Some monopole modifications to DJ16 (change of centroids by ~100-300 keV) can be useful !

*IMSRG results : Stroberg et al, PRL118, 032502 (2017).*

# Two-body effective interaction from NCSM + empirical s.p. energies





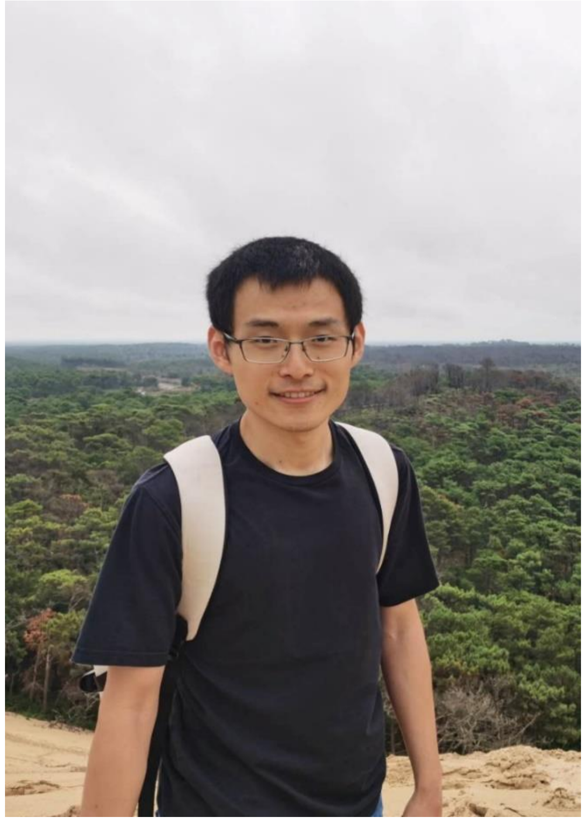
*IMSRG: from Stroberg et al, PRL118, 032502 (2017)*

DJ16$_6$ : rms = 3671 keV

DJ16$_6$A (DJ16$_6$ with monopole modifications):
rms = 235 keV

USDB : rms =467 keV

# II. Brillouin-Wigner Many-body Perturbation theory for closed-shell and open-shell nuclei



*Advances in Many-body Perturbation theory for closed-shell and open-shell nuclei*

Zhen Li, Ph.D. thesis
University of Bordeaux (2020 – 2023)
*Present address : TU Darmstadt

- **Brillouin-Wigner perturbation expansion & convergence criterion**
- Rayleigh-Schrödinger perturbation expansion – extension of the diagrammatic approach (automatic generation and evaluation of Feynman-Goldstone diagrams)

# P-space Schrödinger equation: Exact Solution

❑ **P-space Schrödinger equation with an energy-dependent effective Hamiltonian**

$$H|\Psi_k\rangle = E_k|\Psi_k\rangle \quad \Longrightarrow \quad H_{\text{eff}}(E_k)|\Psi_k^{\mathbb{P}}\rangle = E_k|\Psi_k^{\mathbb{P}}\rangle$$

$$H_{\text{eff}}(E) \equiv PHP + PHQ\frac{1}{E - QHQ}QHP$$

*Bloch, Horowitz, Nucl. Phys. 8, 91 (1958)*
*Feschbach, Ann. Phys. 85, 357 (1958)*

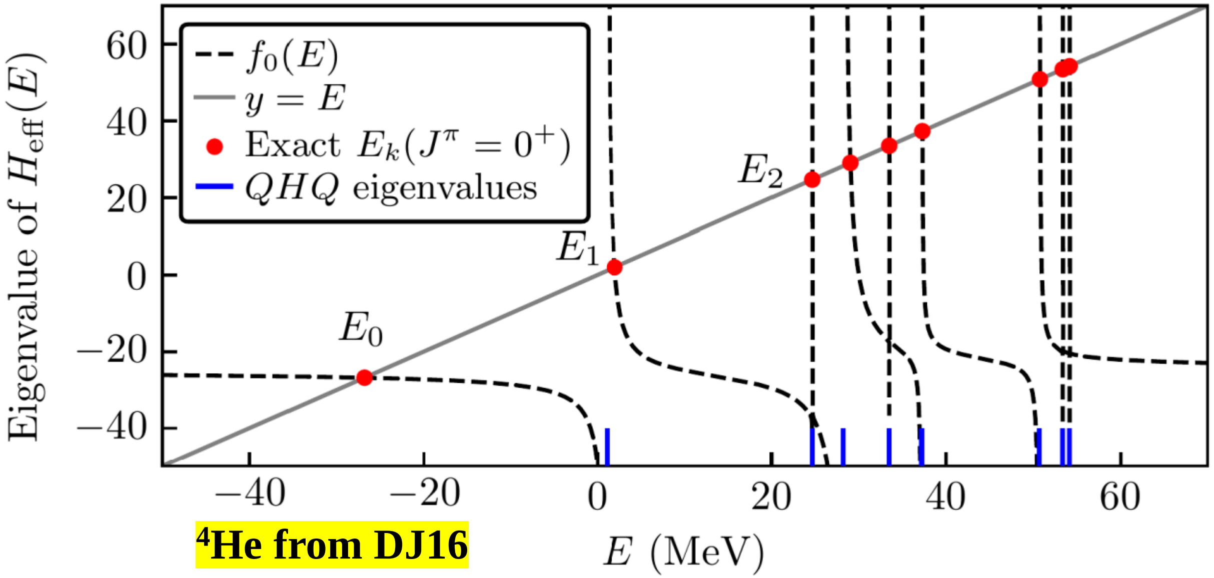
$$\boldsymbol{E}_{\mathbf{k}} \begin{cases} H_{\text{eff}}(E)|\psi_n^{\mathbb{P}}(E)\rangle = f_n(E)|\psi_n^{\mathbb{P}}(E)\rangle \\ f_n(E) \;=\; E \end{cases}$$

- Singularities at the eigenvalues of *QHQ*

$$|\Psi_k\rangle = P|\Psi_k\rangle + Q|\Psi_k\rangle$$

$$f_n'(E) \leq 0$$

$$f_n'(E_k) = -\frac{\langle\Psi_k|Q|\Psi_k\rangle}{\langle\Psi_k|P|\Psi_k\rangle} \leq 0$$



**$^4$He from DJ16**

**$\hbar\omega$ = 18 MeV, $N_{\text{max}}$ = 2**

**Matrix Inversion**

dim(P) =1

# Brillouin – Wigner MBPT : Convergence Criterion

- ☐ **Constructing the effective Hamiltonian by perturbative expansion**

$$H_{\rm eff}(E) \equiv PHP + PHQ\frac{1}{E - QHQ}QHP$$

$$\frac{1}{X-Y} = \frac{1}{X} + \frac{1}{X}Y\frac{1}{X-Y} = \frac{1}{X} + \frac{1}{X-Y}Y\frac{1}{X}$$

$$\frac{1}{E - QHQ} = \frac{1}{\underbrace{(E - QH_0Q - Q\xi Q)}_{X} - \underbrace{(QH_1Q - Q\xi Q)}_{Y}}$$

$$= \frac{1}{X} + \frac{1}{X}Y\frac{1}{X} + \frac{1}{X}Y\frac{1}{X}Y\frac{1}{X} + \cdots = \lim_{n\to\infty}\sum_{k=0}^{n} R^k\frac{1}{X},$$

  - ➢ Ratio of geometric series (*E*-dependent)
  - ➢ Hamiltonian partitioning parameter: $\xi$

$$R \equiv \frac{1}{X}Y = 1 + \frac{1}{E - Q(H_0 + \xi)Q}(QHQ - E)$$

- ☐ **Convergence Criterion : the spectral radius of R should be smaller than 1**

$$\rho(R) < 1$$

As long as $E < E_1^{QHQ}$ the BW perturbation series can always be made convergent,
i.e. for the lowest states of each $J^\pi$ (in particular, ground state) due to the variational principle.

***Universal conclusion, independent of the choice of basis (HO or HF) or the choice of the internucleon interaction (soft or hard).***

*Zhen Li, Smirnova, Phys. Lett. B854, 138749 (2024)*

# MBPT in BW Formalism: *K*-Box Iterative Calculations

- ☐ **High perturbative order calculations by direct *QRQ* matrix multiplication**

$$H_{\text{eff}}(E) = PHP + PHQ\left(\lim_{n\to\infty}\sum_{k=0}^{n} R^{k}\right)\frac{1}{E - QH_0Q - Q\xi Q}QHP,$$

Time complexity in each multiplication ~ $O(d_q^3)$

- ☐ **High perturbative order calculations by *K*-box iterations (Zhen Li, PhD thesis)**

$$H_{\text{eff}}(E) = PHP + P\hat{K}(E)Q\frac{1}{E - QH_0Q - Q\xi Q}QHP.$$

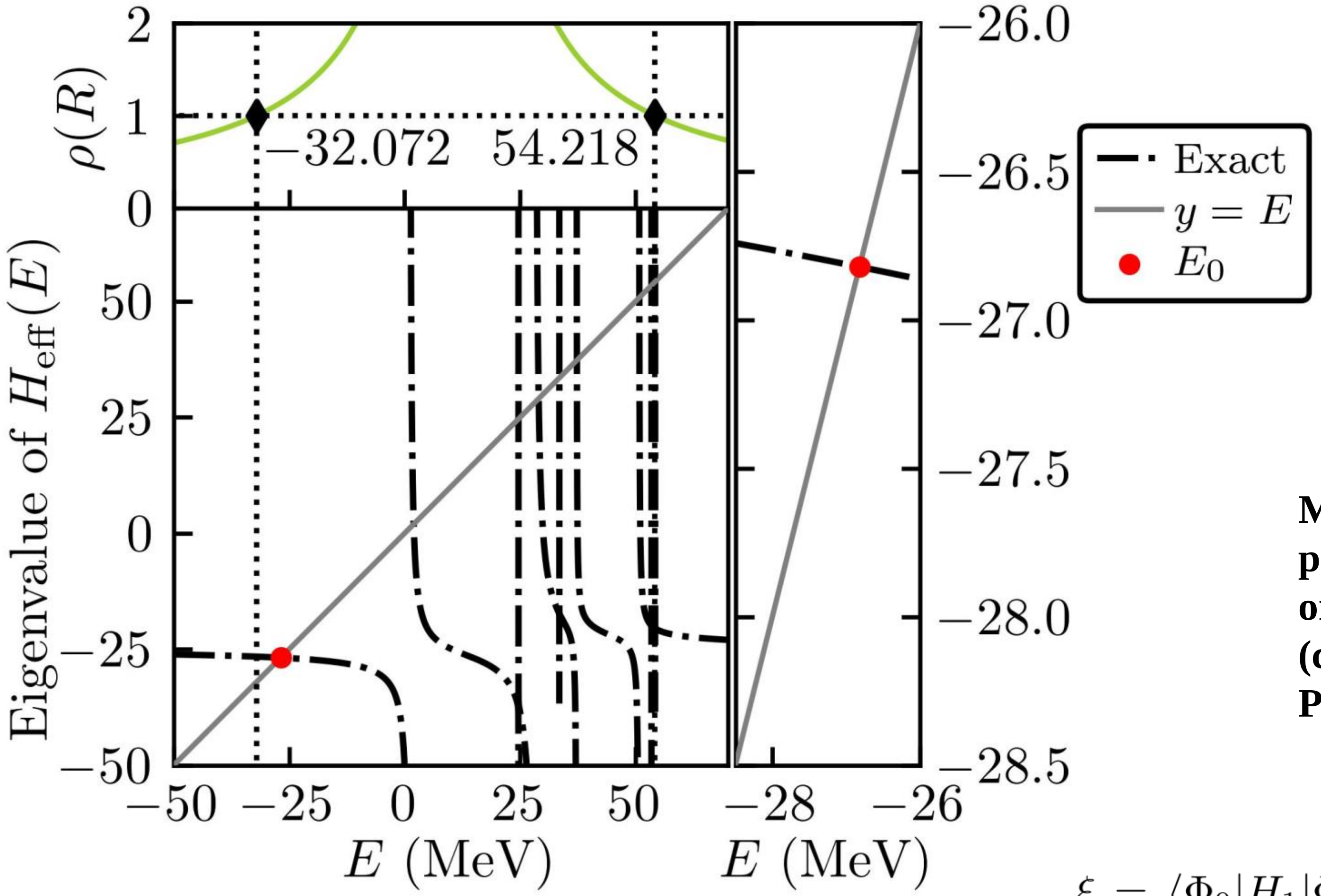
$$\begin{aligned}\hat{K}(E) &\equiv PHQ + PHQ\frac{1}{E - QHQ}(QH_1Q - Q\xi Q)\\ &= PHQ + P\hat{K}(E)Q\frac{1}{E - QH_0Q - Q\xi Q}(QH_1Q - Q\xi Q)\end{aligned}$$

$$\hat{K}^{(n+1)}(E) = PHQ + P\hat{K}^{(n)}(E)Q\frac{1}{E - QH_0Q - Q\xi Q}(QH_1Q - Q\xi Q),\ n = 0, 1, 2, \cdots$$

$$|\Psi_k\rangle = |\Psi_k^{\mathbb{P}}\rangle + \frac{1}{E_k - QH_0Q - Q\xi Q}\hat{K}^{\dagger}(E_k)|\Psi_k^{\mathbb{P}}\rangle$$

Time complexity in each iteration ~ $O(d_p \cdot d_q^2)$

# MBPT in BW Formalism: *K*-Box Iterative Calculations



**Møller-Plesset (MP) partitioning with a normal-ordered Hamiltonian (cf. Roth, Langhammer, PLB683, 282 (2010))**

$$\xi = \langle \Phi_0 | H_1 | \Phi_0 \rangle = -132.927 \text{ MeV}$$

**Ground state energy of $^4$He,**
**DJ16, HO basis, $\hbar\omega = 18$ MeV, $N_{\text{max}}$=2.**
**NCSM: $E_0$ = -26.822 MeV**

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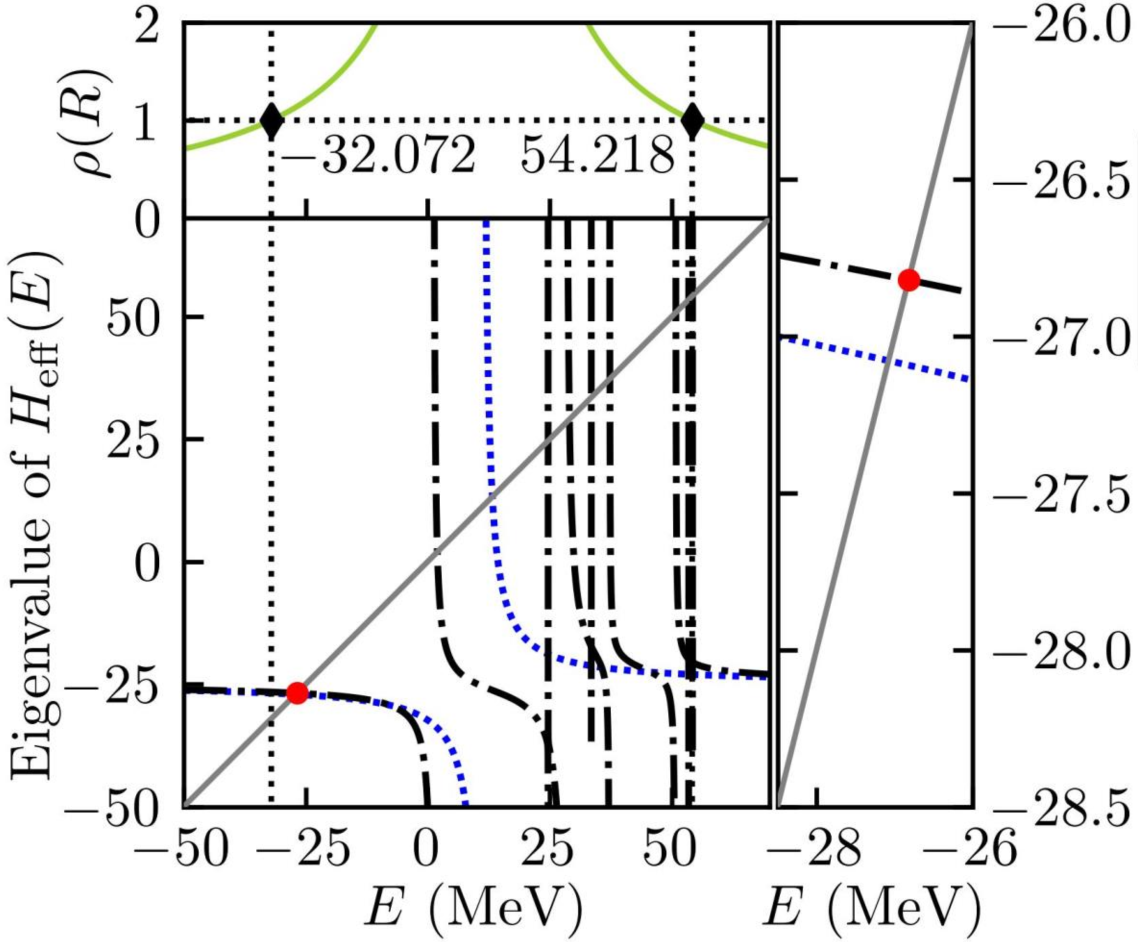

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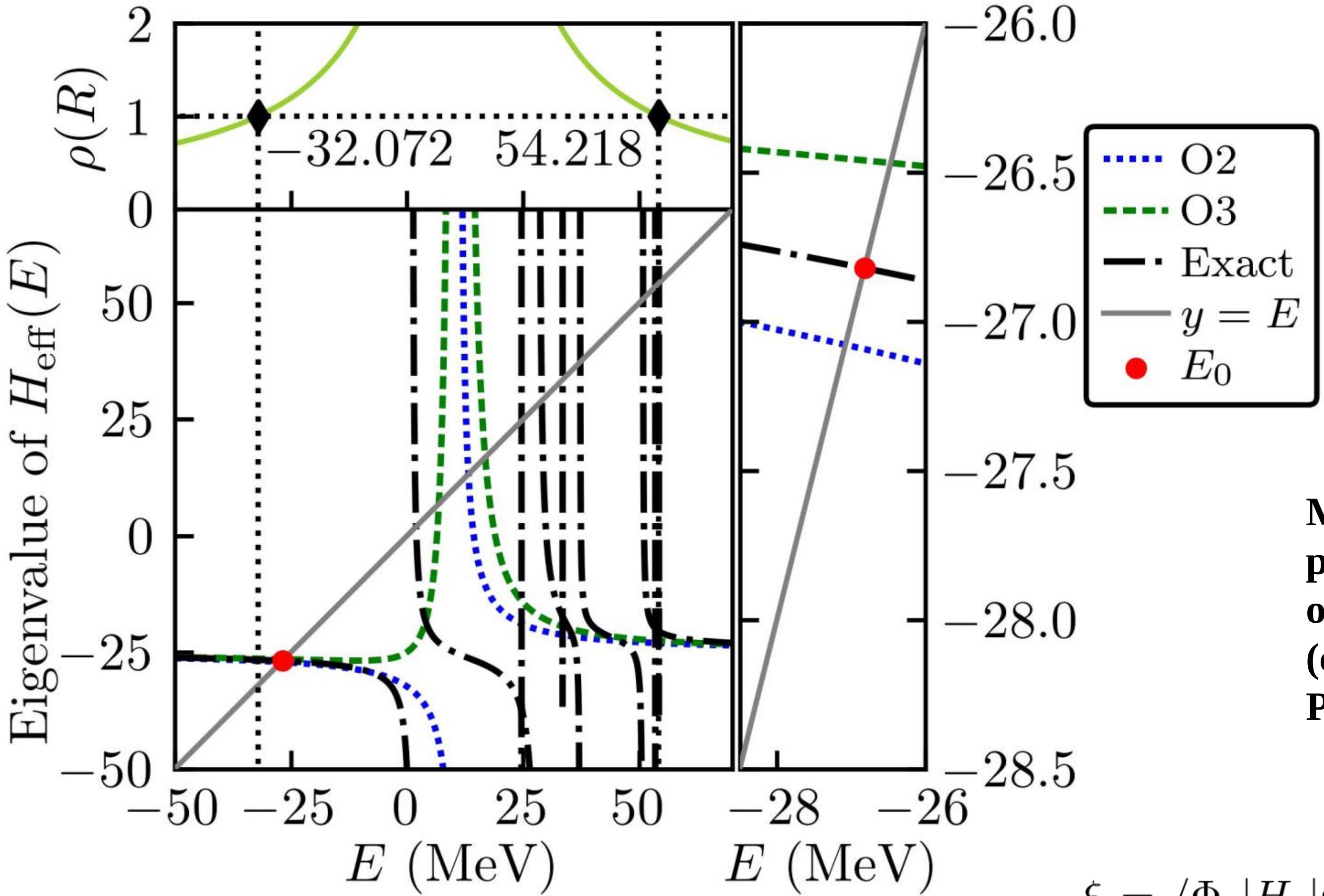

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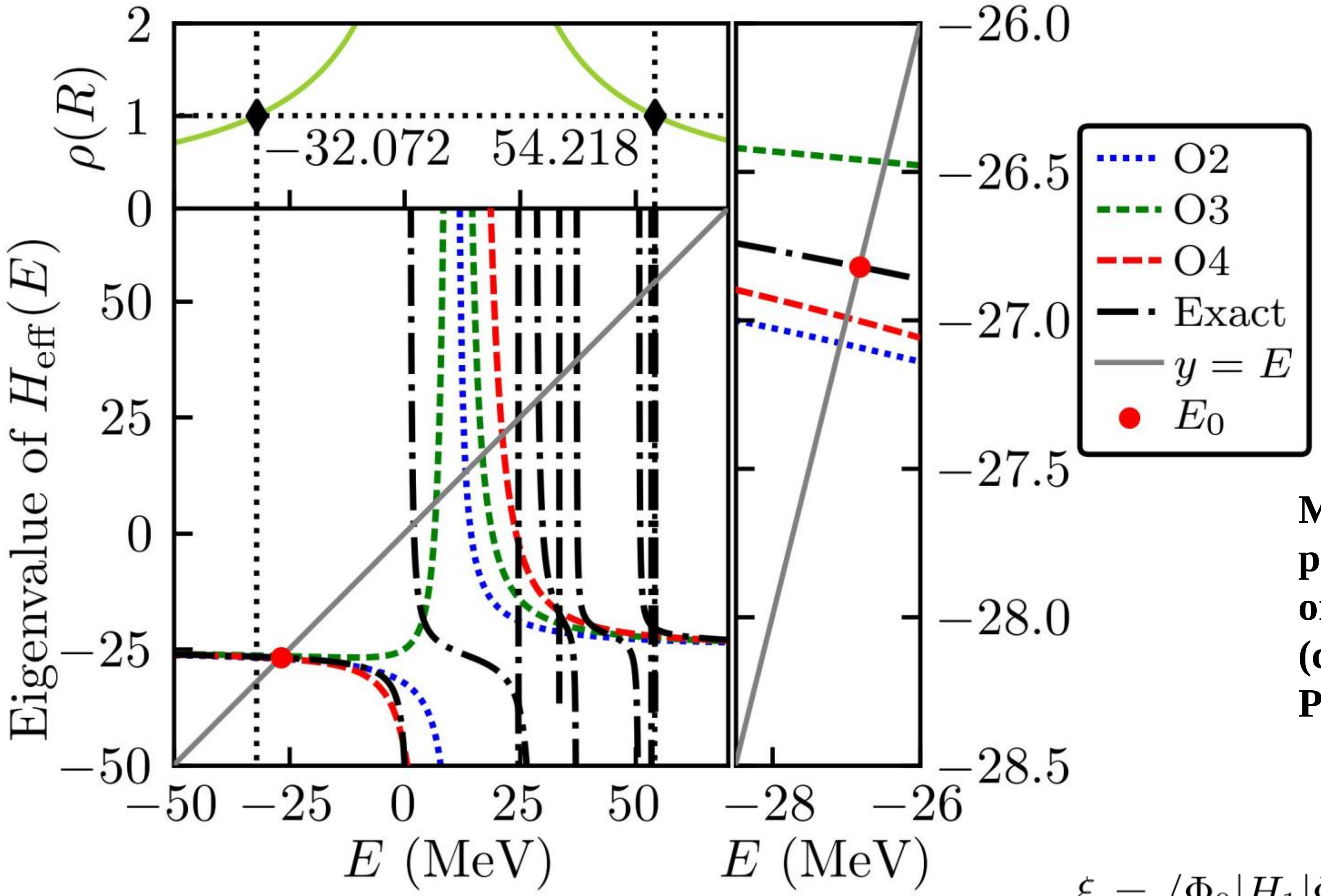

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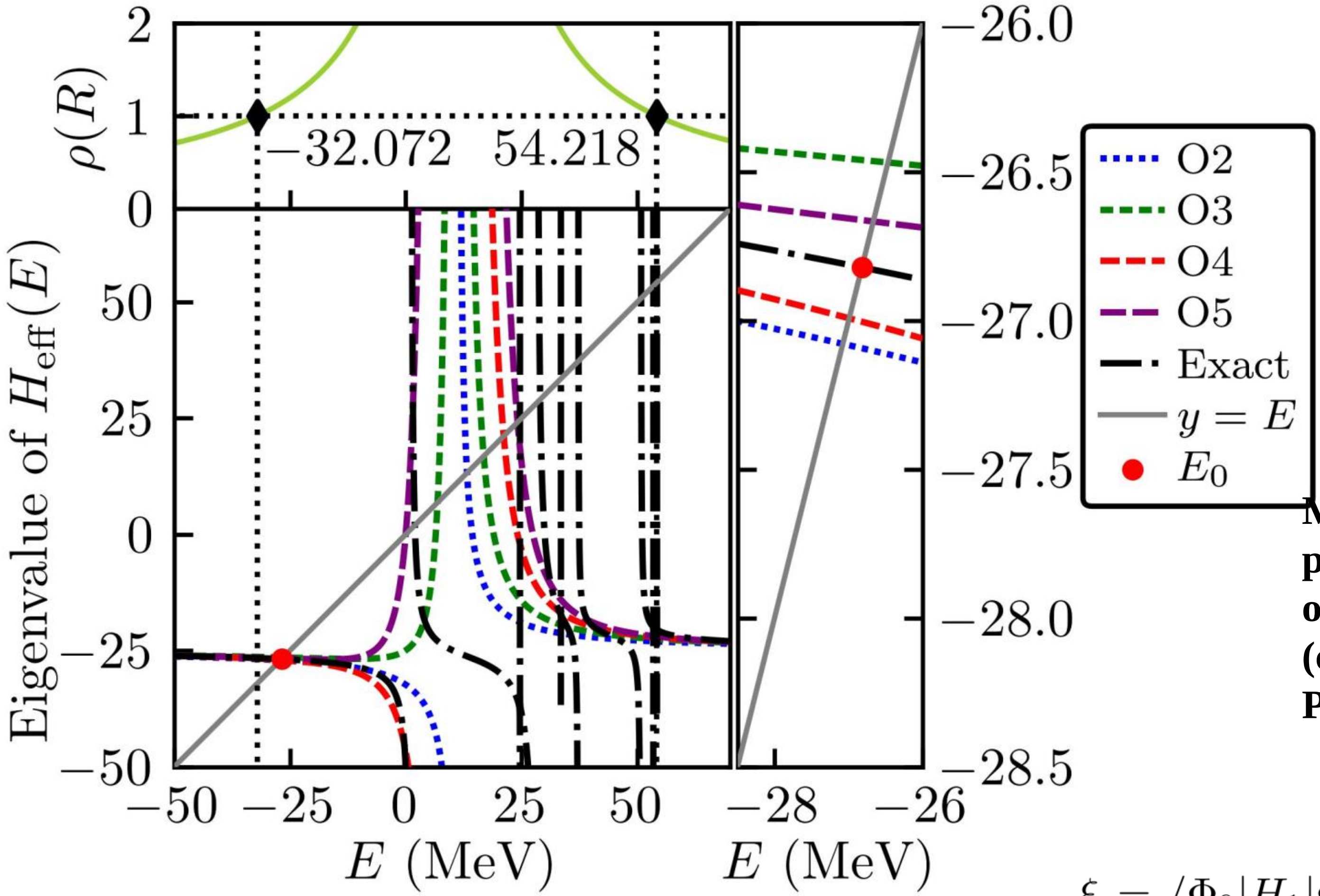

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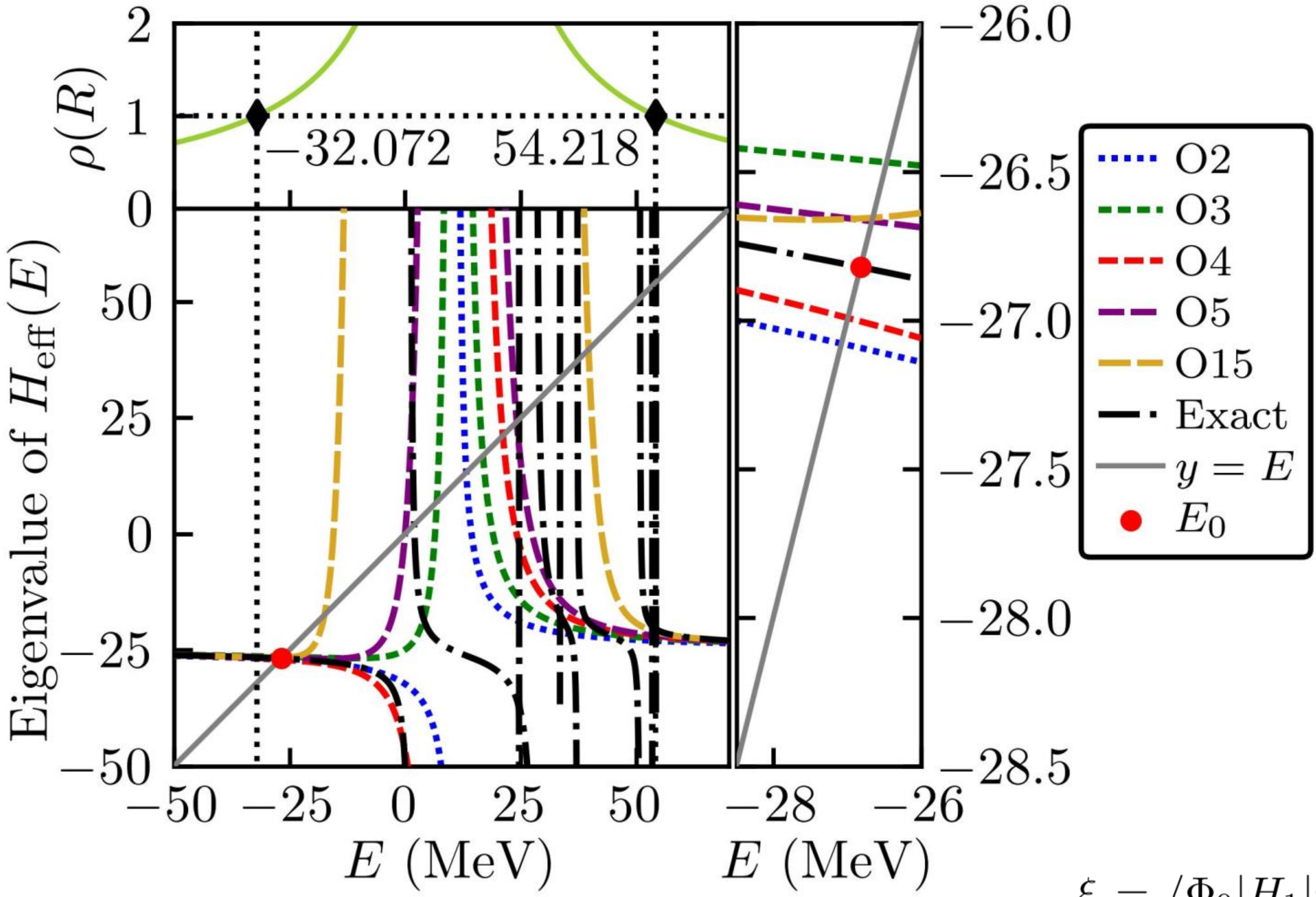
# MBPT in BW Formalism: *K*-Box Iterative Calculations

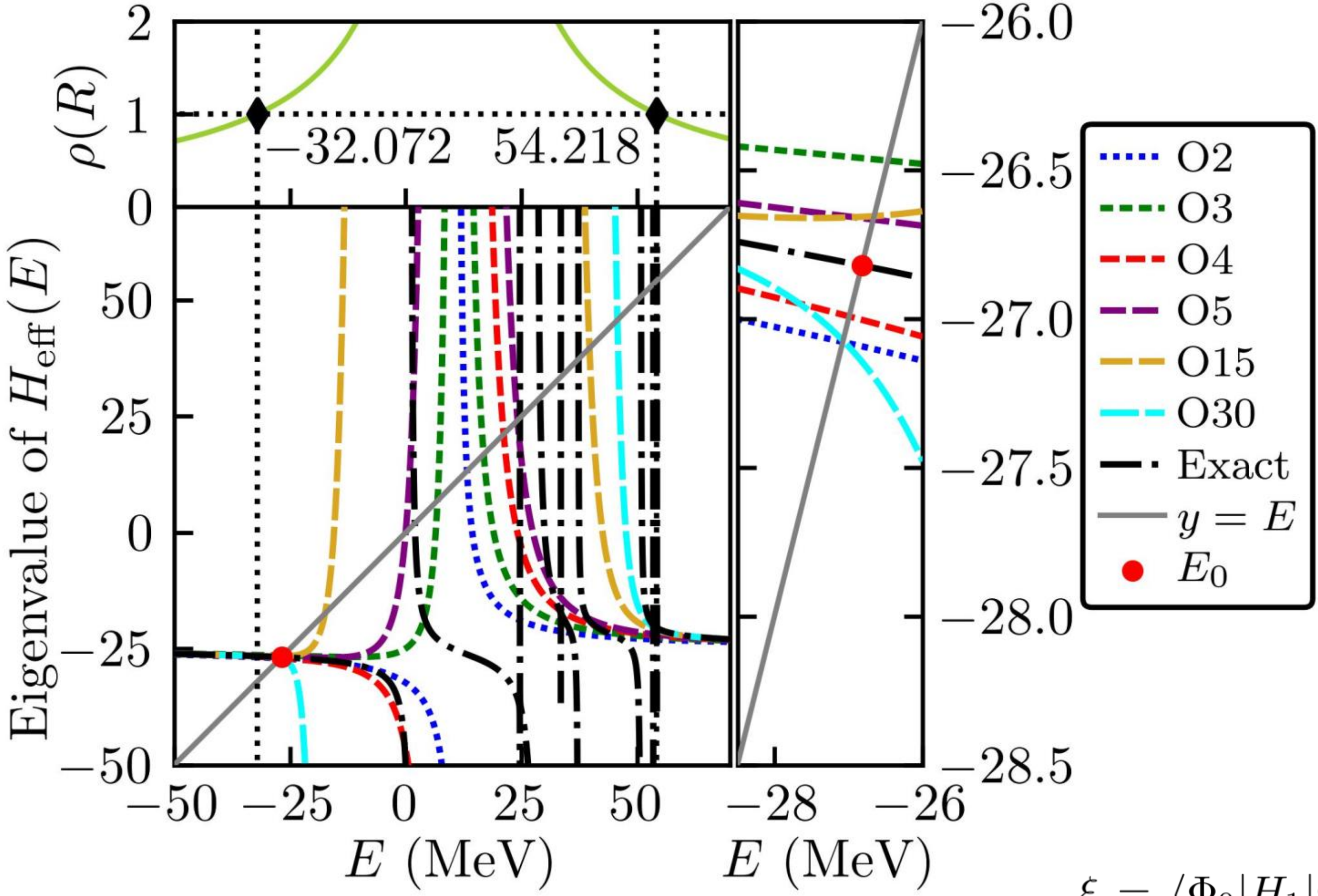


**Møller-Plesset (MP) partitioning with a normal-ordered Hamiltonian**

$$\xi = \langle\Phi_0|H_1|\Phi_0\rangle = -132.927\ \text{MeV}$$

**Ground state energy of $^4$He,**
**DJ16, HO basis,$\hbar\omega = 18$ MeV, $N_{\rm max}$=2.**
**NCSM: $E_0$ = -26.822 MeV**

# MBPT in BW Formalism: *K*-Box Iterative Calculations

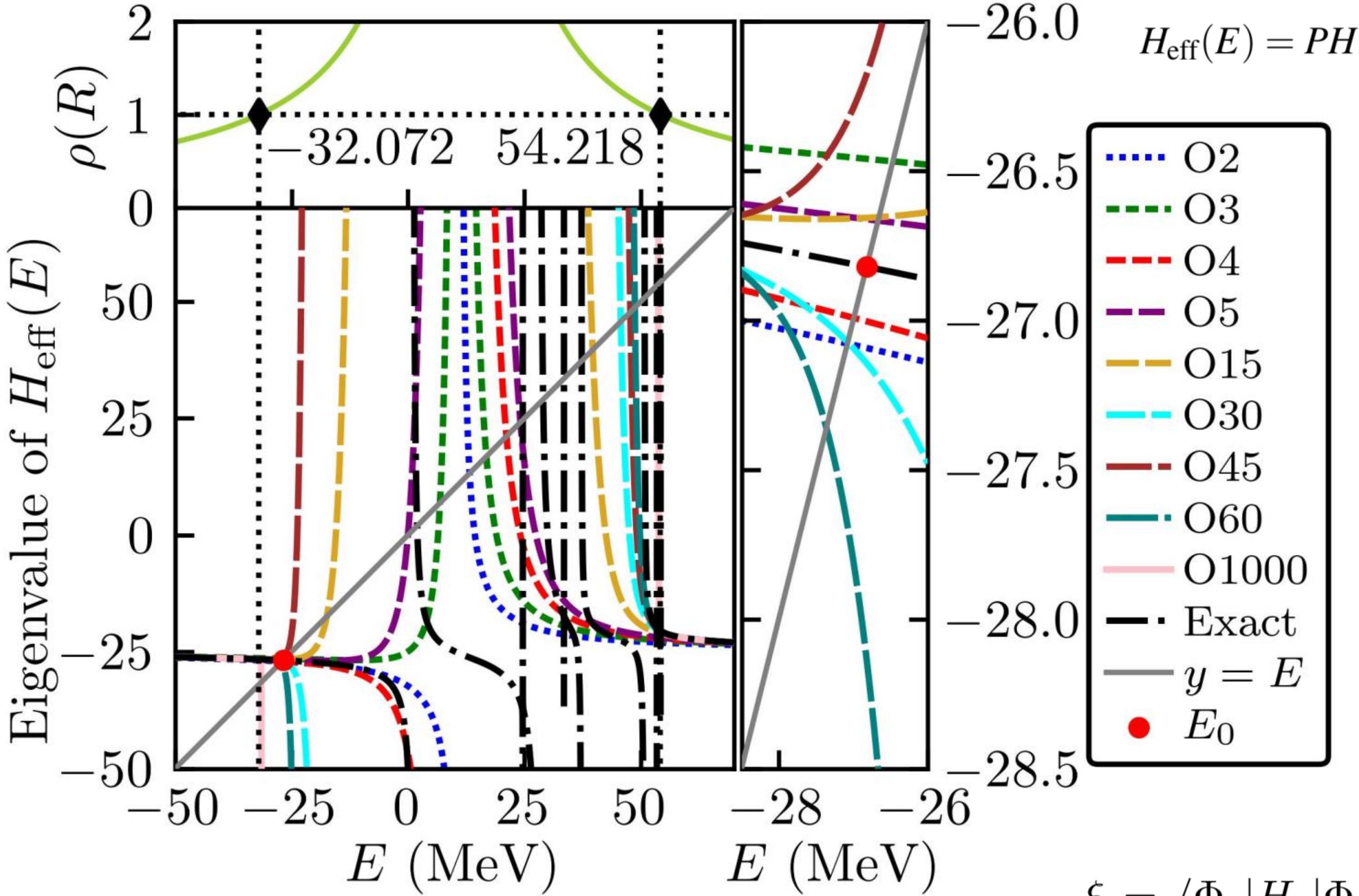


**Møller-Plesset (MP) partitioning with a normal-ordered Hamiltonian (cf. R.Roth, J. Langhammer, PLB683, 282 (2010))**

$$\xi = \langle \Phi_0 | H_1 | \Phi_0 \rangle = -132.927 \text{ MeV}$$

**Ground state energy of $^4$He,**
**DJ16, HO basis,$\hbar\omega = 18$ MeV, $N_{\mathrm{max}}$=2.**
**NCSM: $E_0$ = -26.822 MeV**

# MBPT in BW Formalism: *K*-Box Iterative Calculations



$$H_{\rm eff}(E) = PHP + P\hat{K}(E)Q\frac{1}{E - QH_0Q - Q\xi Q}QHP.$$

**Møller-Plesset (MP) partitioning with a normal-ordered Hamiltonian (cf. R.Roth, J. Langhammer, PLB683, 282 (2010))**

$$\xi = \langle\Phi_0|H_1|\Phi_0\rangle = -132.927\ \mathrm{MeV}$$

**Ground state energy of $^4$He,**
**DJ16, HO basis, $\hbar\omega = 18$ MeV, $N_{\rm max}$=2.**
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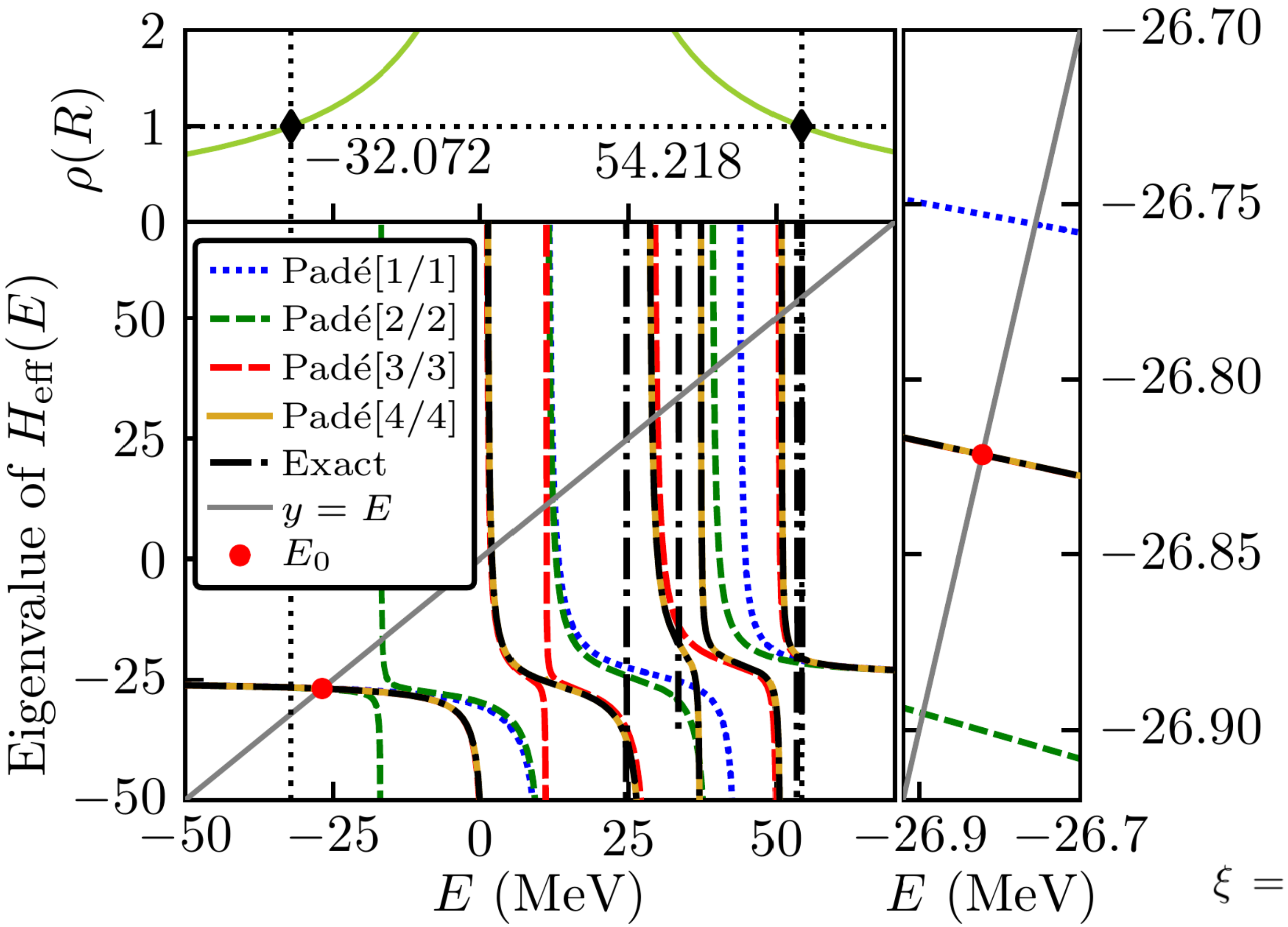
# MBPT in BW Formalism: *K*-Box Iterative Calculations



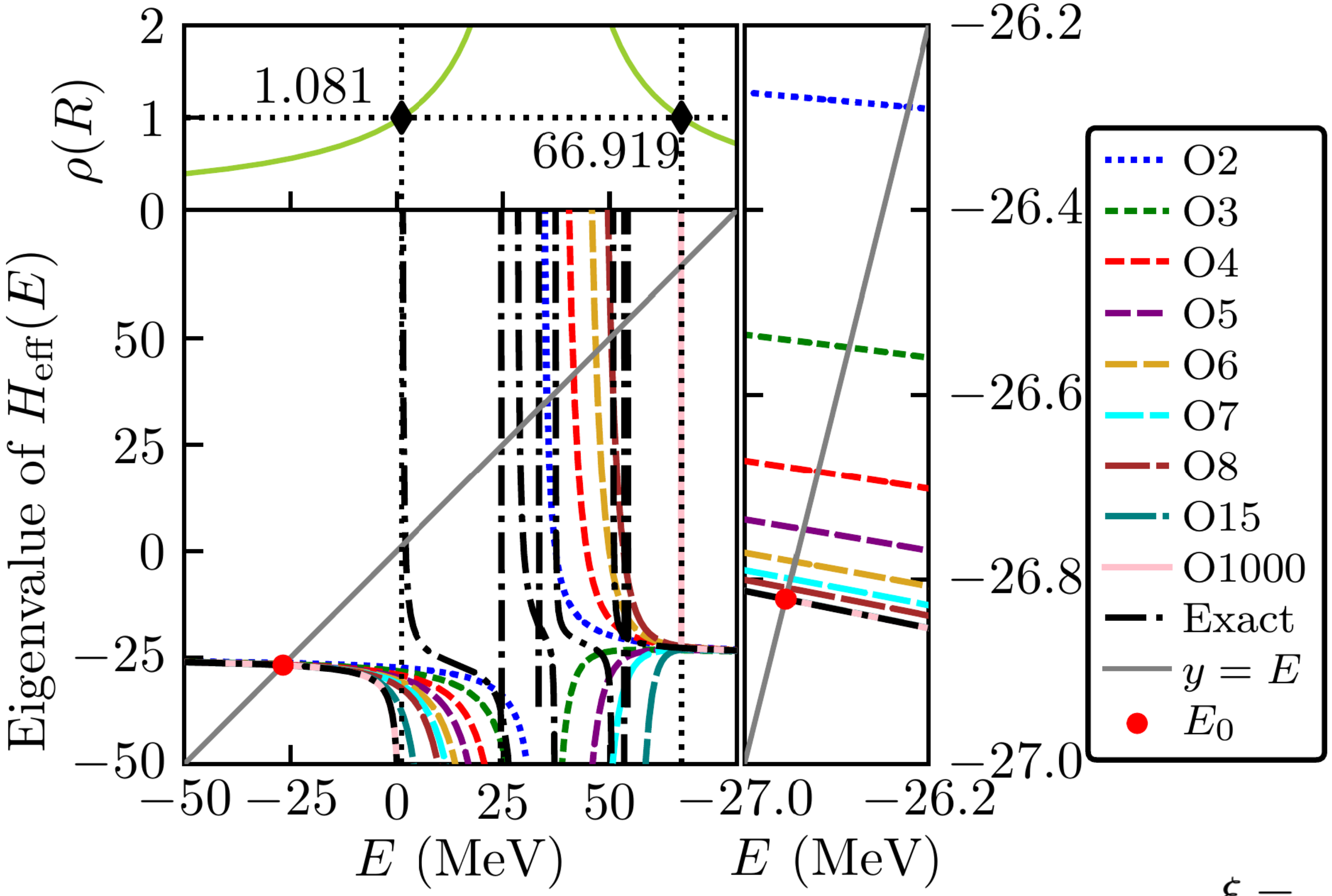
**Ground state energy of $^4$He,**
**DJ16, HO basis,**
**$\hbar\omega$ = 18 MeV, $N_{\mathrm{max}}$=2**
**NCSM: $E_0$ = -26.822 MeV**

**Møller-Plesset (MP) partitioning with a normal-ordered Hamiltonian**

$$\xi = \langle \Phi_0 | H_1 | \Phi_0 \rangle = -132.927 \text{ MeV}$$

$$\text{Padé}[L, M] = \frac{A_L(z)}{B_M(z)} = \frac{a_0 + a_1 z + a_2 z^2 + \cdots + a_L z^L}{b_0 + b_1 z + b_2 z^2 + \cdots + b_M z^M} = \sum_{n=0}^{L+M} c_n z^n + \mathcal{O}(z^{L+M+1}) \qquad f(z) = \sum_{n=0}^{\infty} c_n z^n, \ |z| < R_c$$

# MBPT in BW Formalism: *K*-Box Iterative Calculations

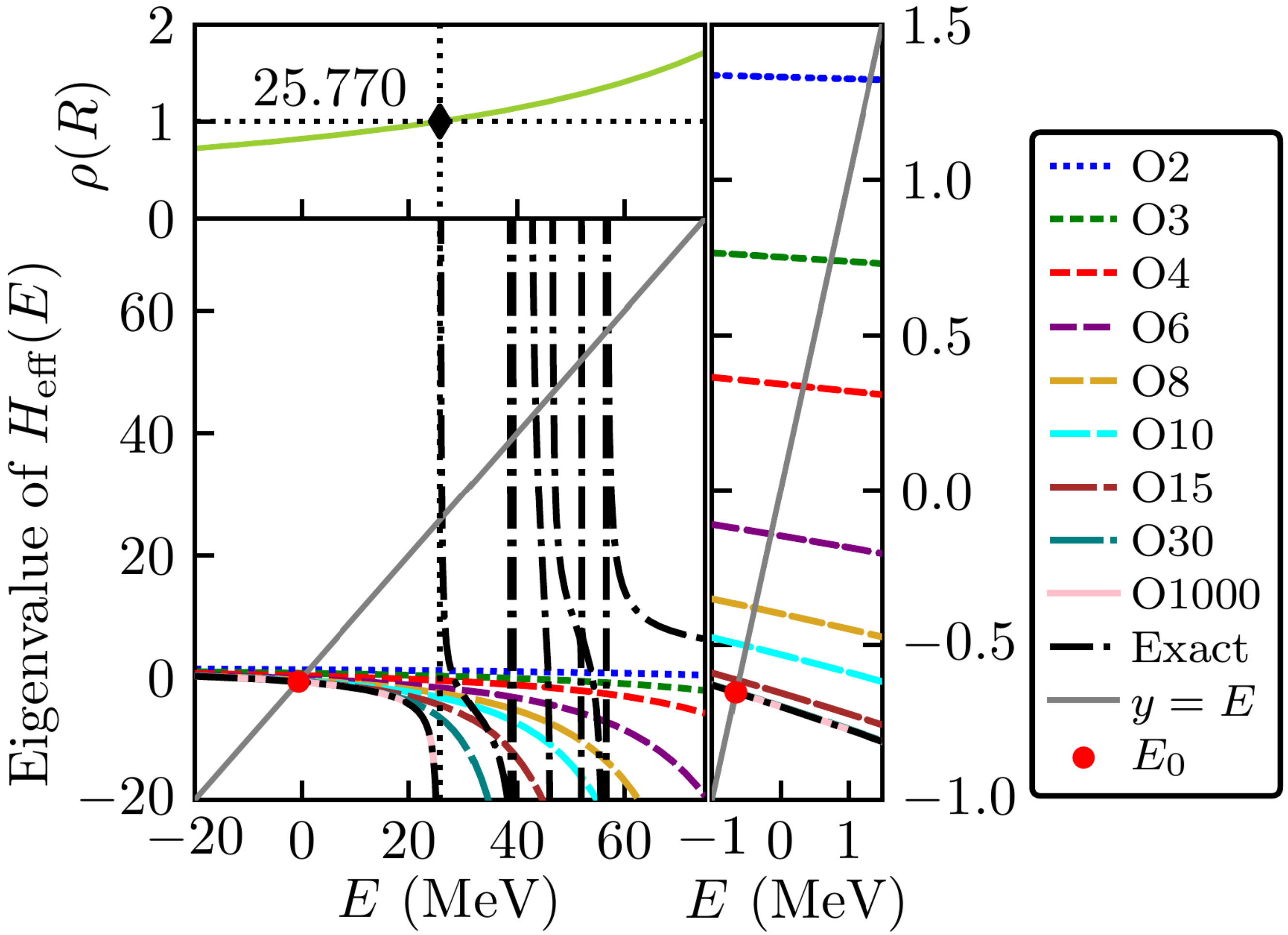


*Zhen Li, PhD Thesis, University of Bordeaux (2023)*

$\xi = -110$ MeV

**Ground state energy of $^4$He,**
**DJ16, HO basis, $\hbar\omega$ = 18 MeV, $N_{\max}$=2.**
**NCSM: $E_0$ = -26.822 MeV**

# MBPT in BW Formalism: *K*-Box Iterative Calculations



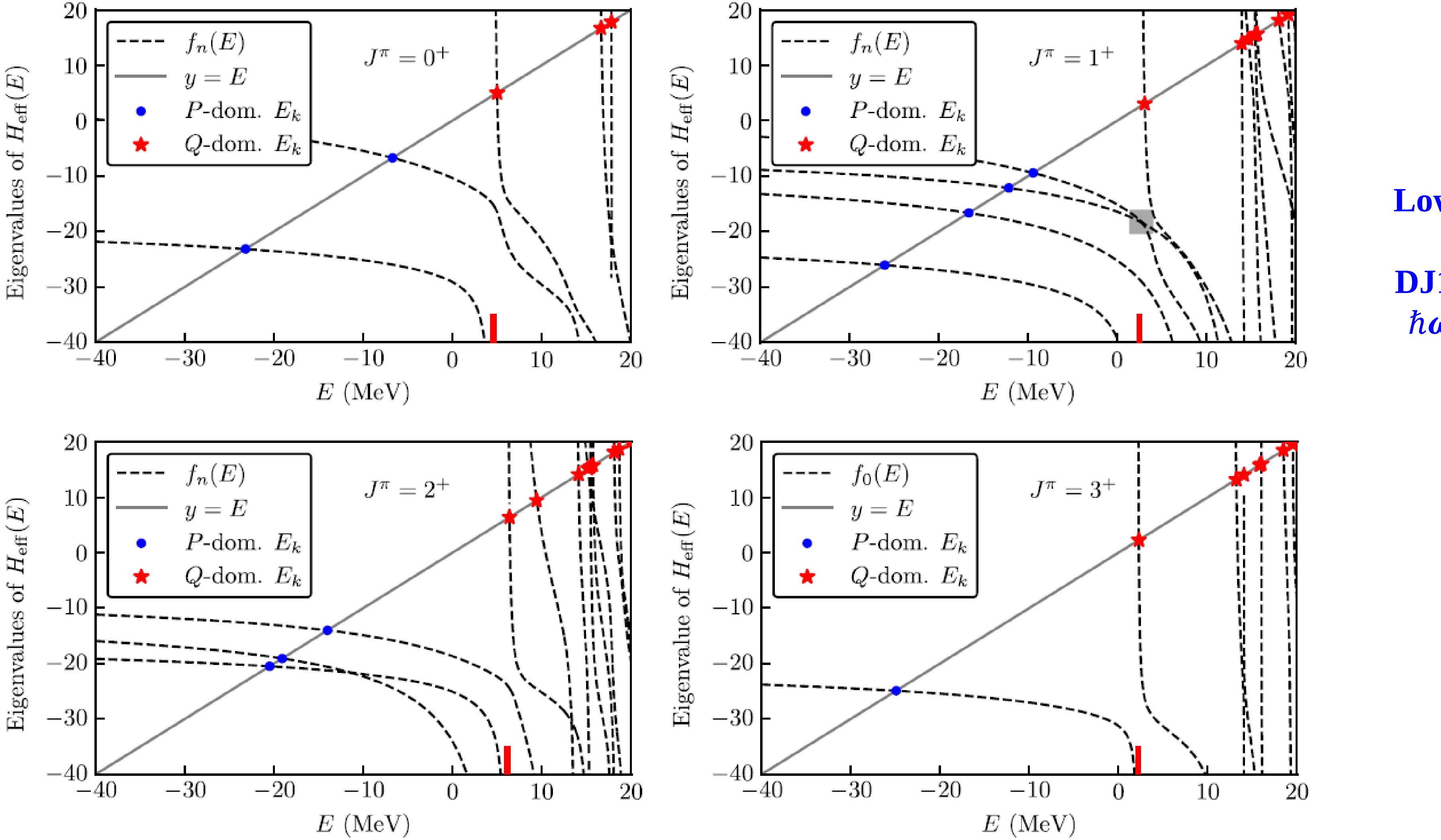
*Zhen Li, PhD Thesis,*
*University of Bordeaux (2023)*

*Zhen Li, Smirnova,*
*Phys. Lett. B854, 138749 (2024)*

$\xi = 0$ MeV

**Ground state energy of $^4$He,**
**bare (unsoftened, hard) N$^3$LO, HO basis, $\hbar\omega$ = 18 MeV, $N_{\text{max}}$=2.**
**NCSM: $E_0$ = -0.653 MeV**

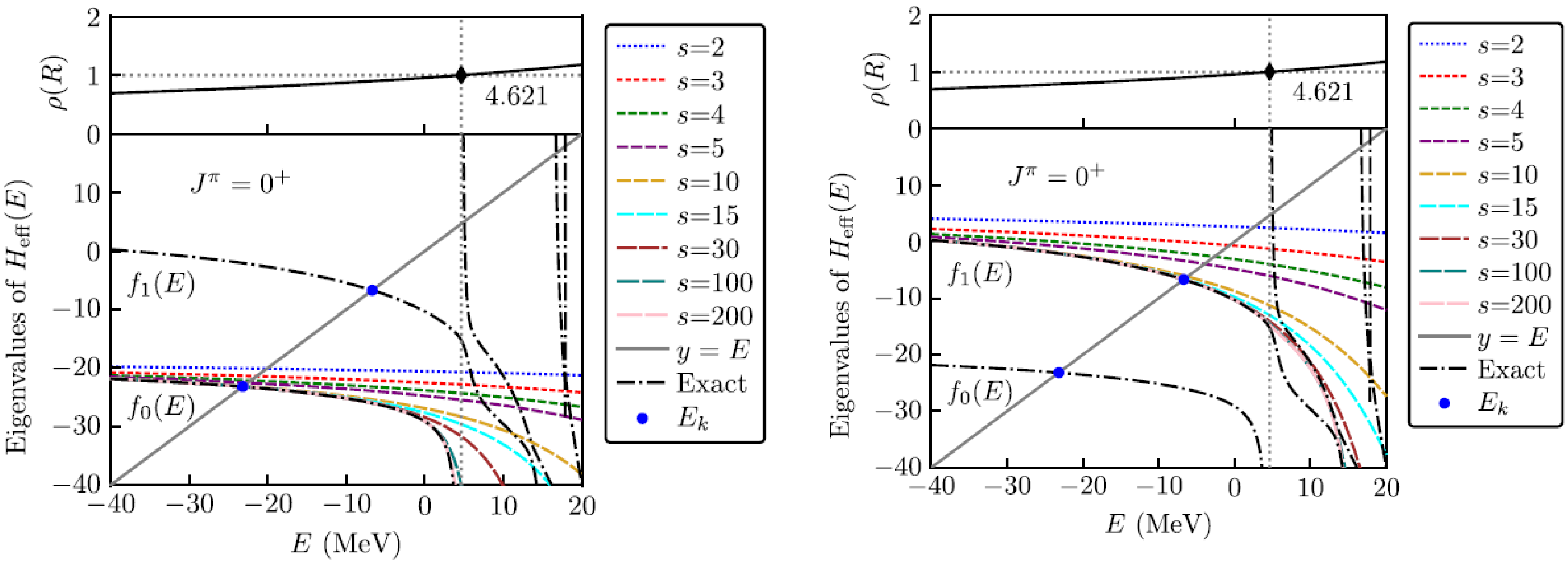
# 6Li : exact solution by matrix inversion



**Low-lying states of $^6$Li, DJ16, HO basis, $\hbar\omega$ = 18 MeV, $N_{\text{max}}$=2.**

*Zhen Li, PhD Thesis, University of Bordeaux (2023)*
*Zhen Li, N. Smirnova, Phys. Rev. C109, 064318 (2024)*

# MBPT in BW Formalism: *K*-Box Iterative Calculations



**0+ states of $^6$Li, DJ16,**
**HO basis, $\hbar\omega$ = 18 MeV, $N_{\text{max}}$=2**

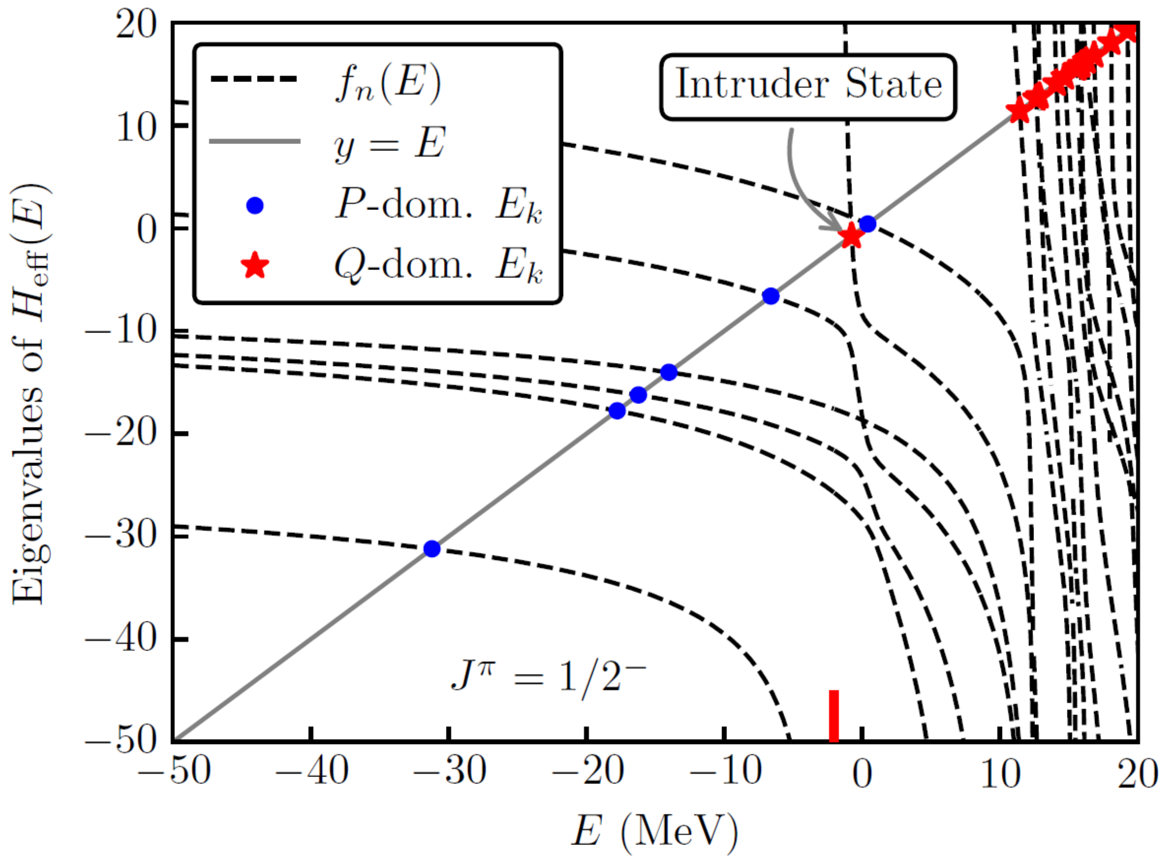
$$\xi = \langle \mathrm{C} | H_1 | \mathrm{C} \rangle$$

*Zhen Li, PhD Thesis, University of Bordeaux (2023)*

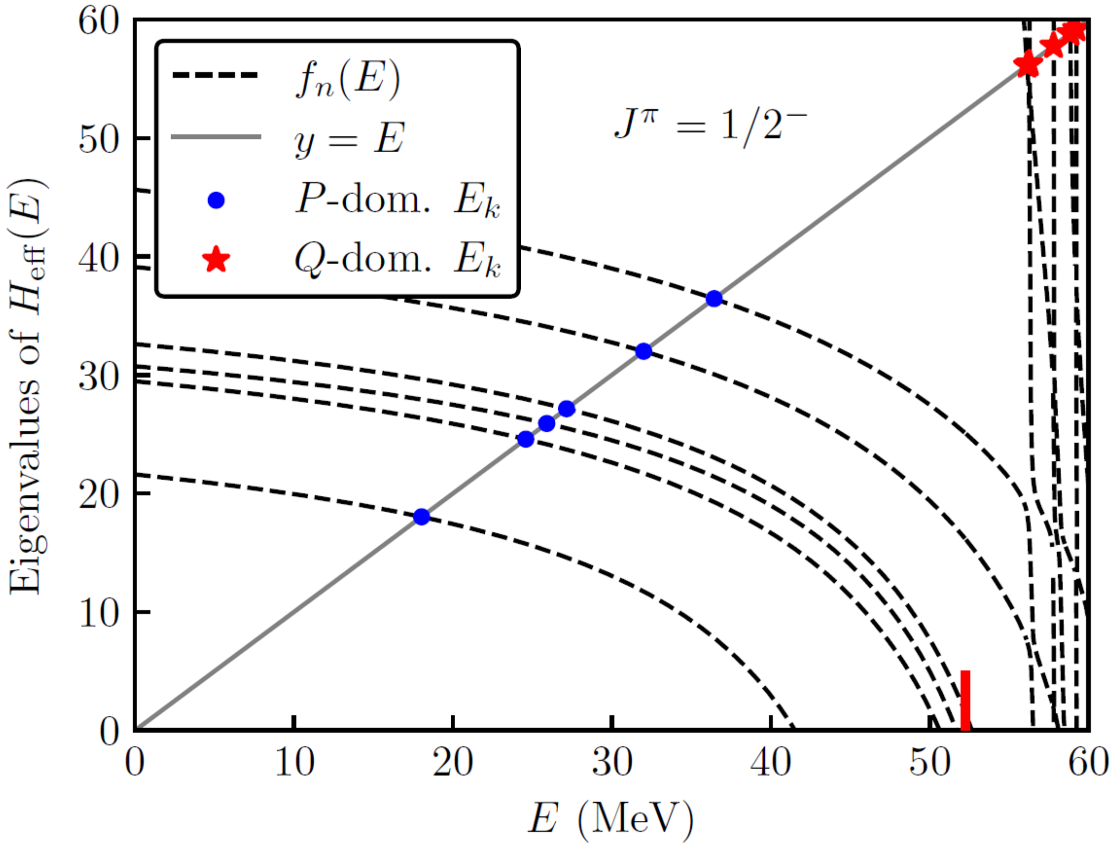
*Zhen Li, Smirnova, Phys. Rev. C109, 064318 (2024)*

# P-space Schrödinger equation for $^7$Li: Exact Solution

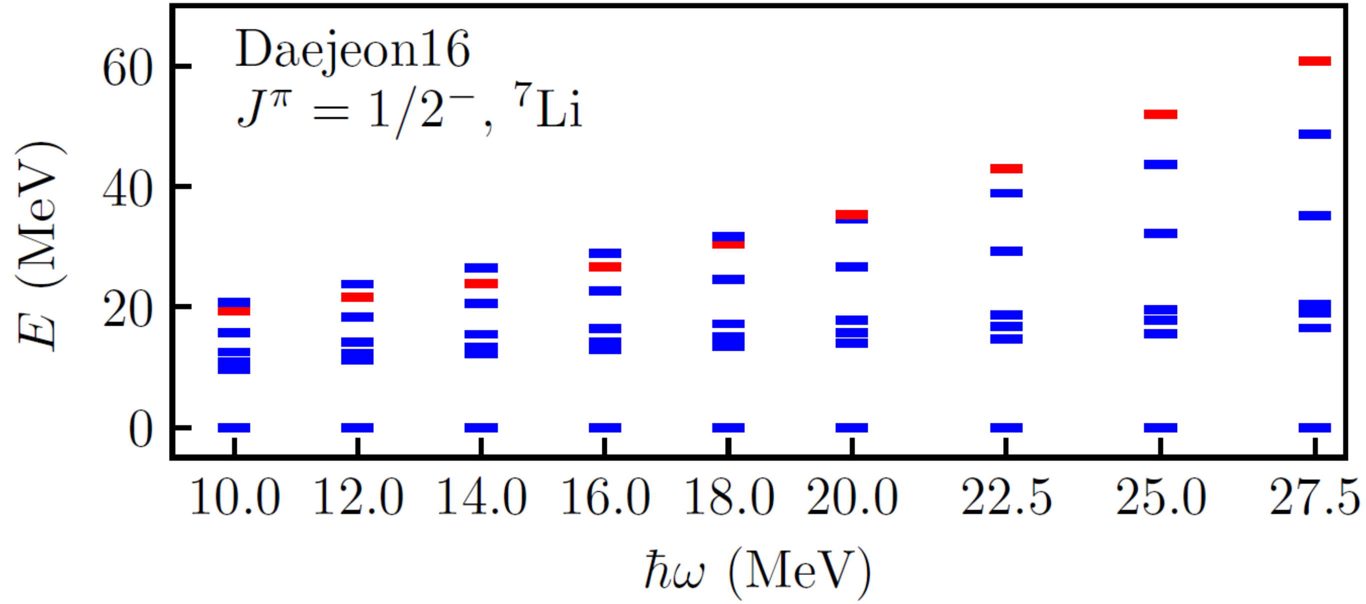
**1/2$^-$ states in $^7$Li with Daejeon16,**
**HO basis : $\hbar\omega$ = 18 MeV, $N_{\max}$=2**



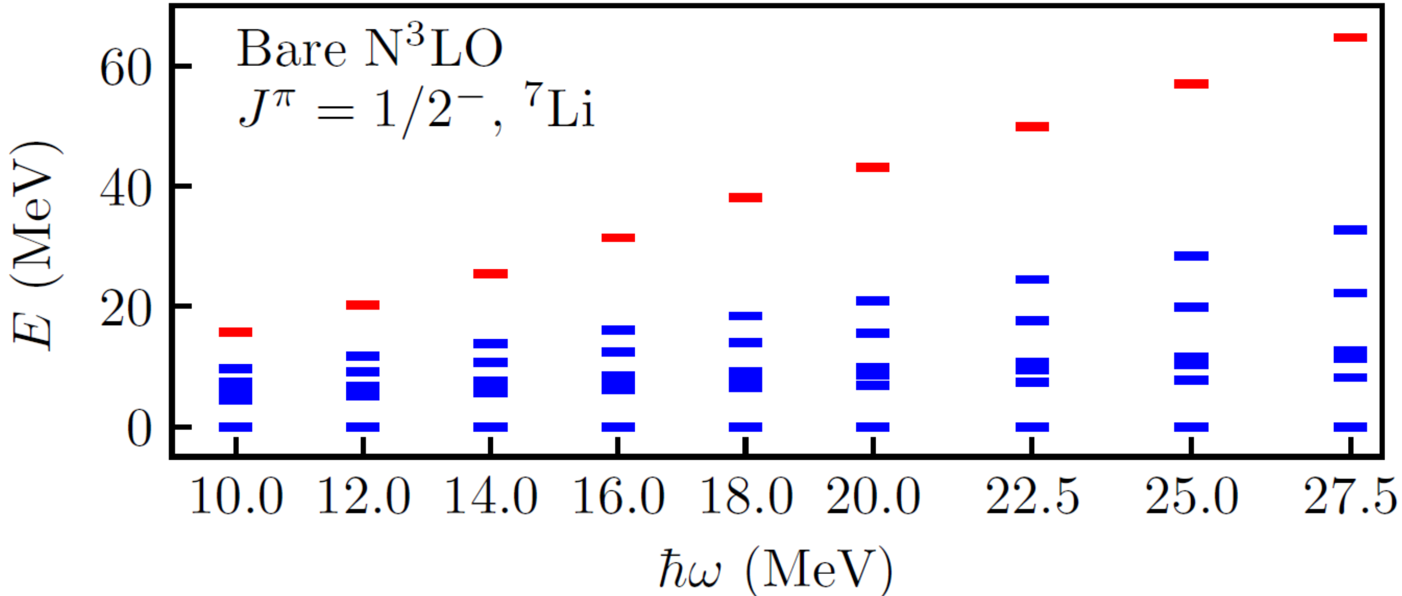
**1/2$^-$ states in $^7$Li with N3LO,**
**HO basis : $\hbar\omega$ = 18 MeV, $N_{\max}$=2**



# NCSM calculation for $^{7}$Li : 1/2$^{-}$ states



**Daejeon16, HO basis,**
**$\hbar\omega$ = 18 MeV, $N_{\text{max}}$=2**



**N3LO, HO basis,**
**$\hbar\omega$ = 18 MeV, $N_{\text{max}}$=2**

# Conclusions and Perspectives

- Microscopic derivation of effective valence-space interaction for the nuclear shell model is still challenging, although it rapidly progresses *(talk by S.R. Stroberg*)

- OLS transformation of the NCSM solution gives encouraging results :

  further steps are foreseen towards larger NCSM spaces and/or larger valence-spaces (*p-sd-pf*).

- MBPT revisited – convergence criterion for BW MBPT - always converging for the lowest $J^{\pi}$ (*PhD thesis of Zhen LI* ) => further implications for RS MBPT ?

- Importance of microscopic approaches to effective interactions and transition operators as first-principles derivation of the Nuclear Shell Model, started 75 years by M. Goeppert-Mayer et al, and towards precision nuclear theory for spectroscopy of exotic nuclei, fundamental interaction studies and astrophysical applications

# BACKUP SLIDES

# Hermitian Effective Hamiltonian

$$
\begin{aligned}
H_{\text{eff}}^{\text{her}} &= \sum_{\alpha\in\mathbb{P}} E_\alpha |\tilde{\Psi}_\alpha^{\mathbb{P}}\rangle\langle\tilde{\Psi}_\alpha^{\mathbb{P}}| \\
&= \sum_{\alpha\in\mathbb{P}} E_\alpha \frac{1}{\sqrt{\mathscr{V}\mathscr{V}^\dagger}} |\Psi_\alpha^{\mathbb{P}}\rangle\langle\Psi_\alpha^{\mathbb{P}}| \frac{1}{\sqrt{\mathscr{V}\mathscr{V}^\dagger}} \\
&= \sum_{\alpha\in\mathbb{P}} E_\alpha \frac{1}{\sqrt{\mathscr{V}\mathscr{V}^\dagger}} \mathscr{V}|\Phi_\alpha\rangle\langle\Phi_\alpha|\mathscr{V}^\dagger \frac{1}{\sqrt{\mathscr{V}\mathscr{V}^\dagger}} \\
&= \frac{1}{\sqrt{\mathscr{V}\mathscr{V}^\dagger}} \mathscr{V} \sum_{\alpha\in\mathbb{P}} E_\alpha |\Phi_\alpha\rangle\langle\Phi_\alpha|\mathscr{V}^\dagger \qquad 1 \\
&= \underbrace{\frac{1}{\sqrt{\mathscr{V}\mathscr{V}^\dagger}} \mathscr{V} H_{\text{eff}}^{\text{diag}} \mathscr{V}^\dagger \frac{1}{\sqrt{\mathscr{V}\mathscr{V}^\dagger}}}_{\text{OLS transformation!}},
\end{aligned}
$$

*Zhen Li, PhD thesis (2023)*

$$\mathscr{V} \equiv \sum_{\alpha\in\mathbb{P}} |\Psi_\alpha^{\mathbb{P}}\rangle\langle\Phi_\alpha|,$$

$$\mathscr{V}|\Phi_\alpha\rangle = |\Psi_\alpha^{\mathbb{P}}\rangle, \; |\Phi_\alpha\rangle = \frac{1}{\mathscr{V}}|\Psi_\alpha^{\mathbb{P}}\rangle.$$

$$|\Psi_\alpha^{\mathbb{P}}\rangle = \sum_{\beta\in\mathbb{P}} c_\beta^\alpha |\Phi_\beta\rangle,$$

$$\mathscr{V} \equiv \sum_{\alpha\in\mathbb{P}} |\Psi_\alpha^{\mathbb{P}}\rangle\langle\Phi_\alpha| = \sum_{\alpha\beta\in\mathbb{P}} c_\beta^\alpha |\Phi_\beta\rangle\langle\Phi_\alpha| = \underbrace{\begin{pmatrix} c_1^1 & c_1^2 & c_1^3 & \cdots & c_1^{d_p} \\ c_2^1 & c_2^2 & c_2^3 & \cdots & c_2^{d_p} \\ c_3^1 & c_3^2 & c_3^3 & \cdots & c_3^{d_p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ c_{d_p}^1 & c_{d_p}^2 & c_{d_p}^3 & \cdots & c_{d_p}^{d_p} \end{pmatrix}}_{U_P},$$

# **BW MBPT:** Practical Calculations for Closed-Shell Nuclei

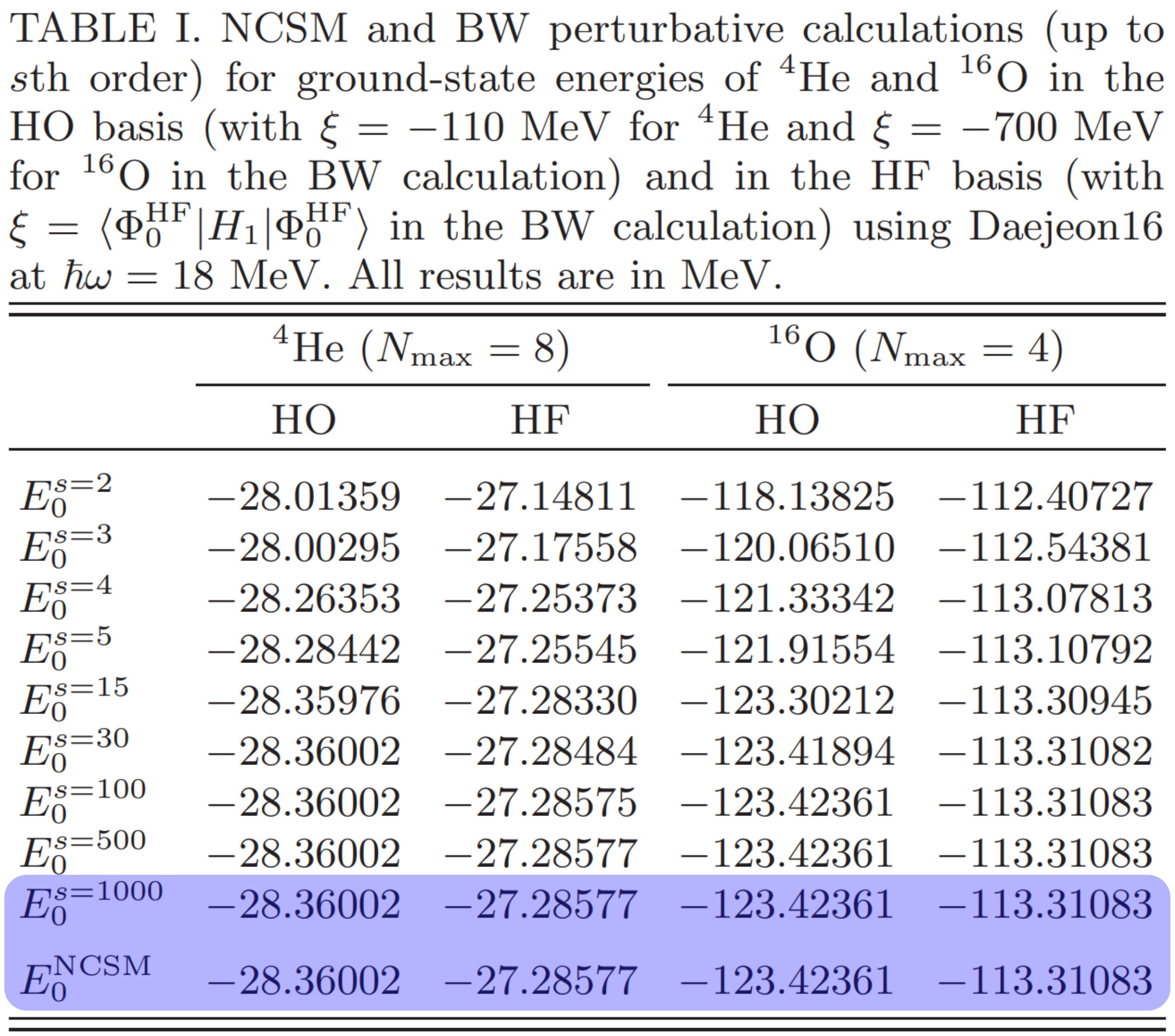


TABLE I. NCSM and BW perturbative calculations (up to $s$th order) for ground-state energies of $^4$He and $^{16}$O in the HO basis (with $\xi = -110$ MeV for $^4$He and $\xi = -700$ MeV for $^{16}$O in the BW calculation) and in the HF basis (with $\xi = \langle \Phi_0^{\mathrm{HF}} | H_1 | \Phi_0^{\mathrm{HF}} \rangle$ in the BW calculation) using Daejeon16 at $\hbar\omega = 18$ MeV. All results are in MeV.

| | $^4$He ($N_{\max} = 8$) | | $^{16}$O ($N_{\max} = 4$) | |
|---|---|---|---|---|
| | HO | HF | HO | HF |
| $E_0^{s=2}$ | −28.01359 | −27.14811 | −118.13825 | −112.40727 |
| $E_0^{s=3}$ | −28.00295 | −27.17558 | −120.06510 | −112.54381 |
| $E_0^{s=4}$ | −28.26353 | −27.25373 | −121.33342 | −113.07813 |
| $E_0^{s=5}$ | −28.28442 | −27.25545 | −121.91554 | −113.10792 |
| $E_0^{s=15}$ | −28.35976 | −27.28330 | −123.30212 | −113.30945 |
| $E_0^{s=30}$ | −28.36002 | −27.28484 | −123.41894 | −113.31082 |
| $E_0^{s=100}$ | −28.36002 | −27.28575 | −123.42361 | −113.31083 |
| $E_0^{s=500}$ | −28.36002 | −27.28577 | −123.42361 | −113.31083 |
| $E_0^{s=1000}$ | −28.36002 | −27.28577 | −123.42361 | −113.31083 |
| $E_0^{\mathrm{NCSM}}$ | −28.36002 | −27.28577 | −123.42361 | −113.31083 |

**$^4$He, $^{16}$O**
**Daejeon16**
**HO basis**
**HF basis**

# **BW MBPT:** Practical Calculations for Closed-Shell Nuclei

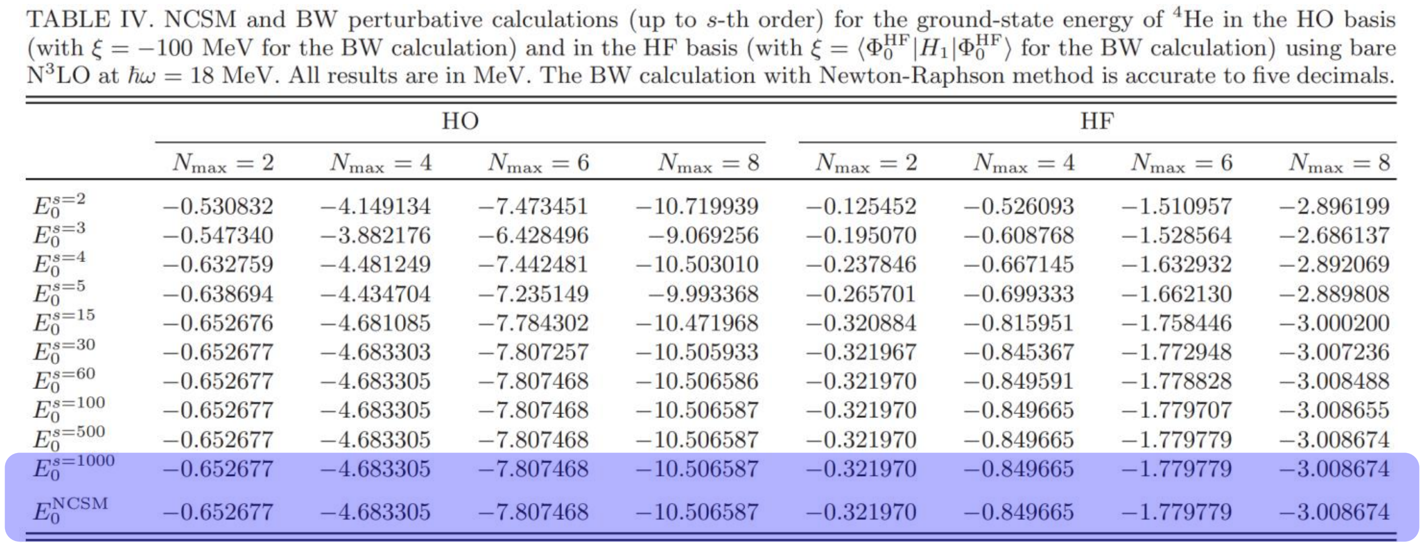


TABLE IV. NCSM and BW perturbative calculations (up to $s$-th order) for the ground-state energy of $^4$He in the HO basis (with $\xi = -100$ MeV for the BW calculation) and in the HF basis (with $\xi = \langle \Phi_0^{\mathrm{HF}} | H_1 | \Phi_0^{\mathrm{HF}} \rangle$ for the BW calculation) using bare N$^3$LO at $\hbar\omega = 18$ MeV. All results are in MeV. The BW calculation with Newton-Raphson method is accurate to five decimals.

| | HO | | | | HF | | | |
|---|---|---|---|---|---|---|---|---|
| | $N_{\max}=2$ | $N_{\max}=4$ | $N_{\max}=6$ | $N_{\max}=8$ | $N_{\max}=2$ | $N_{\max}=4$ | $N_{\max}=6$ | $N_{\max}=8$ |
| $E_0^{s=2}$ | −0.530832 | −4.149134 | −7.473451 | −10.719939 | −0.125452 | −0.526093 | −1.510957 | −2.896199 |
| $E_0^{s=3}$ | −0.547340 | −3.882176 | −6.428496 | −9.069256 | −0.195070 | −0.608768 | −1.528564 | −2.686137 |
| $E_0^{s=4}$ | −0.632759 | −4.481249 | −7.442481 | −10.503010 | −0.237846 | −0.667145 | −1.632932 | −2.892069 |
| $E_0^{s=5}$ | −0.638694 | −4.434704 | −7.235149 | −9.993368 | −0.265701 | −0.699333 | −1.662130 | −2.889808 |
| $E_0^{s=15}$ | −0.652676 | −4.681085 | −7.784302 | −10.471968 | −0.320884 | −0.815951 | −1.758446 | −3.000200 |
| $E_0^{s=30}$ | −0.652677 | −4.683303 | −7.807257 | −10.505933 | −0.321967 | −0.845367 | −1.772948 | −3.007236 |
| $E_0^{s=60}$ | −0.652677 | −4.683305 | −7.807468 | −10.506586 | −0.321970 | −0.849591 | −1.778828 | −3.008488 |
| $E_0^{s=100}$ | −0.652677 | −4.683305 | −7.807468 | −10.506587 | −0.321970 | −0.849665 | −1.779707 | −3.008655 |
| $E_0^{s=500}$ | −0.652677 | −4.683305 | −7.807468 | −10.506587 | −0.321970 | −0.849665 | −1.779779 | −3.008674 |
| $E_0^{s=1000}$ | −0.652677 | −4.683305 | −7.807468 | −10.506587 | −0.321970 | −0.849665 | −1.779779 | −3.008674 |
| $E_0^{\mathrm{NCSM}}$ | −0.652677 | −4.683305 | −7.807468 | −10.506587 | −0.321970 | −0.849665 | −1.779779 | −3.008674 |

**$^4$He**
**bare N$^3$LO**
**HO basis**
**HF basis**

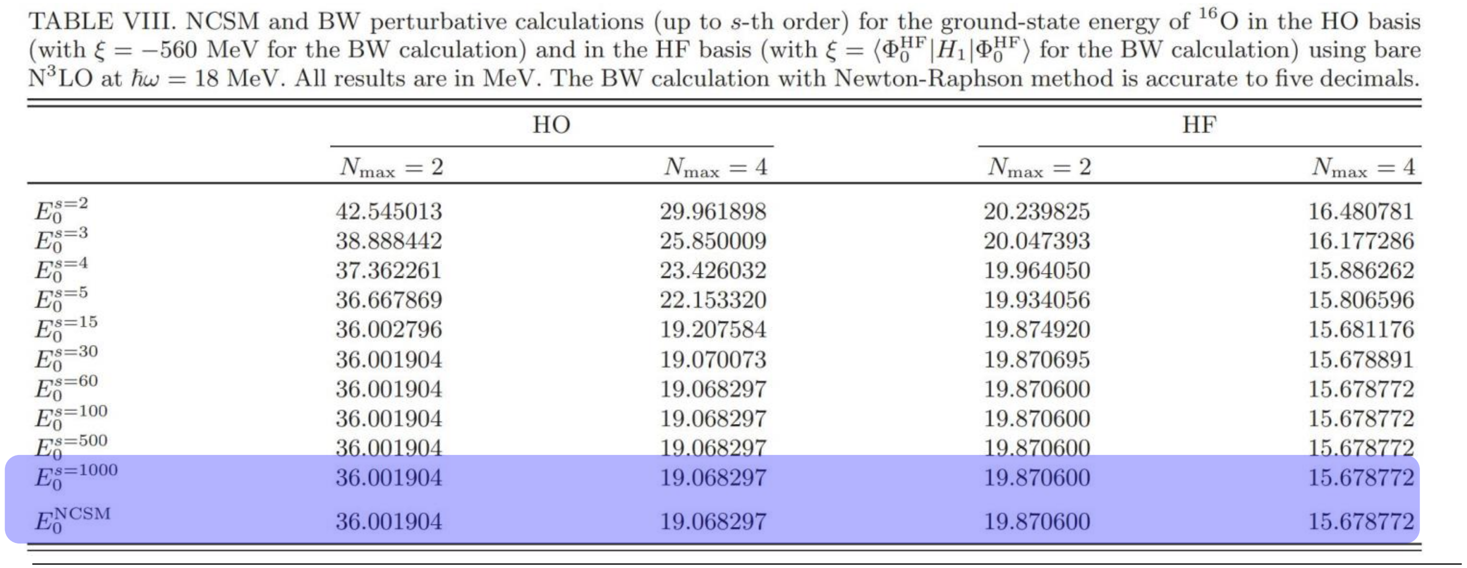


TABLE VIII. NCSM and BW perturbative calculations (up to $s$-th order) for the ground-state energy of $^{16}$O in the HO basis (with $\xi = -560$ MeV for the BW calculation) and in the HF basis (with $\xi = \langle \Phi_0^{\mathrm{HF}} | H_1 | \Phi_0^{\mathrm{HF}} \rangle$ for the BW calculation) using bare N$^3$LO at $\hbar\omega = 18$ MeV. All results are in MeV. The BW calculation with Newton-Raphson method is accurate to five decimals.

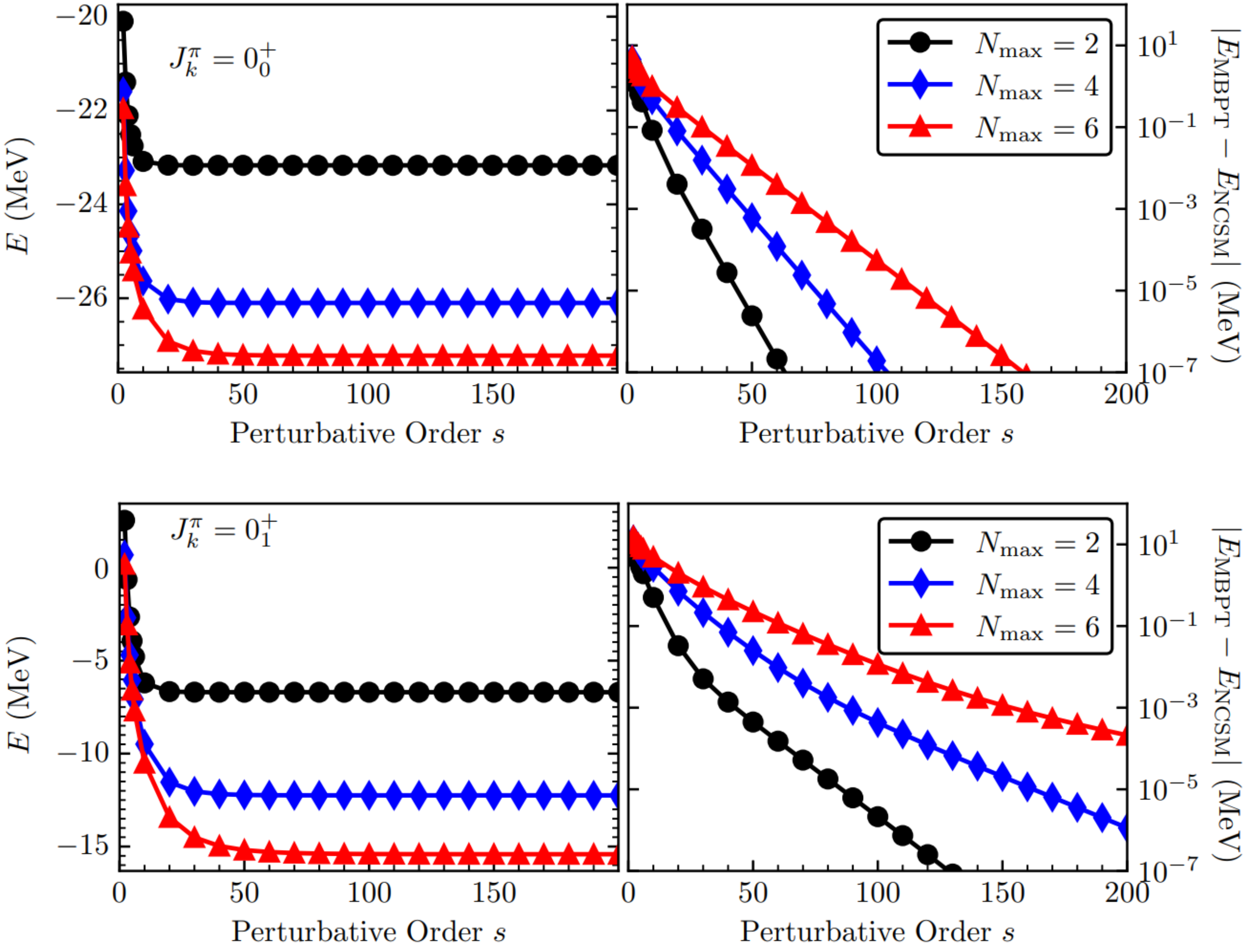
| | HO | | HF | |
|---|---|---|---|---|
| | $N_{\max}=2$ | $N_{\max}=4$ | $N_{\max}=2$ | $N_{\max}=4$ |
| $E_0^{s=2}$ | 42.545013 | 29.961898 | 20.239825 | 16.480781 |
| $E_0^{s=3}$ | 38.888442 | 25.850009 | 20.047393 | 16.177286 |
| $E_0^{s=4}$ | 37.362261 | 23.426032 | 19.964050 | 15.886262 |
| $E_0^{s=5}$ | 36.667869 | 22.153320 | 19.934056 | 15.806596 |
| $E_0^{s=15}$ | 36.002796 | 19.207584 | 19.874920 | 15.681176 |
| $E_0^{s=30}$ | 36.001904 | 19.070073 | 19.870695 | 15.678891 |
| $E_0^{s=60}$ | 36.001904 | 19.068297 | 19.870600 | 15.678772 |
| $E_0^{s=100}$ | 36.001904 | 19.068297 | 19.870600 | 15.678772 |
| $E_0^{s=500}$ | 36.001904 | 19.068297 | 19.870600 | 15.678772 |
| $E_0^{s=1000}$ | 36.001904 | 19.068297 | 19.870600 | 15.678772 |
| $E_0^{\mathrm{NCSM}}$ | 36.001904 | 19.068297 | 19.870600 | 15.678772 |

**$^{16}$O**
**bare N$^3$LO**
**HO basis**
**HF basis**

# **BW MBPT:** Convergence Behavior of Open-Shell Nuclei

**$0^+$ states of $^6$Li, Daejeon16, $\hbar\omega = 18$ MeV**

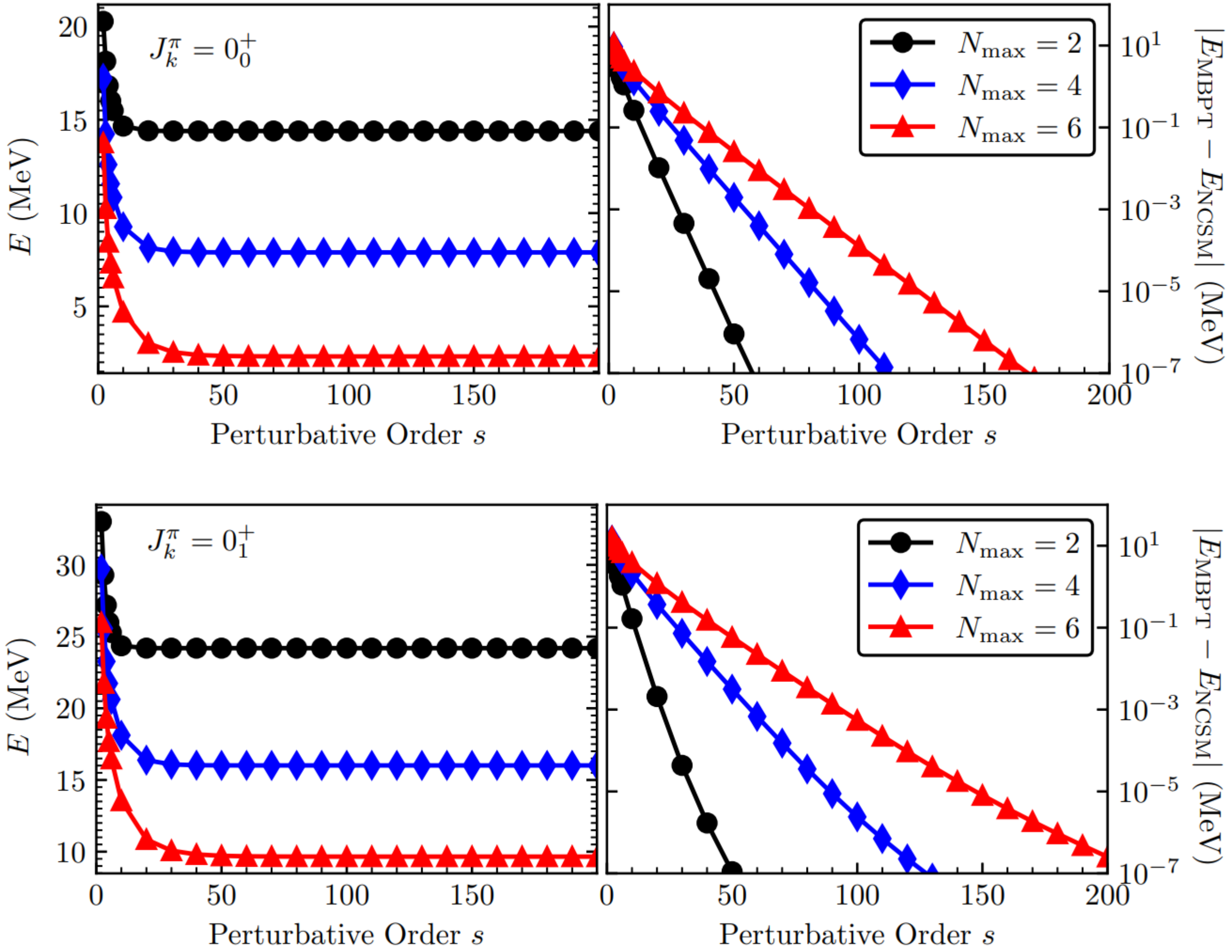
$\xi = \langle \mathrm{C}|H_1|\mathrm{C}\rangle$



# **BW MBPT:** Convergence Behavior of Open-Shell Nuclei

$0^+$ states of $^6$Li, Bare N3LO, $\hbar\omega = 18$ MeV

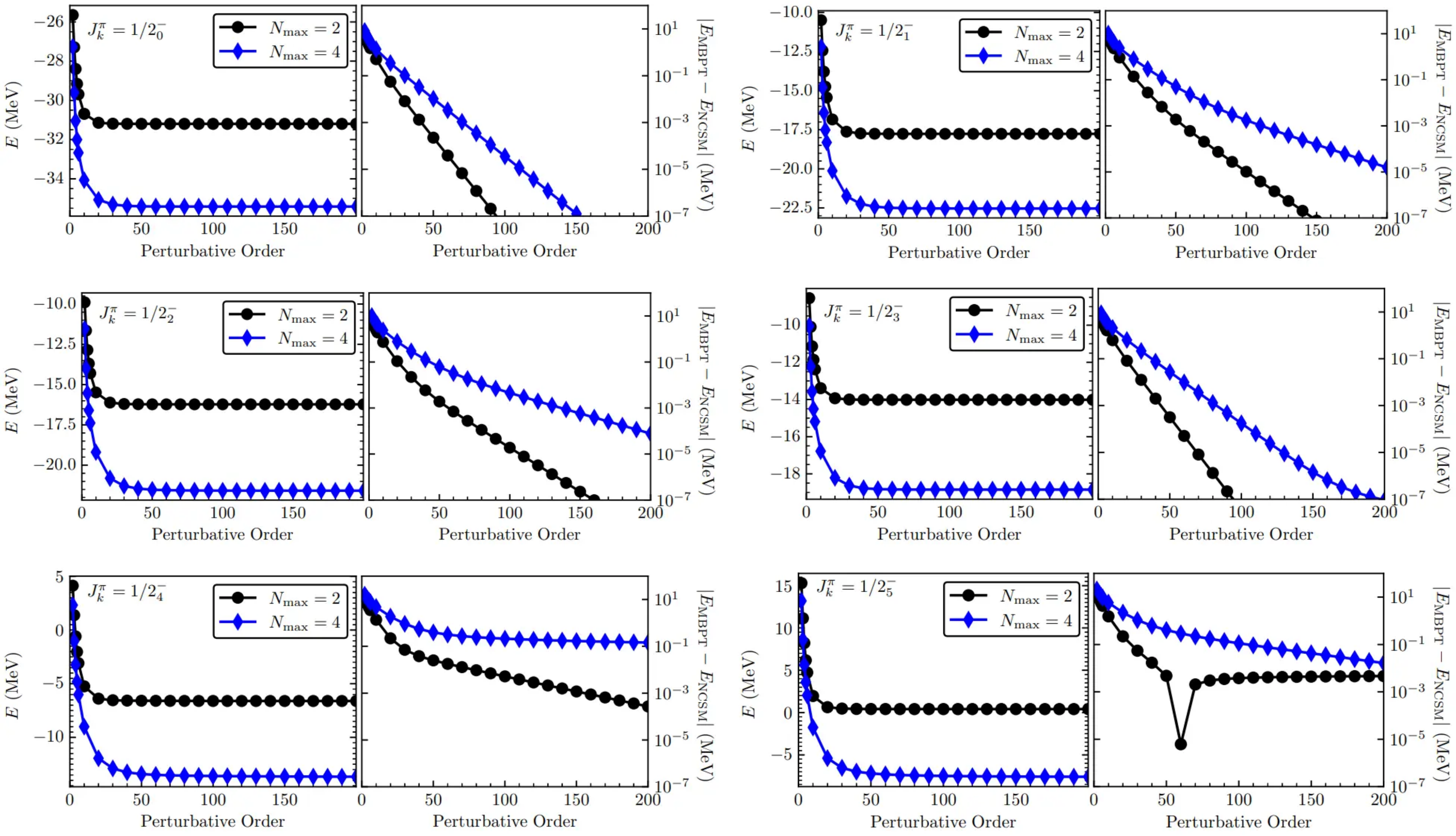
$$\xi = \langle \mathrm{C}|H_1|\mathrm{C}\rangle$$



# **BW MBPT:** Convergence Behavior of Open-Shell Nuclei

**$1/2^-$ states $^7$Li, Daejeon16, $\hbar\omega = 18$ MeV**

$$\xi = \langle \mathrm{C}|H_1|\mathrm{C}\rangle$$



# BW MBPT: Convergence Behavior of Open-Shell Nuclei

**$1/2^-$ states $^7$Li, Bare N$^3$LO, $\hbar\omega = 18$ MeV**

$$\xi = \langle \mathrm{C}|H_1|\mathrm{C}\rangle$$