Nuclear Shell Model Effective Interactions from Many-Body Perturbation Theory

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Nuclear Many Body Problem

A-Body Schrödinger Equation for Nucleus A

$$\hat{H}|\Psi_\alpha\rangle = E_\alpha|\Psi_\alpha\rangle$$

$$\hat{H} = \hat{T} + \hat{V} = \sum_{i=1}^{A} \frac{\hat{\boldsymbol{p}}_i^2}{2m} + \sum_{i<j}^{A} \hat{V}(|\boldsymbol{r}_i - \boldsymbol{r}_j|)$$

Nucleon-Nucleon Interactions

- **Chiral Potentials**: from chiral effective field theory (χEFT), Machleidt et al., Phys. Rep. 503, 1 (2011)
- **Bonn Potentials**: based on meson-exchange models (π, η, $\rho(770)$, $\omega(782)$), Machleidt et al., Phys. Rep. 149, 1 (1987), Machleidt, Phys. Rev. C 63, 024001 (2001)
- **Daejeon16 Potential**: based on renormalized chiral potential N^3LO, fitted to energies of 11 states up to $A = 16$, Shirokov et al., Phys. Lett. B 761, 87 (2016)
- **Argonne Potentials**: Wiringa et al., Phys. Rev. C 51, 38 (1995)
- ...

Nuclear Many Body Problem

Many-Body Methods for Nuclear System

- **Monte-Carlo methods (VMC, GFMC, AFDMC, etc.)**
  - J. Carlson et al., Rev. Mod. Phys. 87, 1067 (2015).
- **Configuration Interaction (CI) methods (SM, NCSM, CC, IM-SRG)**
  - E. Caurier et al., Rev. Mod. Phys. 77, 427 (2005).
  - B. R. Barrett, et al., Prog. Part. Nucl. Phys. 69, 131 (2013).
  - G. Hagen, et al., Rep. Prog. Phys. 77, 096302 (2014).
  - H. Hergert et al., Phys. Rep. 621, 165 (2016).
- **Self-Consistent Green's Function (SCGF) method**
  - W. H. Dickhoff et al., Prog. Part. Nucl. Phys. 52, 377 (2004).
- **Many-Body Perturbation Theory (MBPT)**
  - A. Tichai et al., Front. Phys. 8, 164 (2020).
- **Density Functional Theory (DFT)**
  - M. Bender et al., Rev. Mod. Phys. 75, 121 (2003).
- **HF, GCM, AMD, $\cdots$**

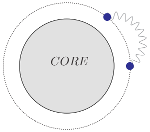
Shell Model

- **Approximations in Shell Model (Interacting Shell Model, Shell Model with a Core, or Valence Shell Model):**
  1. separate the model space into three parts: *Filled Space*, *Valence Space* and *Empty Space*
  2. only consider valence nucleons moving in the *Valence Space*

N	d_N	$\Sigma_N d_N$	*Shells*		*Parity*
⋮	⋮	⋮	⋮		⋮
9	110	440	$0l, 1j, 2h, 3f, 4p$		$-$
8	90	330	$0k, 1i, 2g, 3d, 4s$		$+$
7	72	240	$0j, 1h, 2f, 3p$		$-$
6	56	168	$0i, 1g, 2d, 3s$		$+$
5	42	112	$0h, 1f, 2p$		$-$
4	30	70	$0g, 1d, 2s$		$+$
3	20	40	$0f, 1p$	*Empty Space*	$-$
2	12	20	$0d, 1s$	*Valence Space*	$+$
1	6	8	$0p$		$-$
				Filled Space	
0	2	2	$0s$		$+$

For example (^{18}O):

- *Filled Space*: $0s$ and $0p$ shells, with $4 + 12 = 16$ nucleons (being inert **core**, double magic nucleus)
- *Valence Space*: $0d$-$1s$ shell, with 2 nucleons (the so-called **valence nucleons**)
- *Empty Space*: other shells, without nucleons



Shell Model

▶ **Original *A*-Body Problem:**

$$\hat{H}|\Psi_\alpha\rangle = E_\alpha|\Psi_\alpha\rangle$$

▶ **Shell Model:** reduce the *A*-body problem to a valence-particle problem inside the valence space

$$\hat{H}_{\text{eff}}^{(\text{v})}|\Psi_\alpha^{\mathbb{P}}\rangle = (E_\alpha - E_c)|\Psi_\alpha^{\mathbb{P}}\rangle$$

- $\hat{H}_{\text{eff}}^{(\text{v})}$: effective Hamiltonian of valence nucleons in valence space
- $|\Psi_\alpha^{\mathbb{P}}\rangle$: wavefuntions of valence nucleons in valence space
- E_α: low-lying energies of nucleus A
- E_c: ground state energy of the core nucleus

Shell Model Effective Hamiltonian

Effective Hamiltonian of Shell Model

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

- ε_α: single-particle energy
- V_{eff}: effective interaction

Shell Model Effective Hamiltonian

Effective Hamiltonian for the Shell Model

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

Effective Interaction $V_{\rm eff}$

- **Empirical Effective Interactions:**
  - *p*-shell: Cohen-Kurath
  - *sd*-shell: USD, **USDB**
- **Microscopic Effective Interactions (from realistic nucleon-nucleon interaction):**
  - **Many-Body Perturbation Theory (MBPT): from 60s, see L. Coraggio et al., Prog. Part. Nucl. Phys. 62, 135 (2009), M. Hjorth-Jensen et al., Phys. Rep. 261, 125 (1995) and references therein.**
  - **No-Core Shell Model:** A. F. Lisetskiy et al., Phys. Rev. C 78, 044302 (2008), E. Dikmen et al., Phys. Rev. C 91, 064301 (2015), N. A. Smirnova et al., Phys. Rev. C 100, 054329 (2019).
  - **Coupled Cluster:** G. R. Jansen et al., Phys Rev Lett. 113, 142502 (2014) and Phys. Rev. C 94, 011301 (2016), Sun et al., Phys. Rev. C 98, 054320 (2018).
  - **In-Medium Similarity Renormalization Group:** S. K. Bogner et al., Phys Rev Lett. 113, 142501 (2014), S. R. Stroberg, et al., Phys Rev Lett. 118, 032502 (2017).

Effective Interactions from MBPT ($\hat{Q}$-box, or FDT)

Two-body $\hat{Q}$-Box[1]: valence-linked irreducible diagrams

$$\langle\alpha\beta|\hat{Q}(\omega)|\gamma\delta\rangle = \langle \text{CORE}|c_\beta c_\alpha H_1(t=0)U_I(0,-\infty)c_\gamma^\dagger c_\delta^\dagger|\text{CORE}\rangle_{\text{v}},$$

$$H_1 = V - U = \frac{1}{4}\sum_{ijkl} v_{ij,kl} c_i^\dagger c_j^\dagger c_l c_k - \sum_{ij} U_{i,j} c_i^\dagger c_j,$$

$$U_I(0,-\infty) = \lim_{t'\to-\infty(1-i0^+)} \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_{t'}^{0} \mathrm{d}t_1 \int_{t'}^{t_1} \mathrm{d}t_2 \cdots \int_{t'}^{t_{n-1}} \mathrm{d}t_n H_1(t_1)H_1(t_2)\cdots H_1(t_n)$$

Krenciglowa-Kuo Iteration Equation[1]

$$V_{\text{eff}}^{(0)} = \hat{Q}(\omega),\;\; V_{\text{eff}}^{(n)} = \hat{Q}(\omega) + \sum_{m=1}^{\infty}\hat{Q}_m(\omega)\left\{V_{\text{eff}}^{(n-1)}\right\}^m,\;\; n\geq 1,\;\; \hat{Q}_m(\omega) \equiv \frac{1}{m!}\left[\frac{\mathrm{d}^m\hat{Q}(\omega')}{\mathrm{d}\omega'^m}\right]_{\omega'=\omega}$$

Lee-Suzuki Iteration Equation[1]

$$V_{\text{eff}}^{(1)} = \hat{Q}(\omega),\;\; V_{\text{eff}}^{(n)} = \left\{1 - \hat{Q}_1(\omega) - \sum_{m=2}^{n-1}\hat{Q}_m(\omega)\prod_{k=n-m+1}^{n-1} V_{\text{eff}}^{(k)}\right\}^{-1}\hat{Q}(\omega),\;\; n\geq 2$$

[1] T.T.Kuo and E. Osnes, *Folded-diagram theory of the effective interaction in nuclei, atoms and molecules*, Springer-Verlag (1990); E.M. Krenciglowa and T.T.S. Kuo, Nucl. Phys. A 235, 171 (1974); K. Suzuki and S.Y. Lee, Prog. Theor. Phys. 64, 2091 (1980); L. Coraggio et al., Prog. Part. Nucl. Phys. 62, 135 (2009), M. Hjorth-Jensen et al., Phys. Rep. 261, 125 (1995).

Effective Interactions from MBPT

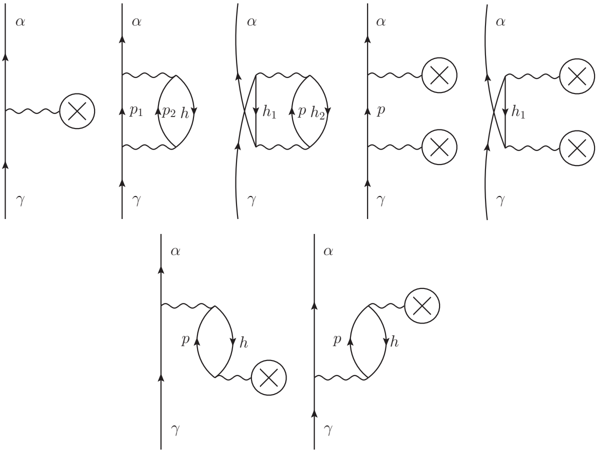


Figure: One-body $\hat{Q}$-box diagrams up to second order.

Effective Interactions from MBPT

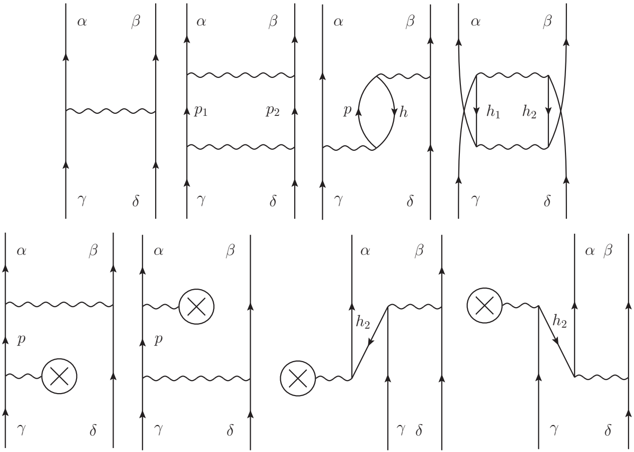
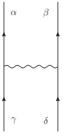


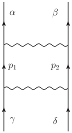
Figure: Two-body $\hat{Q}$-box diagrams up to second order.

Effective Interactions from MBPT

- **Diagram Expressions:**

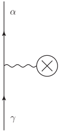


$$= \langle \alpha\beta | V | \gamma\delta \rangle,$$

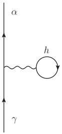


$$= \frac{1}{2} \sum_{p_1 p_2} \frac{\langle \alpha\beta | V | p_1 p_2 \rangle \langle p_1 p_2 | V | \gamma\delta \rangle}{\varepsilon_\gamma + \varepsilon_\delta - \varepsilon_{p_1} - \varepsilon_{p_2}}, \cdots$$

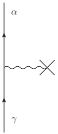
- **$(V\text{-}U)$-insertion diagrams:**



$$\equiv$$



$$+$$



$$= \sum_h \langle \alpha h | V | \gamma h \rangle + \langle \alpha | (-U) | \gamma \rangle, \cdots$$

- $(V\text{-}U)$-insertion diagrams are usually neglected in most applications, assuming that the single-particle wavefunctions of HO and HF are the same;
- $\hbar\omega$ dependence of effective interaction will present without including $(V\text{-}U)$-insertion diagrams order by order[1].

[1] L. Coraggio, et al., Annals of Physics 327, 2125 (2012).

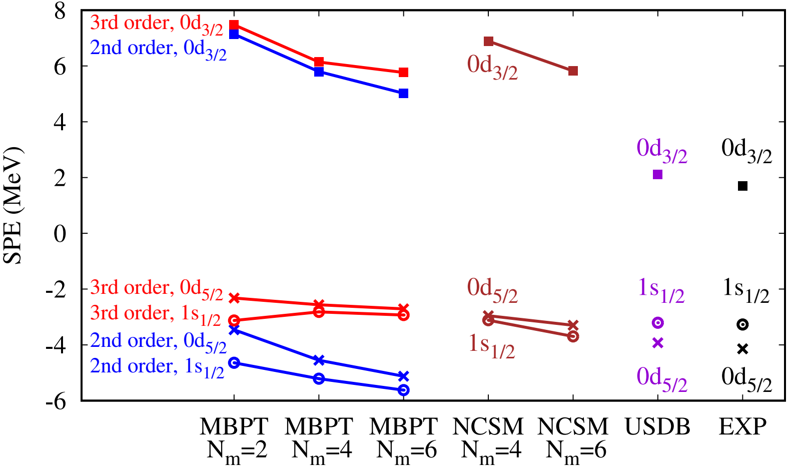
sd-shell results

- **Our work: we have developed a m-scheme Fortran code that allows us to calculate shell model effective Hamiltonians (single-particle energies + effective interactions) in the framework of MBPT (or the so-called $\hat{Q}$-box method, folded-diagram theory) with (V-U)-insertion diagrams order by order.**
- **Preliminary results: *sd*-shell single-particle energies and effective interactions were derived from realistic interaction Daejeon16 (DJ16) with up to third order diagrams.**

sd-shell single-particle energies

sd-shell results, single-particle energies

- **Theoretical Single Particle Energy (SPE) from DJ16:**



NCSM: N. A. Smirnova, et al., Phys. Rev. C 100, 5 (2019); I. J. Shin, et al., to be published;
EXP: N. Schwierz, et al., arXiv:0709.3525;
USDB: B.A. Brown et al., Phys. Rev. C 74, 034315 (2006).

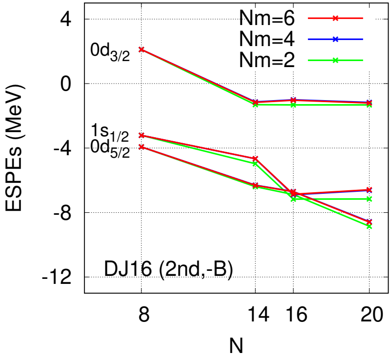
sd-shell effective interactions

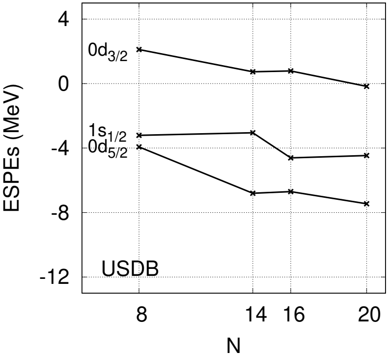
sd-shell results, effective interactions

Effective Single-Particle Energies (ESPEs)[1]: single particle energy in the mean filed approximation

$$\tilde{\varepsilon}_k^{\rho} = \varepsilon_k^{\rho} + \sum_{k'\rho'} V_{kk'}^{\rho\rho'} n_{k'}^{\rho'}, \quad V_{kk'}^{\rho\rho'} = \frac{\sum_J \langle k_\rho k'_{\rho'} | V | k_\rho k'_{\rho'} \rangle_J (2J+1)}{\sum_J (2J+1)}$$

▶ **Neutron ESPEs of Oxygen isotopes at sub-shell closures $N = 8, 14, 16, 20$ derived from DJ16 at 2nd order, without $(V\text{-}U)$-insertion diagrams**





[1] R. K. Bansal and J. B. French, Phys. Lett. 11, 145 (1964), T. Otsuka et al., Prog. Part. Nucl. Phys. 47, 319 (2001), N. A. Smirnova et al., Phys. Lett. B 686, 109 (2010)

sd-shell results, effective interactions

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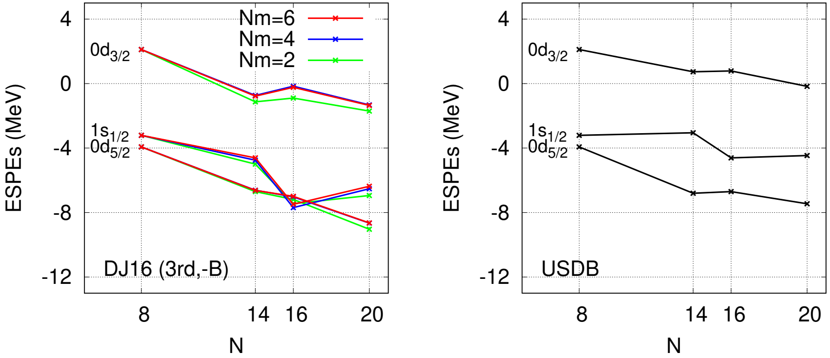

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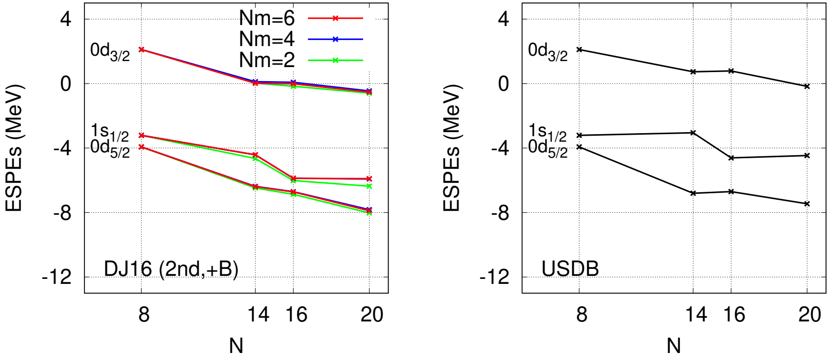

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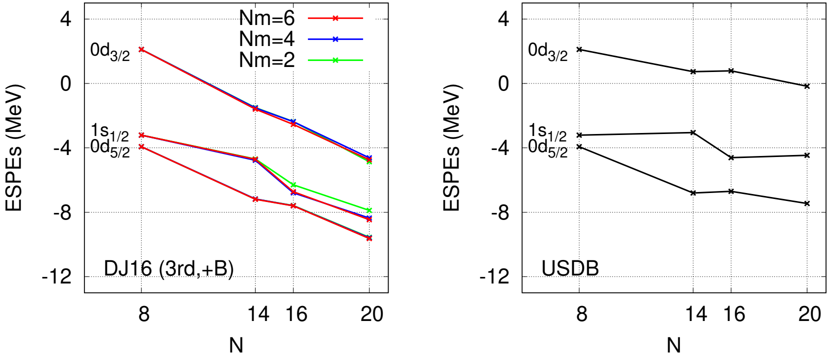

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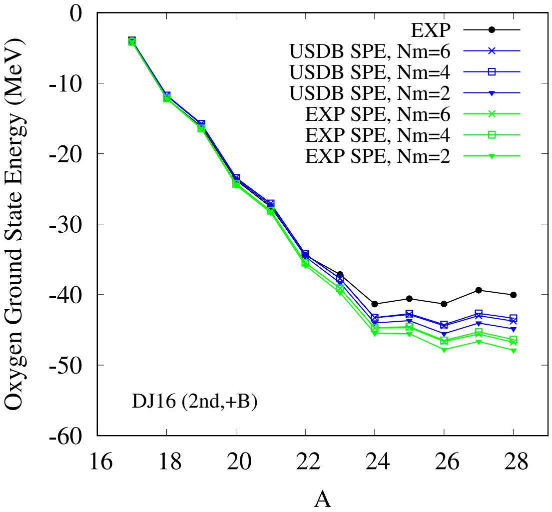
Some *sd*-shell nuclei calculations with the derived effective Hamiltonians (single-particle energies + effective interactions).

sd-shell results, including (V-U)-insertion diagrams order by order

- **Binding Energies[1] of ^{A}O relative to ^{16}O at 2nd order:**



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sd-shell results, including (*V*-*U*)-insertion diagrams order by order

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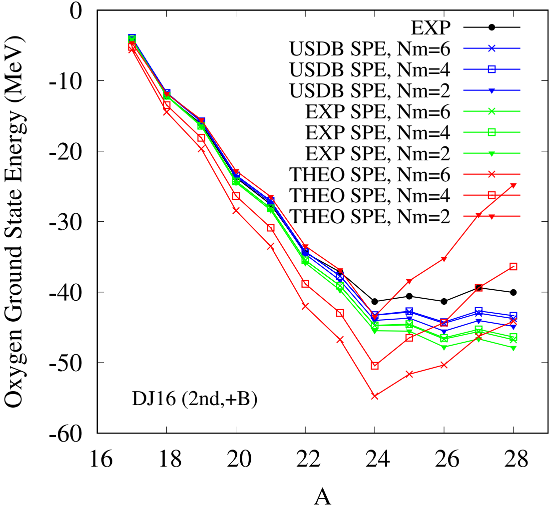

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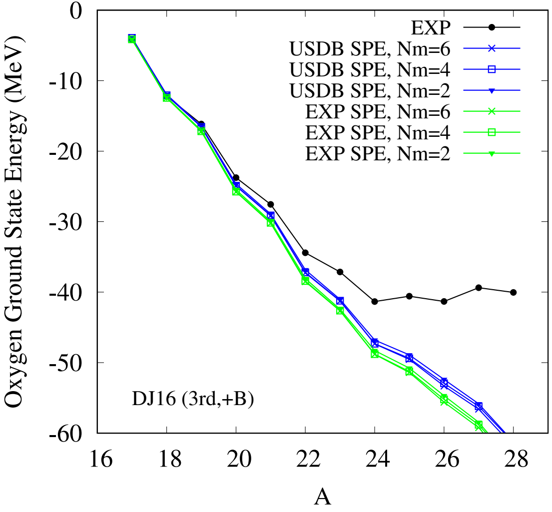

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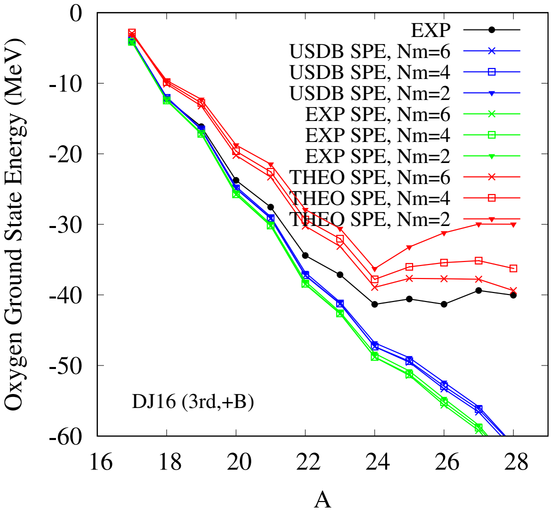

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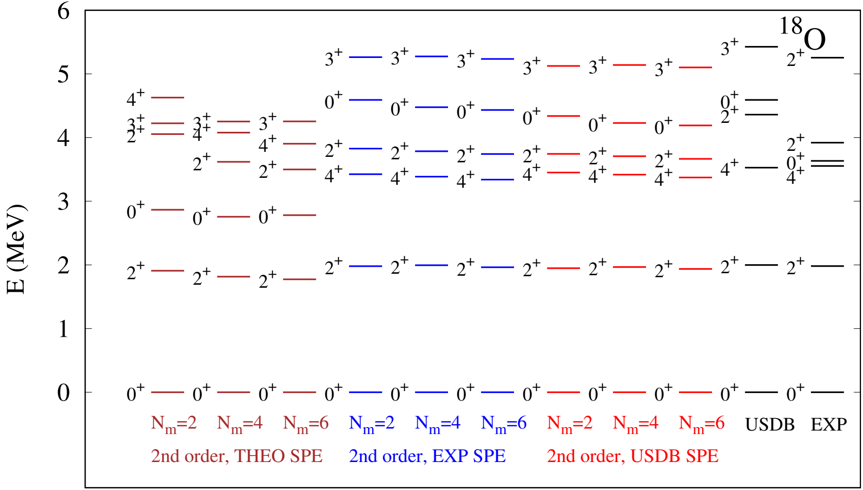
- **Six lowest positive-parity states[1] of ^{18}O at 2nd order:**



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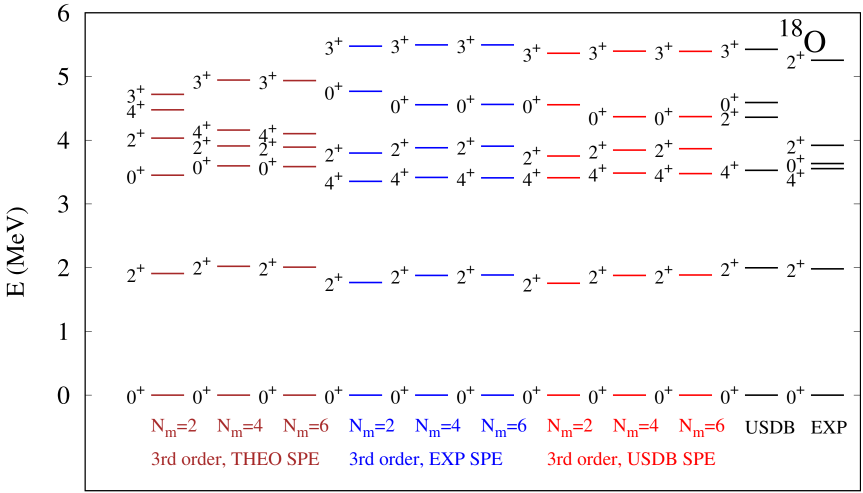

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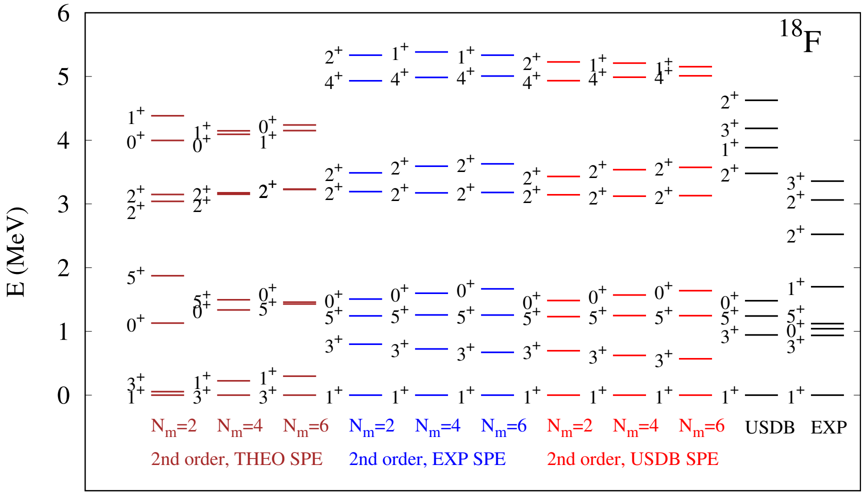
sd-shell results, including (*V*-*U*)-insertion diagrams order by order

- **Eight lowest positive-parity states[1] of ^{18}F at 2nd order:**



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sd-shell results, including (V-U)-insertion diagrams order by order

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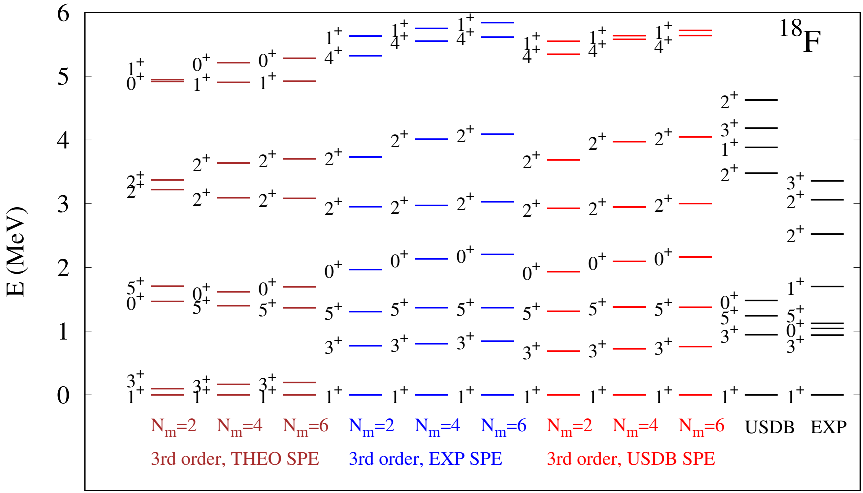

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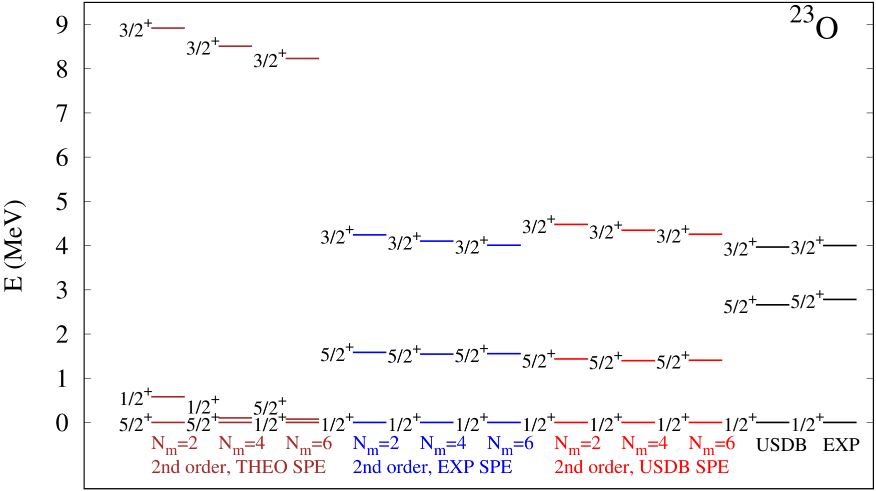
sd-shell results, including (*V*-*U*)-insertion diagrams order by order

- **Three lowest positive-parity states[1] of ^{23}O at 2nd order:**



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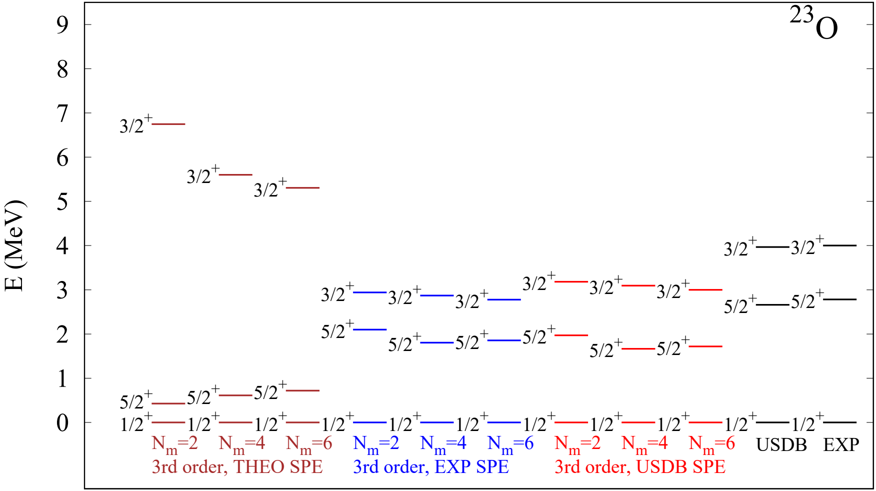

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Summary

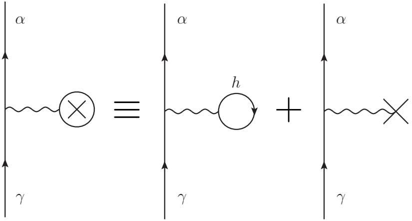
- A Fortran code to calculate effective Hamiltonian was developed in the framework of MBPT.
- *sd*-shell single-particle energies and effective interactions are derived from DJ16 using MBPT with up to third order diagrams.
- The single-particle energies derived at third order are similar to the NCSM results.
- The centroids of the derived effective interactions are too attractive, which results in too small sub-shell gaps. This deficiency leads to overbinding problems in the description of neutron-rich nuclei, and poor spectroscopy of nuclei in the vicinity of sub-shell closures.
- The $(V\text{-}U)$-insertion diagrams can improve the deficient centrodis.
- Third order results give better spectroscopy of nuclei but worse binding energies of neutron-rich nuclei compared to second order results. Therefore, higher order diagrams are expected to give some corrections.

Thank you for your attention

Backup

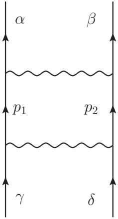
$$U = \sum_{i=1}^{A} u_i = \sum_{i=1}^{A} \left\{ \frac{1}{2} m\omega^2 r_i^2 + \Delta \right\}$$

$$\varepsilon_\alpha = (2n + l + \frac{3}{2})\hbar\omega + \Delta$$



$$= \sum_h \langle \alpha h | V | \gamma h \rangle + \langle \alpha | (-U) | \gamma \rangle$$

Backup



$$= \frac{1}{2} \sum_{p_1 p_2} \frac{\langle \alpha\beta | V | p_1 p_2 \rangle \langle p_1 p_2 | V | \gamma\delta \rangle}{\varepsilon_\gamma + \varepsilon_\delta - \varepsilon_{p_1} - \varepsilon_{p_2}}$$

$$|N_\gamma + N_\delta - N_{p_1} - N_{p_2}| \leq N_{\max}$$

$$N = 2n + l$$