Three-body effective interactions in nuclear structure studies

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Nuclear structure calculations

Aim: derive properties of selected nuclear systems from microscopic point of view.

1. Start with a realistic nucleon-nucleon potential.
2. Construct a medium-renormalized (effective) interaction.
3. Use the effective interaction to calculate properties of nuclear systems.

Missing elements in nuclear structure calculations

1. **Continuum and resonance coupling**
2. **Three-body interactions**

Three-body interactions

1. **Necessary** for reproducing binding energies of light nuclei.
2. Importance for medium and heavy nuclei is still not fully clarified.

Medium and heavy nuclei

Three-body contributions to the effective interaction

1. The **'true'** three-body forces:
   (CD Bonn + TM99 3NF, AV18 + Illinois 3NF, CFPT (N3LO))
2. Three-body terms of the **effective interaction**

Effective interaction

Want to solve the many-body Schrödinger equation for nuclear systems:

$$H\Psi = E\Psi \quad \text{with} \quad H = H_1 + H_0, \quad H_0 = T + U, \quad H_1 = V - U$$

Practically impossible to solve in the complete Hilbert space - consider the problem in the truncated (model) space. Define projection operators: P (on the model space) and Q (on the excluded space):

$$P + Q = 1 \quad \text{and} \quad PQ = 0$$

Then the complete Hilbert-space eigenvalue problem can be replaced by the model space eigenvalue problem:

$$PH_{eff}P\Psi = EP\Psi \quad \text{with} \quad H_{eff} = H_0 + V_{eff}$$

V_{eff} is the effective interaction, acting solely within the model space.

The folded-diagram theory

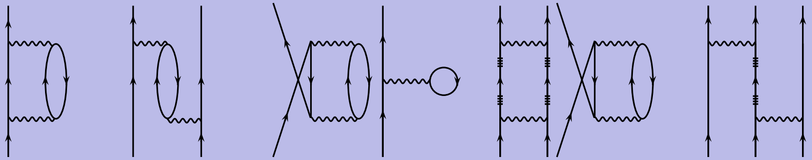
To construct the effective interaction, one starts with introducing the $\hat{Q}$-box[a]:

$$\hat{Q}(\omega) = PH_1P + PH_1Q\frac{1}{\omega - QH_0Q}Q\hat{Q}(\omega)P$$

The $\hat{Q}$-box is a sum of all possible **topologically distinct** diagrams which are:

1. **Irreducible:** the intermediate many-particle states between each pair of vertices belong to the excluded space Q.
2. **Valence linked:** all the interaction vertices are linked (via fermion lines) to at least one valence space line.

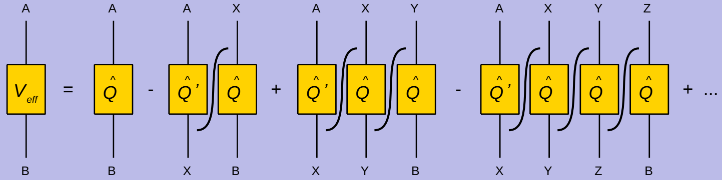
These diagrams can be either connected or disconnected.



[a] T. T. S. Kuo and E. Osnes, Folded-Diagram Theory of the Effective Interaction in Atomic Nuclei, Springer Lecture Noters in Physics (Springer, Berlin, 1990) Vol. 364

The folded-diagram theory

The effective interaction is given by the infinite series of folded $\widehat{Q}$-box diagrams:



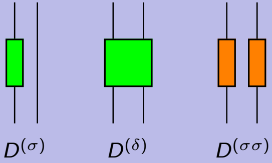
The $\int$ sign stands for the generalized folding operation. A,B,X,Y,Z denote many-body states.

One possibility to evaluate the infinite folded-diagrams series is to employ the Lee-Suzuki resummation scheme. For the **degenerate** model space:

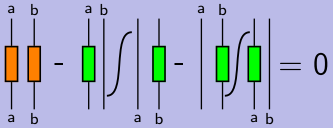
$$V^{(n)} = \frac{1}{1 - Q_1 - \sum_{m=2}^{n-1} \widehat{Q}_m \prod_{k=n-m+1}^{n-1} V^{(k)}} \widehat{Q}(\omega_0) \qquad \text{with} \qquad \widehat{Q}_m = \frac{1}{m!} \frac{d^m \widehat{Q}(\omega_0)}{d\omega^m}$$

where ω_0 is the true model space energy, appropriate for the nuclear system of interest.

The two-body $\widehat{Q}$-box terms



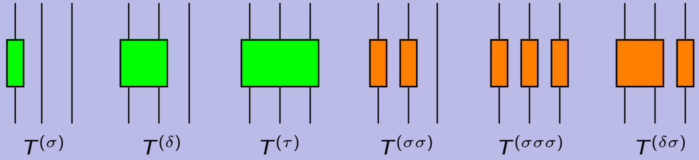
Common practice is to neglect the disconnected two-body $\widehat{Q}$-box terms, $D^{(\sigma\sigma)}$. Negligible for two-body V_{eff}, may not be so for three-body V_{eff}. Can be easily calculated using cancellation property of disconnected diagrams.



$$D^{(\sigma\sigma)}_{ab,ab} - S_{a,a}\int S_{b,b} - S_{b,b}\int S_{a,a} = D^{(\sigma\sigma)}_{ab,ab} + \frac{dS_{a,a}}{d\omega}S_{b,b} + \frac{dS_{b,b}}{d\omega}S_{a,a} = 0$$

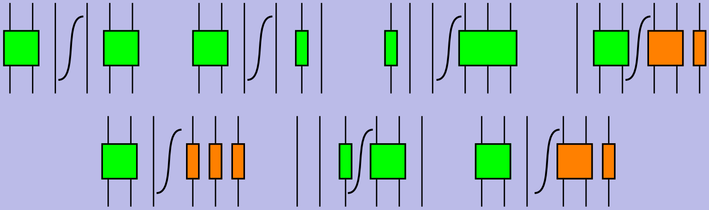
$$\mathbf{D^{(\sigma\sigma)}_{ab,ab}(\omega_0) = -\frac{d}{d\omega}\left[S_{a,a}(\omega)\, S_{b,b}(\omega)\right]_{\omega_0}}$$

The three-body $\hat{Q}$-box terms



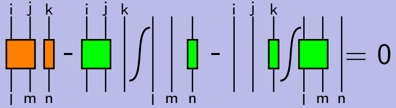
Three-body contributions to the V*eff*

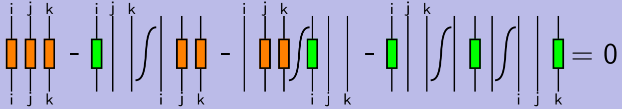
1. Three-body $\widehat{Q}$-box diagrams: T^{τ}, $T^{\sigma\sigma\sigma}$, $T^{\delta\sigma}$.
2. Folded diagrams.



Disconnected terms of the three-body $\hat{Q}$-box

Disconnected diagrams from different folds and with the same amount of interaction vectices cancel out exactly.





$$\langle \mathbf{ijk}|\, \mathbf{T}^{(\sigma\sigma)}\, |\mathbf{lmn}\rangle = -\frac{d}{d\omega}(S_{i,j}S_{j,m} + S_{i,j}S_{k,n} + S_{j,m}S_{k,n})\,\delta_{ij}\,\delta_{jm}\,\delta_{kn}$$

$$\langle \mathbf{ijk}|\, \mathbf{T}^{(\delta\sigma)}\, |\mathbf{lmn}\rangle = -\frac{d}{d\omega}\Big[D^{(\delta)}_{ij,lm}\,S_{k,n} - D^{(\delta)}_{ij,ln}\,S_{k,m} - D^{(\delta)}_{ij,nm}\,S_{k,l} - D^{(\delta)}_{ik,lm}\,S_{j,n} + D^{(\delta)}_{ik,ln}\,S_{j,m} + D^{(\delta)}_{ik,nm}\,S_{j,l} - D^{(\delta)}_{kj,lm}\,S_{i,n} + D^{(\delta)}_{kj,ln}\,S_{i,m} + D^{(\delta)}_{kj,nm}\,S_{i,l}\Big]$$

$$\langle \mathbf{ijk}|\, \mathbf{T}^{(\sigma\sigma\sigma)}\, |\mathbf{lmn}\rangle = \frac{1}{2}\left[\frac{d^2 I}{d\omega^2}(J+K)^2 + \frac{d^2 J}{d\omega^2}(I+K)^2 + \frac{d^2 J}{d\omega^2}(I+J)^2\right]\delta_{il}\,\delta_{jm}\,\delta_{kn} + \left[\frac{dI}{d\omega}\frac{dJ}{d\omega}(I+J+2K) + \frac{dI}{d\omega}\frac{dK}{d\omega}(I+K+2J) + \frac{dJ}{d\omega}\frac{dK}{d\omega}(J+K+2I)\right]\delta_{il}\,\delta_{jm}\,\delta_{kn}$$

where $I = S_{i,i}$, $J = S_{j,j}$, $K = S_{k,k}$.

Separation of two-body and three-body components of V_{eff}

Need to separate two-body and three-body components of the effective interaction to proceed with shell-model calculations. [a]

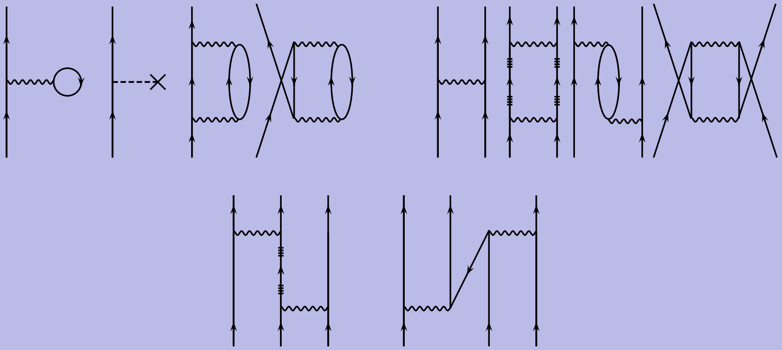
$$\langle ab|\, V\, |cd\rangle = \langle ab|\, V^{(2)}\, |cd\rangle + \Big(\langle a|\, V^{(1)}\, |a\rangle + \langle b|\, V^{(1)}\, |b\rangle\Big)\, \delta_{ac}\, \delta_{bd}$$

$$\begin{aligned}\langle ijk|\, V\, |lmn\rangle = \langle ijk|\, V^{(3)}\, |lmn\rangle + \quad & \langle ij|\, V\, |lm\rangle\, \delta_{kn} - \langle ij|\, V\, |ln\rangle\, \delta_{km} - \langle ij|\, V\, |nm\rangle\, \delta_{kl} - \\ & \langle ik|\, V\, |lm\rangle\, \delta_{jn} + \langle ik|\, V\, |ln\rangle\, \delta_{jm} + \langle ik|\, V\, |nm\rangle\, \delta_{jl} - \\ & \langle kj|\, V\, |lm\rangle\, \delta_{in} + \langle kj|\, V\, |ln\rangle\, \delta_{im} + \langle kj|\, V\, |nm\rangle\, \delta_{il} - \\ & \quad (\langle i|\, V\, |l\rangle + \langle j|\, V\, |m\rangle + \langle k|\, V\, |n\rangle)\, \delta_{il}\, \delta_{jm}\, \delta_{kn}\end{aligned}$$

[a] P.J.Ellis et al,Phys.Rev. **C71** 034301,2005

Calculation details

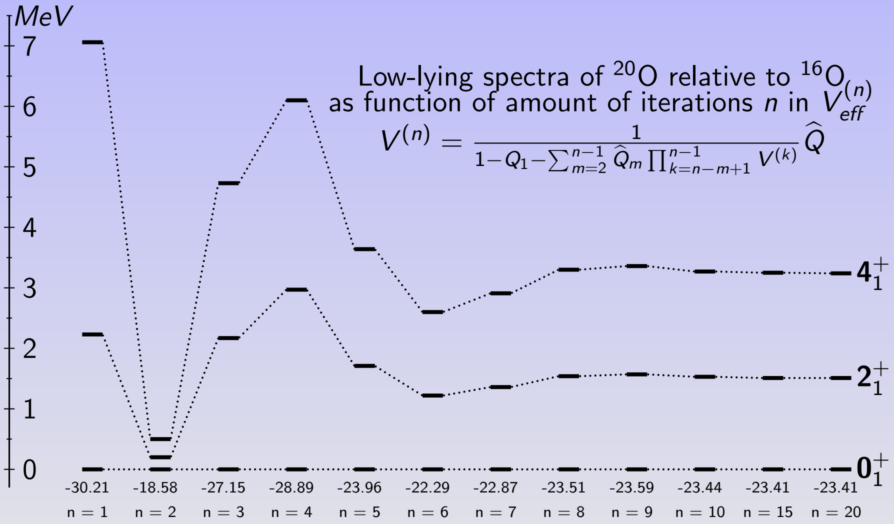
1. *NN*-interaction: *G*-matrix obtained with N3LO CFPT potential, H.O. s.p. basis, $N_{max} = 10$.
2. Degenerate perturbation theory.
3. $\widehat{Q}$-box derivatives are included up to 3rd order.
4. Connected $\widehat{Q}$-box terms are evaluated up to 2nd order in G.



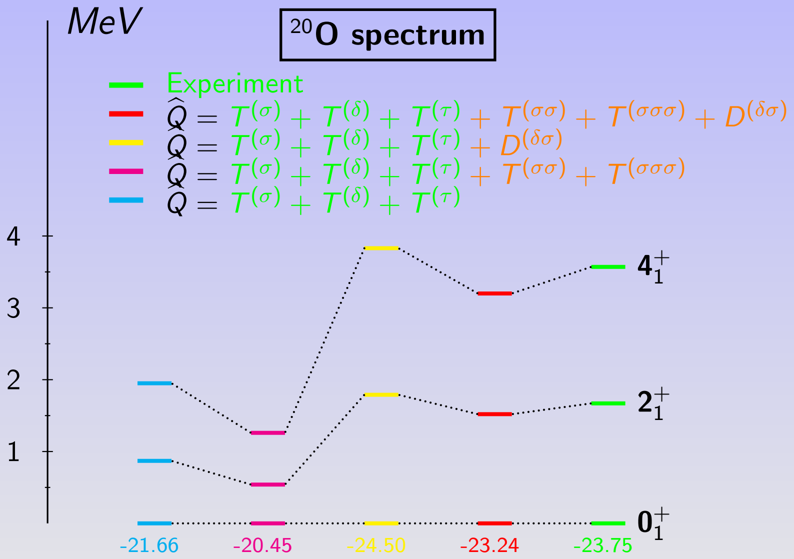
Convergence of the iterative scheme

Low-lying spectra of ^{20}O relative to ^{16}O as function of amount of iterations n in $V_{eff}^{(n)}$

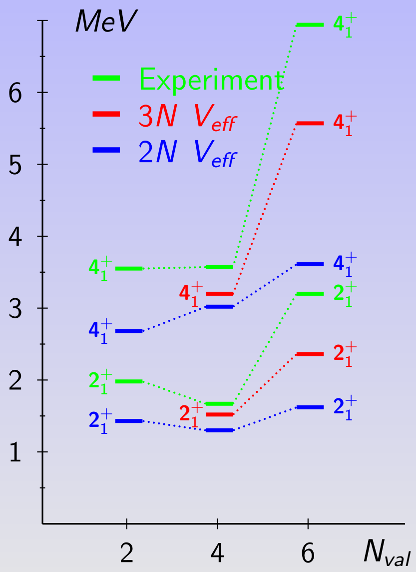
$$V^{(n)} = \frac{1}{1-Q_1-\sum_{m=2}^{n-1} \widehat{Q}_m \prod_{k=n-m+1}^{n-1} V^{(k)}} \widehat{Q}$$



Terms of the three-body V_{eff}



Shell-model calculations of even ^{16}O isotopes



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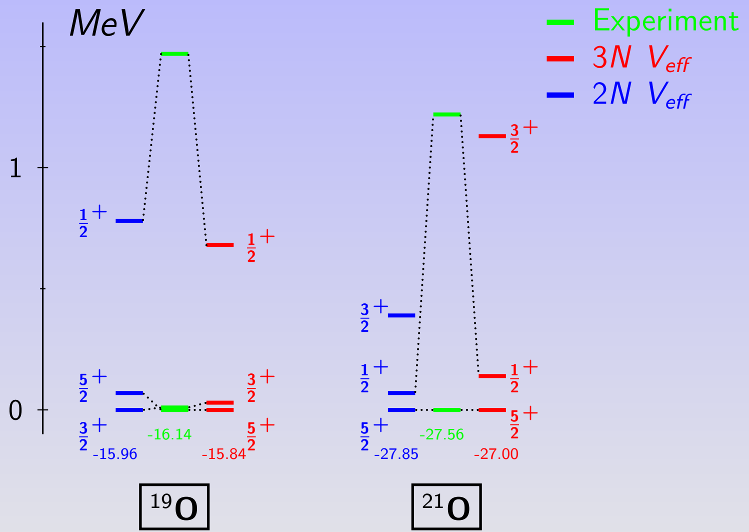
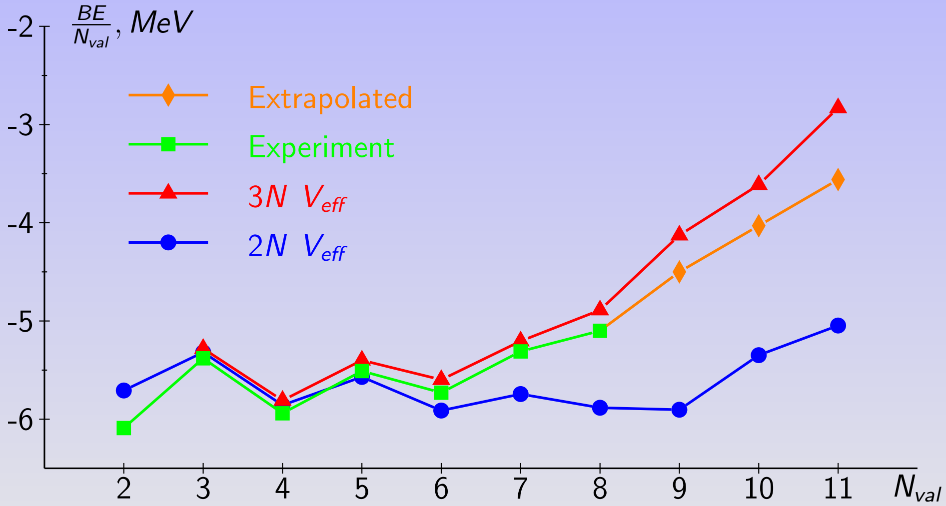


BE/N_{val} trends



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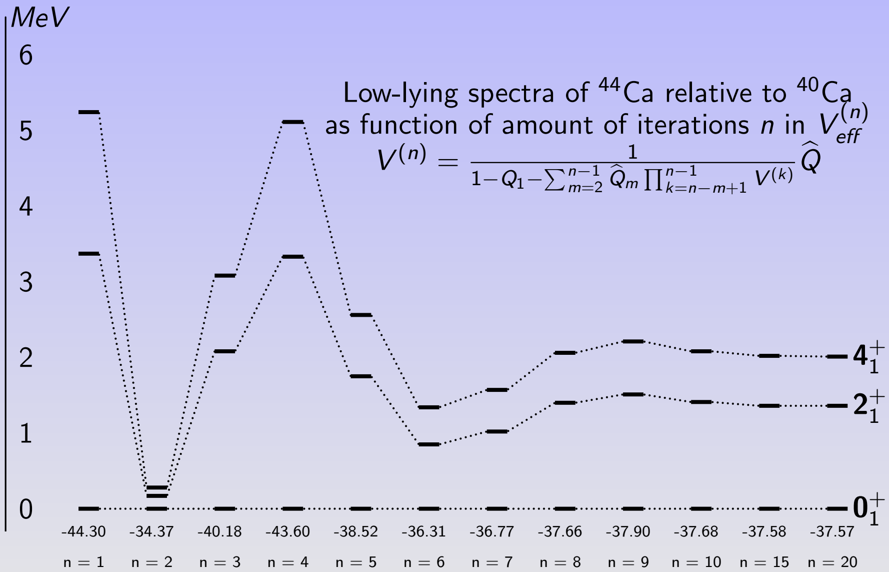

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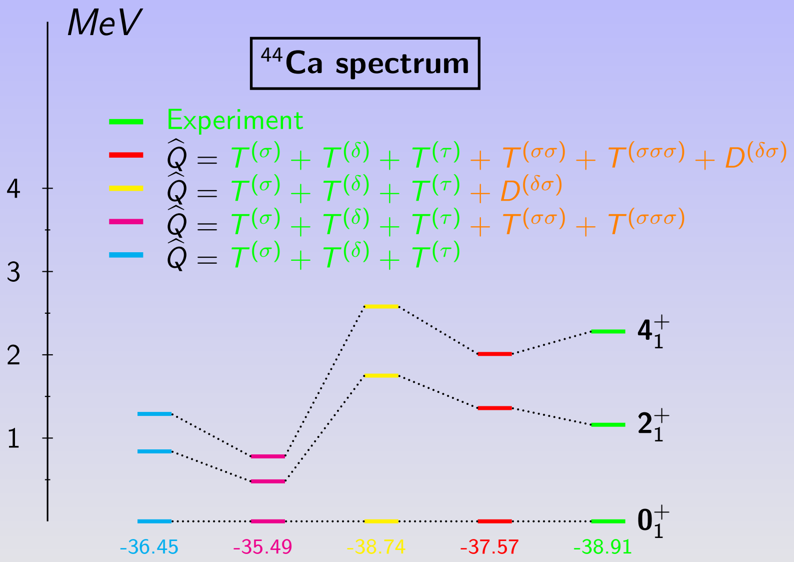
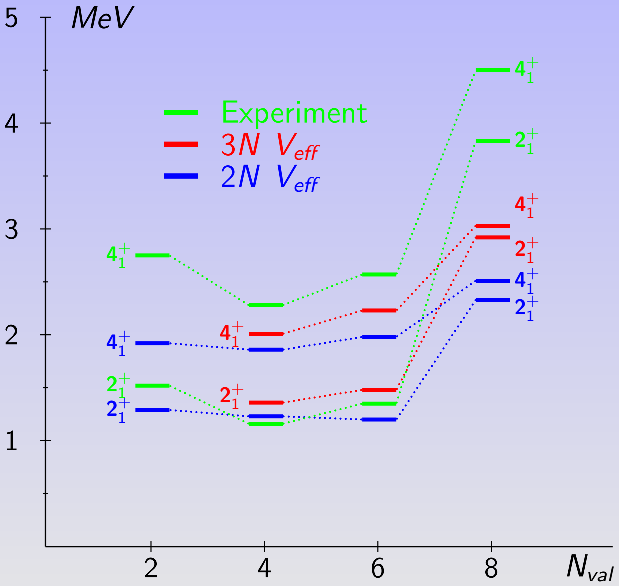
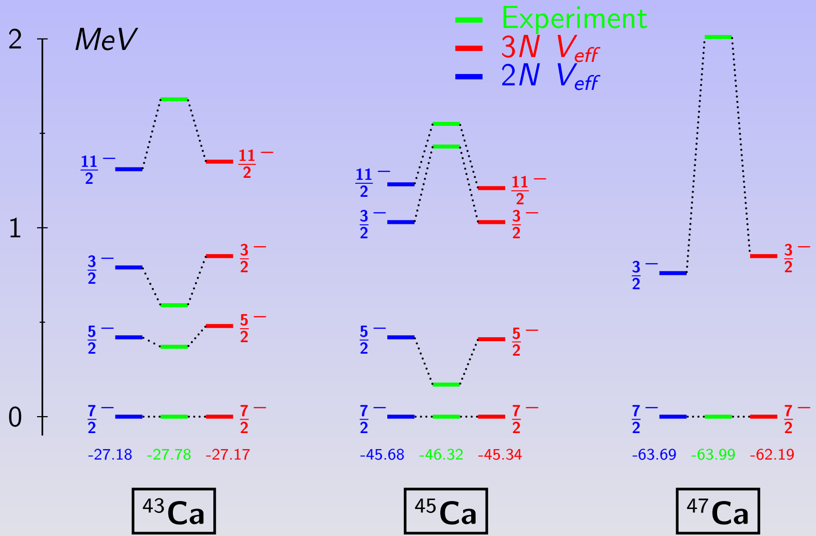


Shell-model calculations of even ^{40}Ca isotopes



Shell-model calculations of odd ^{40}Ca isotopes



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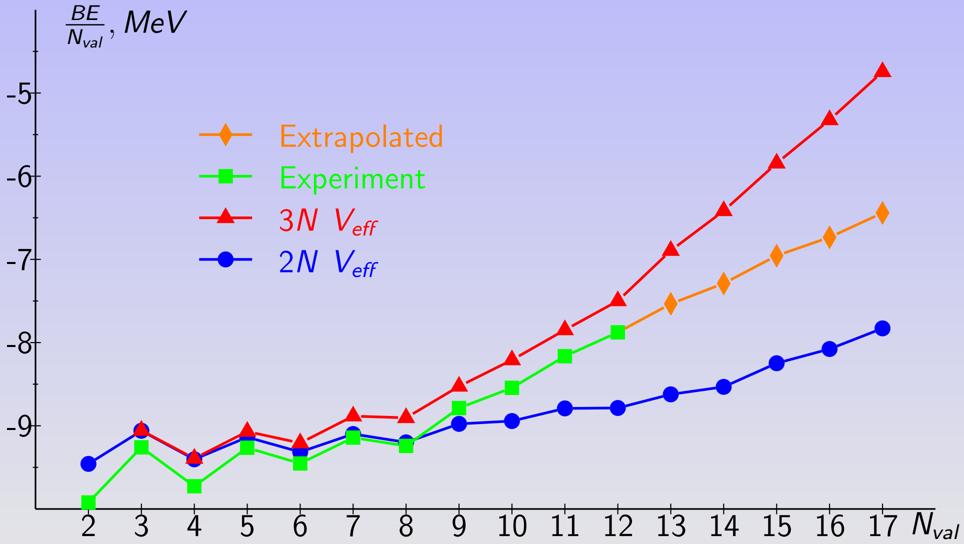

Conclusions

1. Contributions from the three-body V_{eff} terms cannot be neglected.
2. Three-body V_{eff} reproduces binding energy trends of ^{16}O and ^{40}Ca isotopes.
3. Three-body V_{eff} gives more **repulsion** compared two-body V_{eff}.
4. The disconnected terms of the three-body $\hat{Q}$-box must be taken into account.

Work in progress

1. Inclusion of the **'true'** three-body forces: CFPT NNLO.
2. Implementation of the Folded-Diagram Theory for **non-degenerate model space**.
3. Comparison with other schemes for constructing effective interactions (LS similarity transformation).