Ab Initio Nuclear Structure and Reactions with Chiral Three-Body Forces
Outline

- What we are aiming for...
- Ingredients from Three-Body Technology
- 3N Forces in the NCSM/RGM and NCSMC
  - Nucleon-$^4\text{He}$ scattering
  - Continuum effects on the $^9\text{Be}$ energy levels
- Conclusions
What we are aiming for...

Realistic ab-initio description of light nuclei

Bound states & spectroscopy

(IT-)NCSM
Ab-initio description of nuclear clusters
What we are aiming for...

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Resonances & scattering states

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(\textit{IT-})NCSM
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Resonances & scattering states

RGM
Describing relative motion of clusters
What we are aiming for...

Realistic ab-initio description of light nuclei

Bound states & spectroscopy

Resonances & scattering states

(IT-)NCSM
Ab-initio description of nuclear clusters

(IT-)NCSM/RGM & NCSMC approaches

RGM
Describing relative motion of clusters

Successfully applied with NN interactions
Now: Inclusion of 3N Forces
Ingredients from Three-Body Technology
The Chiral NN+3N Hamiltonian

- Hierarchy of consistent nuclear NN, 3N,... forces (and currents)

- NN interaction @ N^3LO (Λ=500MeV)
  [Entem, Machleidt, Phys.Rev C 68, 041001(R) (2003)]

- Standard Hamiltonian
  - 3N interaction @ N^2LO(Λ_{3N}=500MeV)
    - LECs c_D, c_E fitted to β-decay halflife & binding energy of \(^3\)H

- Reduced-Cutoff Hamiltonian
  - 3N interaction @ N^2LO(Λ_{3N}=400MeV)
    - c_D=-0.2, c_E fitted to \(^4\)He
The Similarity Renormalization Group

...yields an evolved Hamiltonian with improved convergence properties in many-body calculations

- Unitary transformation of Hamiltonian $H_\alpha = U_\alpha^\dagger H U_\alpha$

Different SRG-Evolved Hamiltonians

- **NN+3N-induced**: start with NN initial Hamiltonian and keep two- and three-body terms
- **NN+3N-full**: start with NN+3N initial Hamiltonian and keep two- and three-body terms
3N Forces
in the
NCSM/RGM and NCSMC

General Approach of NCSM/RGM

- Represent $H \left| \psi^{J\pi T} \right\rangle = E \left| \psi^{J\pi T} \right\rangle$ using the **over-complete basis**

$$
\left| \psi^{J\pi T} \right\rangle = \sum_{\nu} \int drr^2 \frac{g_{\nu}^{J\pi T}(r)}{r} A_{\nu} \left| \phi_{\nu r}^{J\pi T} \right\rangle
$$

with the binary-cluster channel states

$$
\left| \phi^{J\pi T} \right\rangle = \left\{ \left| \Phi(A-a) \right\rangle \otimes \left| \Phi(a) \right\rangle \otimes \left| rl \right\rangle \right\}^{J\pi T}
$$

g_{\nu}^{J\pi T}(r)$ unknown
General Approach of NCSM/RGM

- Represent $H |\psi^{J\pi T}\rangle = E |\psi^{J\pi T}\rangle$ using the **over-complete basis**

$$|\psi^{J\pi T}\rangle = \sum_{\nu} \int drr^2 \frac{g^{J\pi T}_\nu(r)}{r} A_\nu |\phi^{J\pi T}_{\nu r}\rangle$$

with the binary-cluster channel states

$$|\phi^{J\pi T}\rangle = \left\{ |\Phi^{(A-a)}\rangle \otimes |\Phi^{(a)}\rangle \otimes |r l\rangle \right\}^{J\pi T}$$

$g^{J\pi T}_\nu(r)$ unknown

NCSM delivers $|\Phi^{(A-a)}\rangle$ and $|\Phi^{(a)}\rangle$
General Approach of NCSM/RGM

- Represent $H |\psi^{J\pi T}\rangle = E |\psi^{J\pi T}\rangle$ using the **over-complete basis**

$$ |\psi^{J\pi T}\rangle = \sum_{\nu} \int \text{d}rr^2 \frac{g_{\nu}^{J\pi T}(r)}{r} A_{\nu} |\phi_{\nu r}^{J\pi T}\rangle $$

$g_{\nu}^{J\pi T}(r)$ unknown

with the binary-cluster channel states

$$ |\phi^{J\pi T}\rangle = \left\{ |\Phi^{(A-a)}\rangle \otimes |\Phi(a)\rangle \otimes |r l\rangle \right\}^{J\pi T} $$

- Solve **generalized eigenvalue** problem

$$ \sum_{\nu} \int \text{d}rr^2 \left[ H_{\nu, \nu'}^{J\pi T}(r', r) - E N_{\nu, \nu'}^{J\pi T}(r, r') \right] \frac{g_{\nu r}^{J\pi T}}{r} = 0 $$
General Approach of NCSM/RGM

- Represent $H |\psi^{J\pi T}\rangle = E |\psi^{J\pi T}\rangle$ using the **over-complete basis**

$$|\psi^{J\pi T}\rangle = \sum_{\nu} \int drr^2 \frac{g^{\nu T}_\nu(r)}{r} A_\nu |\phi^{J\pi T}_{\nu r}\rangle$$

with the binary-cluster channel states

$$|\phi^{J\pi T}\rangle = \left\{ |\Phi^{(A-a)}\rangle \otimes |\Phi(a)\rangle \otimes |r\rangle \right\}^{J\pi T}$$

- Solve **generalized eigenvalue** problem

$$\sum_{\nu} \int drr^2 \left[ \mathcal{H}^{J\pi T}_{\nu,\nu'}(r', r) - E\mathcal{N}^{J\pi T}_{\nu,\nu'}(r, r') \right] \frac{g^{\nu T}_\nu(r)}{r} = 0$$

Hamiltonian kernel $\langle \phi^{J\pi T}_{\nu r'} | A_\nu H A_\nu |\phi^{J\pi T}_{\nu r}\rangle \propto \langle \Phi^{(A-1)} | a^\dagger a^\dagger a a a |\Phi^{(A-1)}\rangle$

for single-nucleon projectiles and including 3N forces
Nucleon-$^4$He Scattering

In collaboration with
G. Hupin, S. Quaglioni, P. Navrátil & R. Roth

Three-Nucleon Force Effects on Scattering Phase Shifts

Including seven eigenstates of $^4$He

$N_{\text{max}} = 13$
$E_{3\text{max}} = 14$
$\hbar \Omega = 20 \text{ MeV}$
$\alpha = 0.0625 \text{ fm}^4$
$\lambda = 2.0 \text{ fm}^{-1}$

Joachim Langhammer - DPG Tagung Frankfurt - March 2014
$^4\text{He}$

**3N Force Effects on Phase Shifts**


$N_{\text{max}} = 13$

$E_{3\text{max}} = 14$

$\hbar \Omega = 20 \text{ MeV}$

$\alpha = 0.0625 \text{ fm}^4$

$\lambda = 2.0 \text{ fm}^{-1}$

+ Experiment

- - 3N-induced

- - - 3N-full

Good agreement with data for $^2P_{1/2}$, $^2D_{3/2}$ and $^2S_{1/2}$

Including seven eigenstates of $^4\text{He}$

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$^4\text{He}$

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3N Force Effects on Phase Shifts


\[ N_{\text{max}} = 13 \]
\[ E_{3\text{max}} = 14 \]
\[ \hbar \Omega = 20 \text{ MeV} \]
\[ \alpha = 0.0625 \text{ fm}^4 \]
\[ \lambda = 2.0 \text{ fm}^{-1} \]

Figure 13.9 – Comparison of the n-\(^4\)He (left-hand panel) and p-\(^4\)He (right-hand panel) scattering phase shifts for partial wave \(^2P_{1/2}, ^2D_{3/2}\) and \(^2S_{1/2}\) obtained with the NN+3N-induced and NN+3N-full Hamiltonian. The calculations include seven eigenstates of \(^4\)He and use \(N_{\text{max}} = 13\). Remaining parameters are \(E_{3\text{max}} = 14\) and \(\hbar \Omega = 20 \text{ MeV}\). (published in [51]).

Good agreement with data for \(^2P_{1/2}, ^2D_{3/2}\) and \(^2S_{1/2}\)

Including seven eigenstates of \(^4\)He

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Cross Section & Analyzing

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Cross Section & Analyzing


13.3 Cross Sections and Analyzing Powers

Chiral 3N improves agreement with experiment

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Representing $H |\psi^{J\pi T}\rangle = E |\psi^{J\pi T}\rangle$ using the \textbf{over-complete basis}

\[ |\Psi^{J\pi T}\rangle = \sum_{\lambda} c_{\lambda} |\Psi_{A} E_{\lambda} J^{\pi T}\rangle + \sum_{\nu} \int dr r^{2} \frac{\chi_{\nu}(r)}{r} |\xi_{\nu r}^{J\pi T}\rangle \]

- Expansion in A-body (IT-)NCSM eigenstates
- Identical to the NCSM/RGM expansion
NCSMC Formalism with 3N Forces

- Representing $H |\psi^{J\pi T}\rangle = E |\psi^{J\pi T}\rangle$ using the over-complete basis

$$|\psi^{J\pi T}\rangle = \sum_\lambda c_\lambda |\Psi_\lambda E_\lambda J^{\pi T}\rangle + \sum_\nu \int dr r^2 \frac{\chi_\nu(r)}{r} |\xi^{J\pi T}_{\nu r}\rangle$$

Expansion in A-body (IT-)NCSM eigenstates leads to the NCSMC equations

$$\begin{pmatrix} H_{\text{NCSM}} & h \\ h & \mathcal{H} \end{pmatrix} \begin{pmatrix} c \\ \chi(r)/r \end{pmatrix} = E \begin{pmatrix} 1 & g \\ g & 1 \end{pmatrix} \begin{pmatrix} c \\ \chi(r)/r \end{pmatrix}$$

3N forces contribute in

$H_{\text{NCSM}}$ Covered by (IT-)NCSM

$\mathcal{H}$ Contains the NCSM/RGM Hamiltonian kernel

$h$ Given by $\langle \Psi_\lambda E_\lambda J^{\pi T} | \hat{H} | \xi^{J\pi T}_{\nu r}\rangle$
NCSMC Formalism with 3N Forces

- Representing $H \ket{\psi^{J\pi T}} = E \ket{\psi^{J\pi T}}$ using the **over-complete basis**

$$\ket{\psi^{J\pi T}} = \sum_\lambda c_\lambda \ket{\Psi_A E_\lambda J^{\pi T} \chi} + \sum_\nu \int dr r^2 \frac{\chi_\nu(r)}{r} \ket{\xi^{J\pi T}_{\nu r}}$$

Expansion in A-body (IT-)NCSM eigenstates

leads to the NCSMC equations

$$\begin{pmatrix} H_{NCSM} & h \\ h & \mathcal{H} \end{pmatrix} \begin{pmatrix} c \\ \chi(r)/r \end{pmatrix} = E \begin{pmatrix} 1 \\ g \end{pmatrix}$$

3N forces contribute in $H_{NCSM}$

Covered by (IT-)NCSM

$\mathcal{H}$

Given by $\langle \Psi_A E_\lambda J^{\pi T} | H | \xi^{J\pi T}_{\nu r} \rangle$

Contains the NCSM/RGM Hamiltonian kernel

Accessing targets beyond $^4$He using uncoupled densities
Ab-initio Description of $^9$Be via NCSMC

- All excited states are resonances
- Study the impact of the continuum by investigating neutron-$^8$Be scattering
Ab-initio Description of $^9$Be via NCSMC

- All excited states are resonances
- Study the impact of the continuum by investigating neutron-$^8$Be scattering
- NCSM with 3N forces reveals large discrepancies compared to experiment
3N Force Effects on Phase Shifts

broad also true for all remaining non-resonant phase shifts that we do particularly near resonance energies. We note that the initial chiral 3N interactions for the negative-parity than for the positive parity is practically identical for both Hamiltonians. In general, counter roughly the same shift of their resonance position due to the difference in the effective range of the interaction.

$\alpha = 0.0625 \text{ fm}^4$

$\hbar \Omega = 20 \text{ MeV}$

Extract $^9\text{Be}$ energy levels from computed eigenphase shifts...
Figure 14.6 – Negative (left-hand panel) and positive (right-hand panel) parity spectrum of $^9$Be relative to the n-$^8$Be threshold at $N_{\text{max}} = 6$ (7) and 12 for IT-NCSM (first two columns) and NCSMC (last two columns) compared to experiment [148]. Remaining parameters are $\hbar \Omega = 20$ MeV and $\alpha = 0.0625$ fm$^4$. For further explanation see text.

We find excellent agreement for the first and second resonances at $N_{\text{max}} = 12$. Note also that the energy of the $3/2^-$ ground state is lowered by about 0.5 MeV due to continuum contributions and the agreement with experiment is improved. Next we compare the changes for $N_{\text{max}} = 6$ to 12 for both methods, respectively. For the NCSMC energies we find only small effects from the increased model-space size that are slightly larger for the higher-excited states but still remain below 0.5 MeV. Thus, the NCSMC calculations seem to be well converged with respect to $N_{\text{max}}$ as already observed for the eigenphase shifts in the previous subsection. This is different for the IT-NCSM energies, where we find significantly larger effects hinting at less converged calculations. This is of course not unexpected due to the fact that all excited states of $^9$Be are resonances and the IT-NCSM with its basis of $A$-body HO Slater determinants is not designed for a proper description of continuum states.

The discussion of the positive-parity states of $^9$Be in context of the right-hand panel of Figure 14.6 is similar: we find even more dramatic effects of the continuum as evident from comparing the energies for fixed $N_{\text{max}}$ between the two approaches. Again, the NCSMC reduces all energy differences relative to the n-$^8$Be threshold compared to the IT-NCSM, leading to improved agreement with experiment. The agreement is particularly striking for the $S$-wave dominated $1^{+}$ state, which for $N_{\text{max}} = 7$ is shifted by about 5 MeV right on top of its experimental position slightly above the threshold, and remains practically constant for the step to $N_{\text{max}} = 11$ in the NCSMC. Also the $3/2^+$ resonance dominated by the $4S_3/2$ partial wave is found in good agreement with experiment, while the discrepancies remain larger for the $5/2^+$ and $9/2^+$ resonances. Note that one might expect contributions from the broad $4^{+}$ state of $^8$Be that might improve the $9/2^+$ resonance of $^9$Be. As for the negative parities, the NCSMC energies are much less affected by increasing the model-space size from $N_{\text{max}} = 7$ to 11.
9Be Energy Levels: NCSM vs. NCSMC

Figure 14.6 – Negative (left-hand panel) and positive (right-hand panel) parity spectrum of 9Be relative to the n-8Be threshold at N_{max} = 6 (7) and 12 (11) for IT-NCSM (first two columns) and NCSMC (last two columns) compared to experiment [148]. Remaining parameters are \( \hbar \Omega = 20 \text{ MeV} \) and \( \alpha = 0.0625 \text{ fm}^4 \). Further explanation see text.

- The discussion of the negative-parity states of 9Be in context of the left-hand panel of Figure 14.6 is similar: we find excellent agreement for the \( 1 \text{/}2- \) and second \( 3 \text{/}2- \) resonances at N_{max} = 12. Note also that the energy of the \( 3 \text{/}2- \) ground state is lowered by about 0.5 MeV due to continuum contributions and the agreement with experiment is improved. Next we compare the changes for N_{max} = 6 to 12 for both methods, respectively. For the NCSMC energies we find only small effects from the increased model-space size that are slightly larger for the higher-excited states but still remain below 0.5 MeV. Thus, the NCSMC calculations seem to be well converged with respect to N_{max} as already observed for the eigenphase shifts in the previous subsection. This is different for the IT-NCSM energies, where we find significantly larger effects hinting at less converged calculations. This is of course not unexpected due to the fact that all excited states of 9Be are resonances and the IT-NCSM with its basis of \( A \)-body HO Slater determinants is not designed for a proper description of continuum states.

- The discussion of the positive-parity states of 9Be in context of the right-hand panel of Figure 14.6 is similar: we find even more dramatic effects of the continuum as evident from comparing the energies for fixed N_{max} between the two approaches. Again, the NCSMC reduces all energy differences relative to the n-8Be threshold compared to the IT-NCSM, leading to improved agreement with experiment. The agreement is particularly striking for the \( S \)-wave dominated \( 1 \text{/}2+ \) state, which for N_{max} = 7 is shifted by about 5 MeV right on top of its experimental position slightly above the threshold, and remains practically constant for the step to N_{max} = 11 in the NCSMC. Also the \( 3 \text{/}2+ \) resonance dominated by the \( 4 \text{S}_32 \) partial wave is found in good agreement with experiment, while the discrepancies remain larger for the \( 5 \text{/}2+ \) and \( 9 \text{/}2+ \) resonances. Note that one might expect contributions from the broad \( 4 \text{S}_32 \) state of 8Be that might improve the \( 9 \text{/}2+ \) resonance of 9Be. As for the negative parities, the NCSMC energies are much less affected by increasing the model space from N_{max} = 7 to 11.
9Be Energy Levels: NCSM vs. NCSMC

- Significant contributions from the continuum degrees of freedom
- Excellent agreement with experiment for 1/2− & second 5/2− as well as the 1/2+ and 3/2+ states
- NCSMC seems to be well-converged already at moderate Nmax
**Be Energy Levels: NCSM vs. NCSMC**

**Figure 14.7**

Negative (left-hand panel) and positive (right-hand panel) parity spectra of $^9$Be relative to the n-$^8$Be threshold at $N_{\text{max}} = 12$ and 11, respectively. Shown from IT-NCSM (first two columns) and NCSMC (last two columns) results and experiment (middle columns) [148]. The first and last columns contain the energies for the NN+3N-induced and the second and fourth column for the NN+3N-full Hamiltonian, respectively. Remaining parameters are $\hbar = 20$ MeV and $\alpha = 0.0625$ fm$^4$. For further explanation see text.

We add a comment on excitation energies that can be read off Figure 14.6 by the energy differences to the ground-state. The excitation energy of the $5/2^-$ resonance and similarly all excitation energies of the positive-parity states relativ to the $1/2^+$ state are in good agreement with experiment already at the level of IT-NCSM calculations. It seems as if the main issue of the IT-NCSM is to produce the correct threshold energy.

So far we have found significant effects due to the continuum in the $^9$Be energy levels for the NN+3N-full Hamiltonian. In Figure 14.7 we go on with distinguishing effects caused by the SRG-induced 3N interaction from those originating from the initial chiral 3N interaction. Again the left-hand panel covers the negative-parity spectrum at $N_{\text{max}} = 12$, and the right-hand panel contains the energies of positive-parity states at $N_{\text{max}} = 11$. Within each panel the first two columns depict the results from the IT-NCSM while the two last columns cover the results from the NCSMC, and we include the experimental energy in the middle. Furthermore, the first column contains the results from the NN+3N-induced Hamiltonian and the second the energies for NN+3N-full. This is reversed for the columns corresponding to NCSMC (see column labels). In the negative-parity spectrum we find all states, except the first $5/2^-$ resonance, sensitive to the inclusion of the initial chiral 3N interaction with effects of roughly similar size for both, the IT-NCSM and the NCSMC. Except for the ground state the inclusion of the initial chiral 3N interaction increases the energy difference to the threshold. Since the IT-NCSM energy differences for the NN+3N-induced Hamiltonian are typically close to or above the experimental energies, the agreement is better.
Figure 14.7 – Negative (left-hand panel) and positive (right-hand panel) parity spectrum of $^9$Be relative to the $^8$Be threshold at $N_{\text{max}} = 12$ and 11, respectively. Shown from IT-NCSM (first two columns) and NCSMC (last two columns) results and experiment (middle columns) [148]. The first and last columns contain the energies for the NN+3N-induced and the second and fourth column for the NN+3N-full Hamiltonian, respectively. Remaining parameters are $\hbar \Omega = 20 \text{MeV}$ and $\alpha = 0.0625 \text{fm}$. For further explanation see text.

We add a comment on excitation energies that can be read off Figure 14.6 by the energy differences to the ground-state. The excitation energy of the $5/2^-$ resonance and similarly all excitation energies of the positive-parity states relativ to the $^8$Be ground-state are in good agreement with experiment already at the level of IT-NCSM calculations. It seems as if the main issue of the IT-NCSM is to produce the correct threshold energy.

So far we have found significant effects due to the continuum in the $^9$Be energy levels for the NN+3N-full Hamiltonian. In Figure 14.7 we go on with distinguishing effects caused by the SRG-induced 3N interaction from those originating from the initial chiral 3N interaction. Again the left hand-panel covers the negative-parity spectrum at $N_{\text{max}} = 12$, and the right-hand panel contains the energies of positive-parity states at $N_{\text{max}} = 11$. Within each panel the first two columns depict the results from the IT-NCSM while the two last columns cover the results from the NCSMC, and we include the experimental energy in the middle. Furthermore, the first column contains the results from the NN+3N-induced Hamiltonian and the second the energies for NN+3N-full. This is reversed for the columns corresponding to NCSMC (see column labels). In the negative-parity spectrum we find all states, except the first $5/2^-$ resonance, sensitive to the inclusion of the initial chiral 3N interaction with effects of roughly similar size for both, the IT-NCSM and the NCSMC. Except for the ground state the inclusion of the initial chiral 3N interaction increases the energy difference to the threshold. Since the IT-NCSM energy differences for the NN+3N-induced Hamiltonian are typically close to or above the experimental energies, the agreement with experiment is good.
$^9$Be Energy Levels: NCSM vs. NCSMC

Collaboration with Petr Navrátil
Figure 14.7 – Negative (left-hand panel) and positive (right-hand panel) parity spectrum of $^9\text{Be}$ relative to the $^8\text{Be}$ threshold (at $N_{\text{max}} = 12$, respectively). Shown from IT-NCSM (first two columns) and NCSMC (last two columns) results and experiment (middle columns) [148]. The first and last columns contain the energies for the NN+3N-induced and the second and fourth column for the NN+3N-full Hamiltonian, respectively. Remaining parameters are $\hbar\Omega = 20$ MeV and $\alpha = 0.0625$ fm. 

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Collaboration with Petr Navrátil

9Be Energy Levels: NCSM vs. NCSMC
9Be Energy Levels: NCSM vs. NCSMC

- Treatment of continuum important for conclusions about 3N interactions
- First 5/2− insensitive to the chiral 3N interaction
- 7/2− resonance → interaction problem?
Conclusions
Conclusions

- **Inclusion of 3N forces** challenging but **completed** for single- and two-nucleon projectiles

- New computational scheme — heavier targets accessible

- Promising results for n-\(^{8}\)Be (and p-\(^{10}\)C and n-\(^{16}\)C)

- Proper treatment of continuum **vital** for validation of chiral 3N interactions

Nuclear structure and reactions accessible with full 3N treatment via the No-Core Shell Model with Continuum
Epilogue

- **thanks to my group & collaborators**
  - S. Binder, A. Calci, E. Gebrerufael, S. Fischer, H. Krutsch, R. Roth, S. Schulz, C. Stumpf, A. Tichai, R. Trippel, R. Wirth
  - P. Navrátil
    TRIUMF, Vancouver, Canada
  - G. Hupin, S. Quaglioni
    LLNL, Livermore, USA
  - J. Vary, P. Maris
    Iowa State University, USA
  - H. Hergert
    The Ohio State University, USA
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    IPN Orsay, France
  - K. Hebeler
    TU Darmstadt

**Computing Time**

- [Jülich Forschungszentrum](#)
- [NERSC](#)
- [Center for Scientific Computing Frankfurt](#)
Epilogue

- **thanks to my group & collaborators**
  - S. Binder, A. Calci, E. Gebrerufael, S. Fischer, H. Krutsch, R. Roth, S. Schulz, C. Stumpf, A. Tichai, R. Trippel, R. Wirth

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  The Ohio State University, USA

- P. Piecuch, S. Bogner  
  Michigan State University, USA

- H. Feldmeier, T. Neff  
  GSI Helmholtzzentrum

- P. Papakonstantinou  
  IPN Orsay, France

- K. Hebeler  
  TU Darmstadt

Thanks for your attention!
Inclusion of more excited states

Need to switch to NCSMC for full convergence

\[ N_{\text{max}} = 13 \]
\[ E_{3\text{max}} = 14 \]
\[ \hbar \Omega = 20 \text{ MeV} \]
\[ \alpha = 0.0625 \text{ fm}^4 \]
\[ \lambda = 2.0 \text{ fm}^{-1} \]