Large-basis *ab initio* shell model investigations of halo nuclei

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***Work performed at:** Nuclear Theory & Modeling Group, Lawrence Livermore National Laboratory*

In collaboration with:
Petr Navrátil, W. Erich Ormand *(LLNL),* Etienne Caurier *(IRES Strasbourg)*

Workshop on the physics of halo nuclei
ECT*, Trento, Italy, Nov 1, 2006

Outline

- **Introducing the *ab initio* no-core shell model**
- **Applying the method to exotic nuclei and halo states**
- **Selected results** ^{9,11}Be study: spectra, parity inversion, observables (see also P. Navrátil's talk this afternoon)
- **B(E1) strength in ^{11}Be** - some historical and new perspectives
- **Concluding remarks**

Bold claim:

The no-core shell model provides a microscopic understanding of light nuclei, based on the properties of the *NN+NNN* interactions.

The tools are sufficiently robust to yield precision tests of the nuclear Hamiltonians themselves.

The physics of exotic nuclei, explored at RNB facilities, plays a major role in this endeavour.

The microscopic *ab initio* approach

Aiming for truly predictive power:

- **State-of-the-art nuclear Hamiltonians**
  - Can either have roots in QCD or be based on traditional meson-exchange theory
  - Empirical in that they accurately fit a wealth of *NN* scattering data

- **State-of-the-art nuclear many-body methods**
  - A number of methods are available for A ≤ 4:
    Faddev-Yakubovsky, CRCGV, SVM, GFMC, HH variational, EIHH, NCSM
    See benchmark paper: Kamada et al, *PRC64(2001)044001*
  - Very few methods are available for A>4 with the use of realistic interactions
    Green's function Monte Carlo pioneered this path
    NCSM, Coupled-cluster method, Eff. Interaction for HH basis

- **State-of-the-art computing facilities**

The *ab initio* no-core shell model

- It is a general approach for studying strongly interacting, quantum many-body systems.
- A matrix diagonalization technique to solve the translational invariant A-body problem in a finite harmonic oscillator basis

The NCSM approach:

- Start with a *NN* (or *NN* + *NNN*) interaction
- Unitary transformation of the bare Hamiltonian performed to compute model-space dependent effective interaction
- Diagonalize H_n^{eff} in the given model space
- Check convergence by repeating the calculations for
  - increasing model space (or cluster level of the eff. int.)
  - several values of $h\Omega$

See, e.g., P. Navrátil, *et al*, Phys. Rev. C 62, 054311 (2000).

The *ab initio* Hamiltonian

- Modern, high-precision *NN* interactions are available

- Can be based on either traditional meson-exchange theory or have roots in QCD

- Empirical in that they accurately fit a wealth of *NN* scattering data, as well as deuteron properties, see:

  http://nn-online.sci.kun.nl/nn/ (Nijmegen database)

- **Don’t forget: importance of three-nucleon forces!**

See, e.g., P. Navrátil and W. E. Ormand, Phys. Rev. C 68(2003)034305
And ongoing work on applying 3NF from chiral perturbation theory

The NCSM effective interaction

Model space: The NCSM solves the Schrödinger equation in a large, but finite model space P.

Problem: High-momentum components of high-precision NN interactions require enormously large spaces.

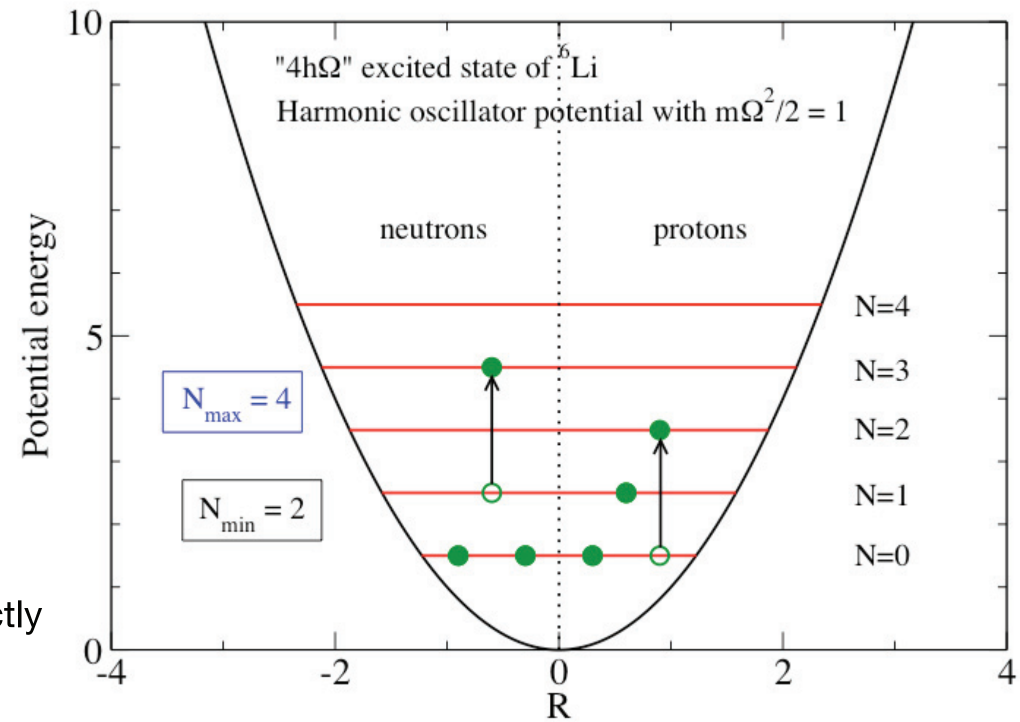
The NCSM model space

Define the "$N_{max}h\Omega$" A-particle model space (P-space) as including all HO excitations up to a total energy cutoff:

$$\sum_{i=1}^{A} \varepsilon_i \le \left(N_m + \frac{3A}{2} \right) \hbar\Omega$$

where $N_m \equiv N_{min} + N_{max}$

Note, translational invariance can be exactly retained by using a Lagrange multiplier.



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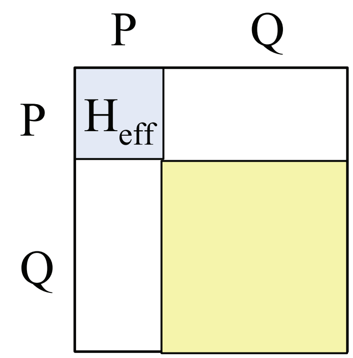
Problem: High-momentum components of high-precision NN interactions require enormously large spaces.

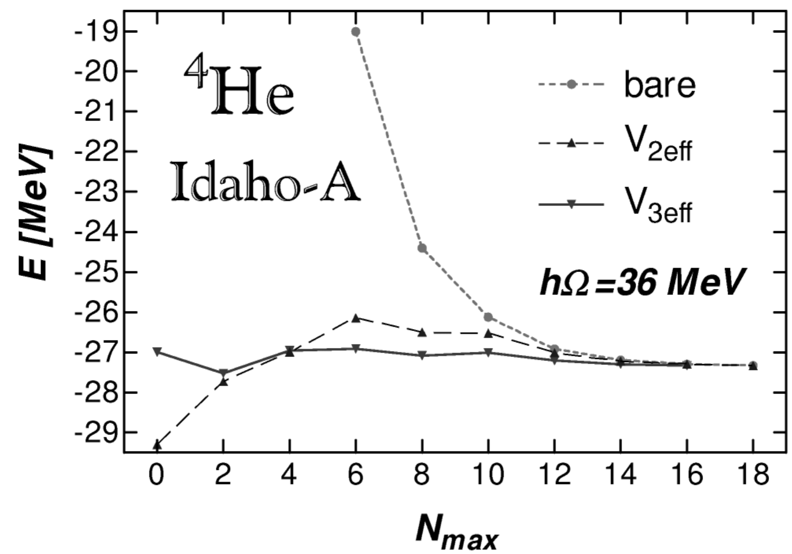
Solution: Follow formal procedure (Lee-Suzuki) to derive an effective interaction acting only in the model space and reproducing exactly a subset of the eigensolutions.

Price: This procedure generates A-body operators and is essentially as difficult to apply as solving the full problem.

Approximation: Generate effective interaction at 2- or 3-body cluster level.



P. Navrátil and W. E. Ormand, Phys. Rev. Lett. 82(2002)152502



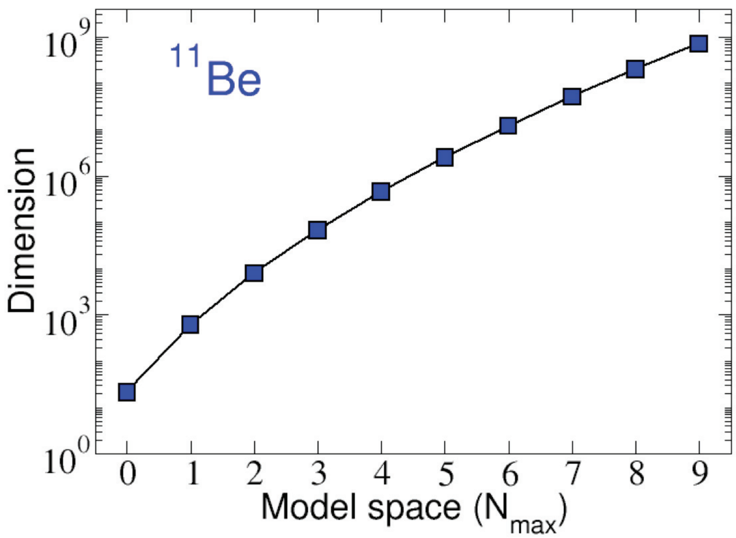
P. Navrátil, J.P. Vary and B.R. Barrett, Phys. Rev. Lett. 84(2000)5728
K. Suzuki and S.Y. Lee, Prog. Theor. Phys. 64(1980)2091

Large-scale shell model calculations

- Diagonalization of huge, but sparse, matrices
- M-scheme shell model codes: MFD, REDSTICK, ANTOINE
- Lanczos algorithm for diagonalization

A quick comparison:
NCSM vs Standard SM

Dimension of ^{11}Be model spaces

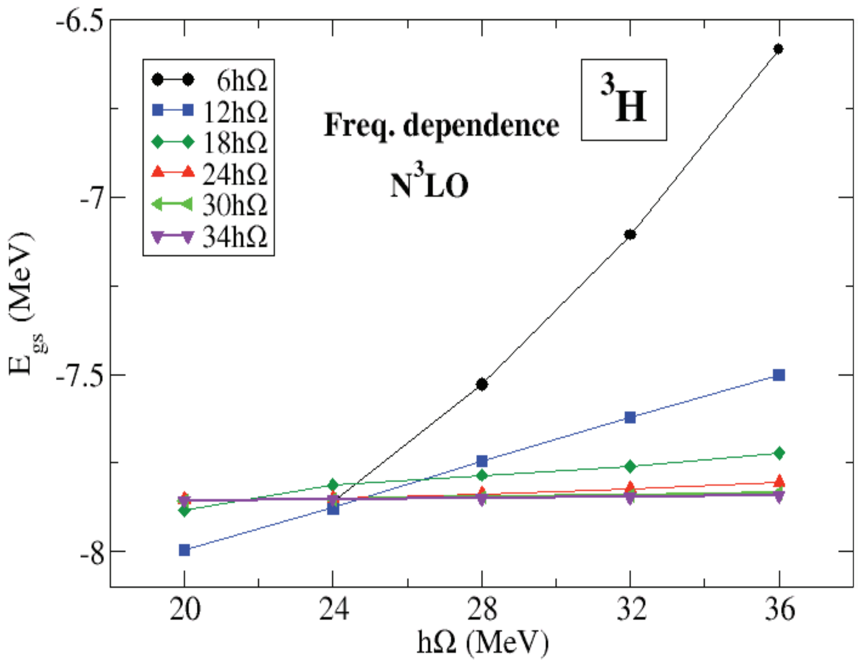


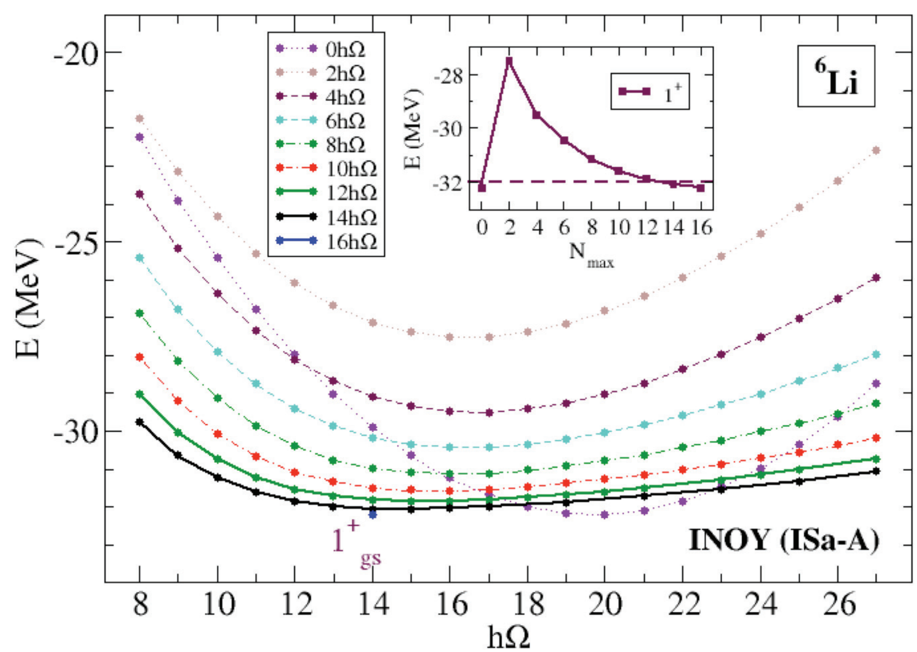
	^{11}Be NCSM: 9hΩ	**^{57}Ni SM: full fp-shell**
Dimension	0.71×10^9	1.4×10^9
Active shells	66	4
nljm-states	572	20
Stored MEs	~70 Gb	~1 Gb

E. Caurier and F. Nowacki, Acta Phys. Pol. B**30**(1999)705

Selected convergence tests and examples

- Independence of Ω when $N_{max} \rightarrow \infty$
- Not a variational calculation
- Convergence as $N_{max} \rightarrow \infty$





C. Forssén, ECT*, Trento, Nov 1, 2006

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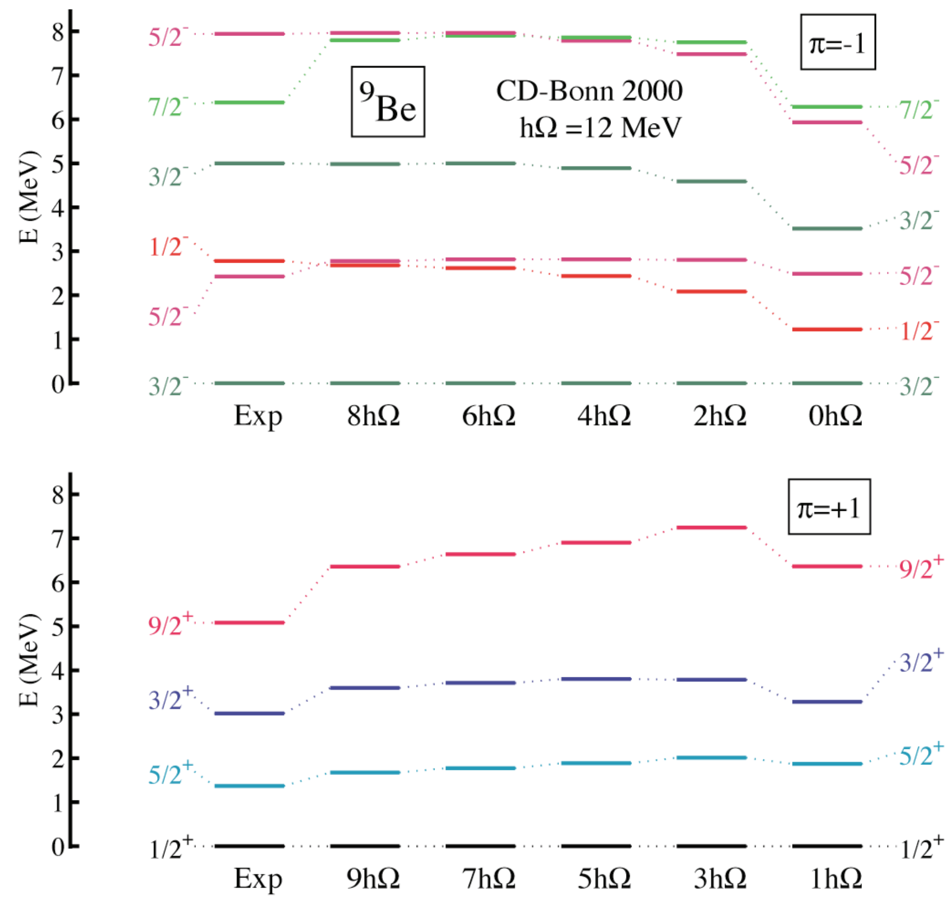
- Convergence of excitation spectra: ^{9}Be example

  see recent β-decay study by

  M. Borge et al, Phys. Scr. T125(2006)103



C. Forssén *et al*, Phys. Rev. C 71 (2005) 044312

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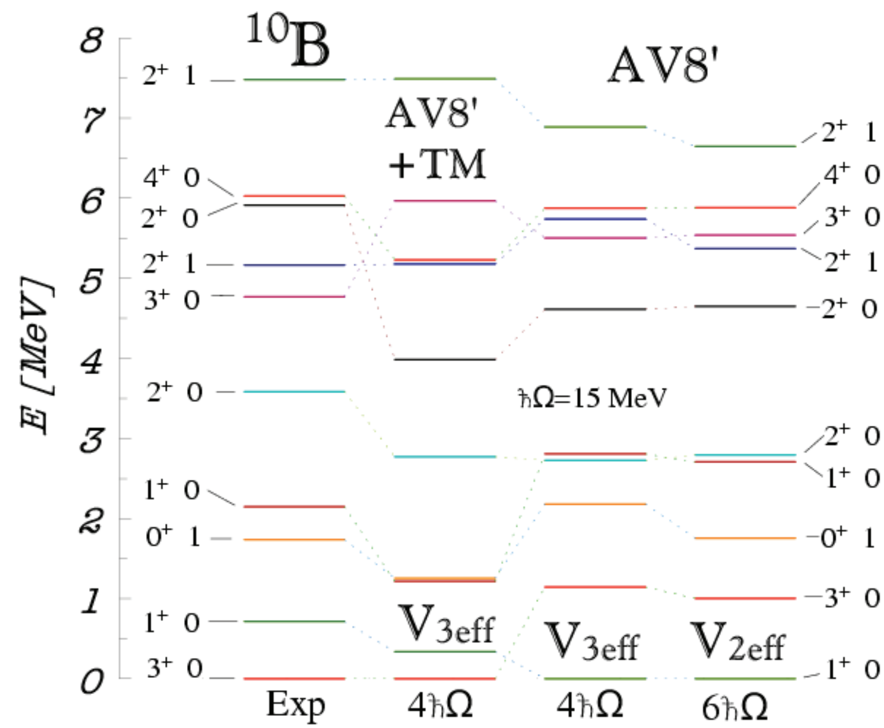
- The 3N-interaction sometimes play a critical role in determining the structure of nuclei:
  ^{10}B example, spin inversion



P. Navrátil and W. E. Ormand, Phys. Rev. C 68(2003)034305

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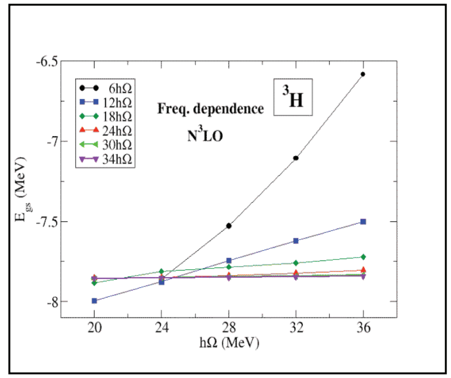

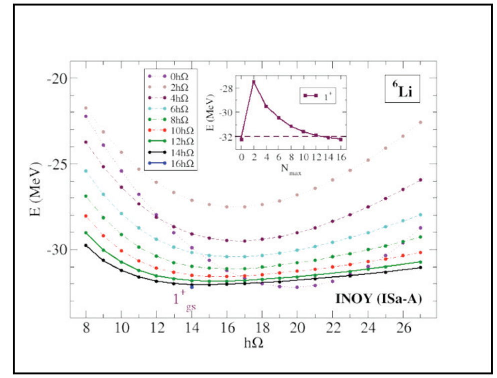

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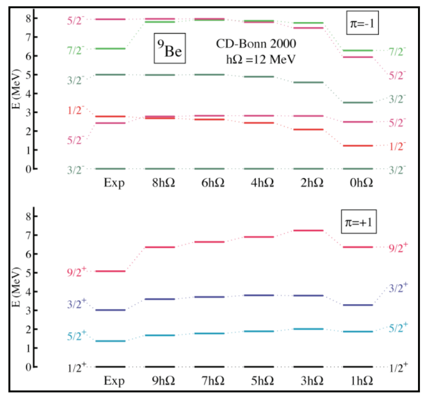

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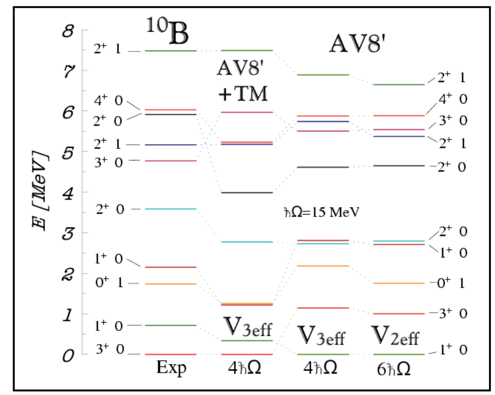


Hamiltonian fitting *NN* (and possibly *NNN*) data

Nuclear spectra and other properties

Application to exotic nuclei

Bold claim from the introduction:

The tools are sufficiently robust to yield precision tests of the nuclear Hamiltonians themselves.

The physics of exotic nuclei, explored at RNB facilities, plays a major role in this endeavour.

Some advantages:

- Basically no restrictions regarding the Hamiltonian
- Preserves the symmetries: Rotational, translational, parity, etc
- Very good convergence properties
- Gives eigenstates and eigenenergies. Spectra can be constructed and operator MEs calculated

Some challenges:

- Expansion in bound-state basis functions
- Dimension grows rapidly with increasing number of nucleons
- Slower convergence for $1\hbar\Omega$– and $2\hbar\Omega$-dominated states
- Cluster limit $a \leq 3$ in eff. int. restricts the description of e.g. α clusterization

Large-scale *ab initio* NCSM study of A=9-11

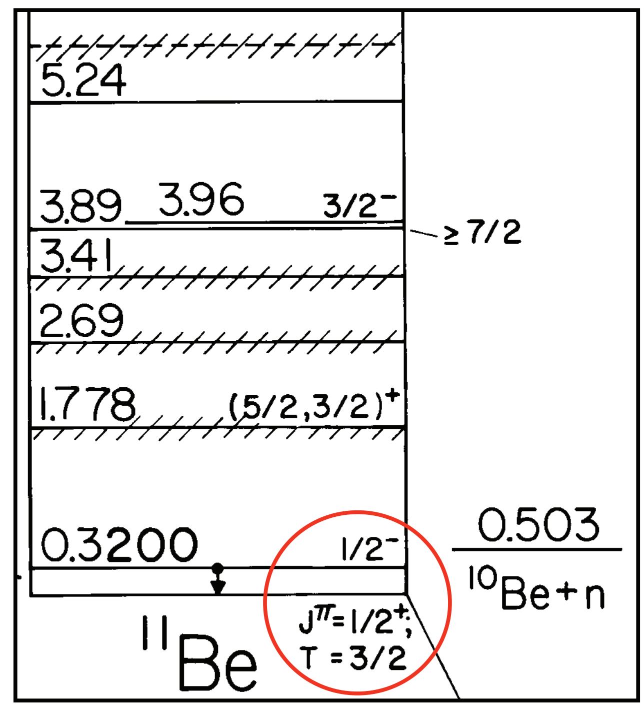
- Large-scale calculations with convergence tests were performed for several A=9-13 isotopes.
- Model spaces exceeding 1×10^9 were reached.
- Effects of different NN interactions on spectroscopy and other observables were studied.
- Particular focus on the quenching of the shell gap. Indications that 3N forces are important.
- Converged wave functions used to investigate cluster overlaps.

C. Forssén *et al*, Phys. Rev. C 71 (2005) 044312

VOLUME 4, NUMBER 9 PHYSICAL REVIEW LETTERS MAY 1, 1960

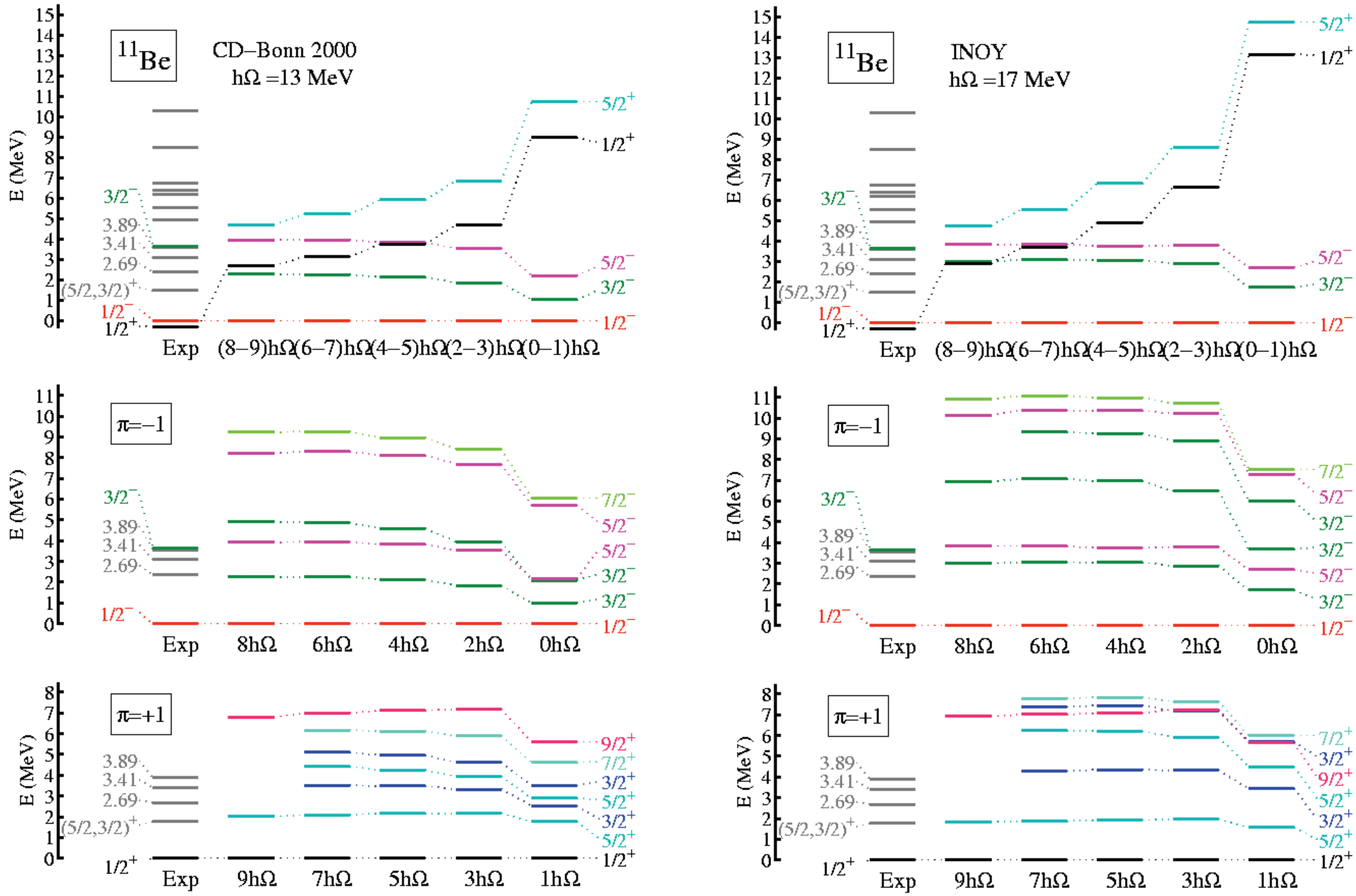
ORDER OF LEVELS IN THE SHELL MODEL AND SPIN OF Be^{11*}

I. Talmi and I. Unna
Department of Physics, The Weizmann Institute of Science, Rehovoth, Israel
(Received April 4, 1960)

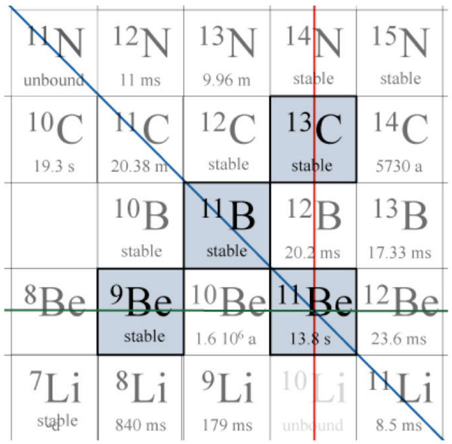


^{11}Be spectrum

- Remarkable agreement between the predictions of different, high-precision *NN* interactions.
- Unnatural-parity states are too high - but dropping.

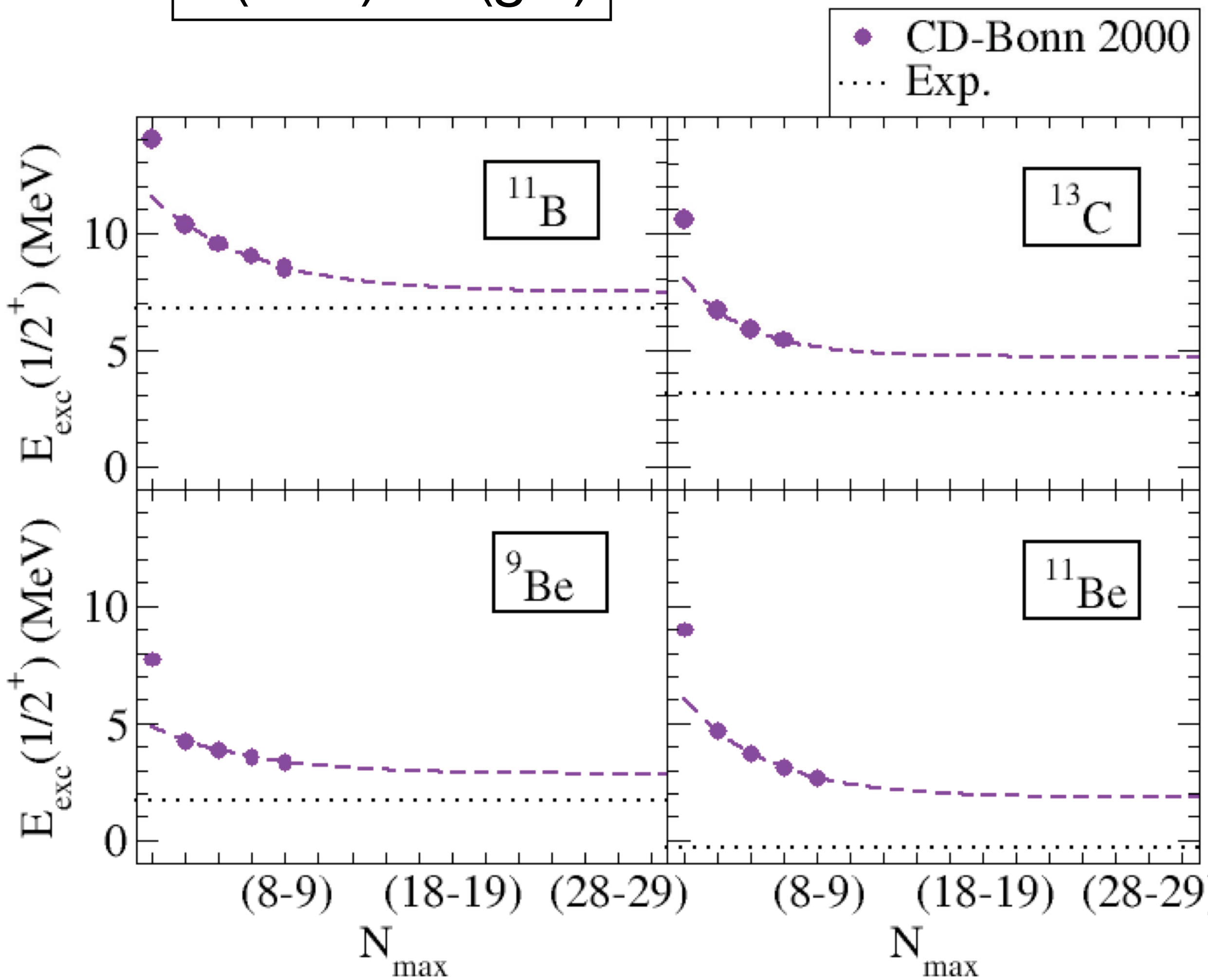


Systematics: first unnatural-parity state



- The position of the first unnatural parity states differ a lot between these isotopes.
- The energy of 1hΩ-dominated states exhibits a slower convergence in the NCSM.
- But the large shifts are reproduced nicely

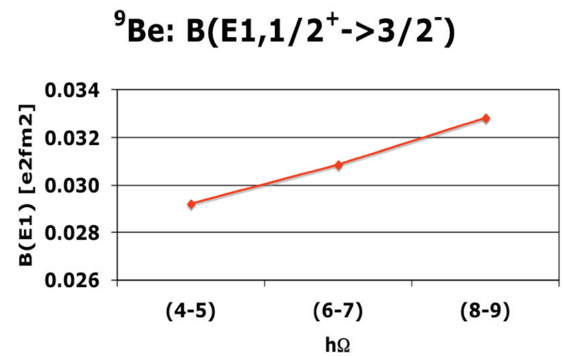
$E(1/2^+) - E(gs^-)$

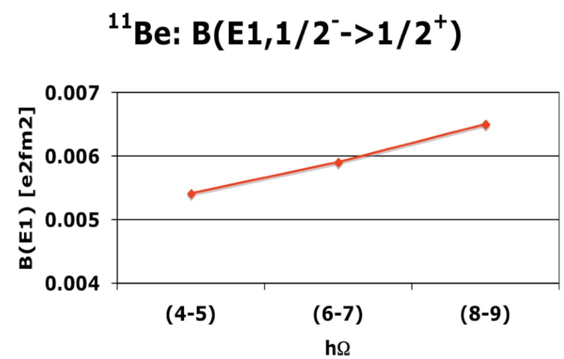


Observables: ^{9,11}Be

	^{9}Be		^{11}Be	
	Exp	AV8'	Exp	AV8'
μ_{gs} [μ_N]	-1.18	-1.22	-1.68	-1.58
Q_{gs} [e^2fm^4]	5.86	4.01		
B(E2) [e^2fm^4]	$5/2^- \rightarrow 3/2^-$			
	27.1	15.0		
B(M1) [μ_N^2]	$5/2^- \rightarrow 3/2^-$			
	0.54	0.37		
B(E1) [e^2fm^2]	$1/2^+ \rightarrow 3/2^-$		$1/2^- \rightarrow 1/2^+$	
	0.061	0.033	0.116	0.0065
r_{mat} [fm]	2.45	2.34	2.86	2.54

Experimental
Converged
Not converged





Note: we have not used effective operators!
(but it would probably not change anything in our 2-body approximation)

Strong E1 transition in ^{11}Be

PHYSICAL REVIEW C VOLUME 3, NUMBER 6 JUNE 1971

Lifetime of the First Excited State of ^{11}Be†

S. S. Hanna,* K. Nagatani, W. R. Harris, and J. W. Olness
Brookhaven National Laboratory, Upton, New York 11973
(Received 5 March 1971)

The mean lifetime of the first excited state of ^{11}Be at 0.32 MeV has been measured by the Doppler-shift-attenuation method. The result 0.18±0.06 psec corresponds to a very strong $E1$ transition, 0.33 W.u. This value is in very good agreement with a simple harmonic-oscil-

Experimental result
$\Gamma(^{11}\text{Be})/\ \Gamma(^{13}\text{C}) = 8.5$

Simple HO picture:
$\Gamma(^{11}\text{Be})/\ \Gamma(^{13}\text{C}) = 0.7$

PHYSICAL REVIEW C VOLUME 28, NUMBER 2 AUGUST 1983

Strong $E1$ transitions in ^{9}Be, ^{11}Be, and ^{13}C

D. J. Millener, J. W. Olness, and E. K. Warburton
Brookhaven National Laboratory, Upton, New York 11973

S. S. Hanna
Stanford University, Stanford, California 94305

attributed to the large increase in the $1s_{1/2}p_{1/2}$ SPME for neutrons loosely bound to the ground state of the ^{10}Be core. Particularly significant is the increase in the $1s_{1/2}p_{1/2}$ SPME relative to the $d_{5/2}p_{3/2}$ SPME, where the particles are coupled to higher core states with correspondingly larger separation energies. The near cancellation of the $1s_{1/2}p_{1/2}$ and $d_{5/2}p_{3/2}$ contributions in the HO calculation is thus removed. We note that to obtain

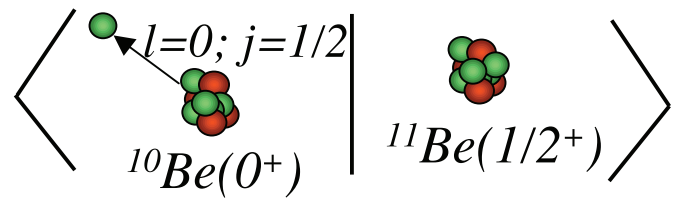
From HO ➡ WS single-particle wfs resulted in B(E1): 0.011 ➡ 0.52 W.u.

How much does $^{11}\mathrm{Be}_{gs}$ look like $^{10}\mathrm{Be}_{gs}$+n ?

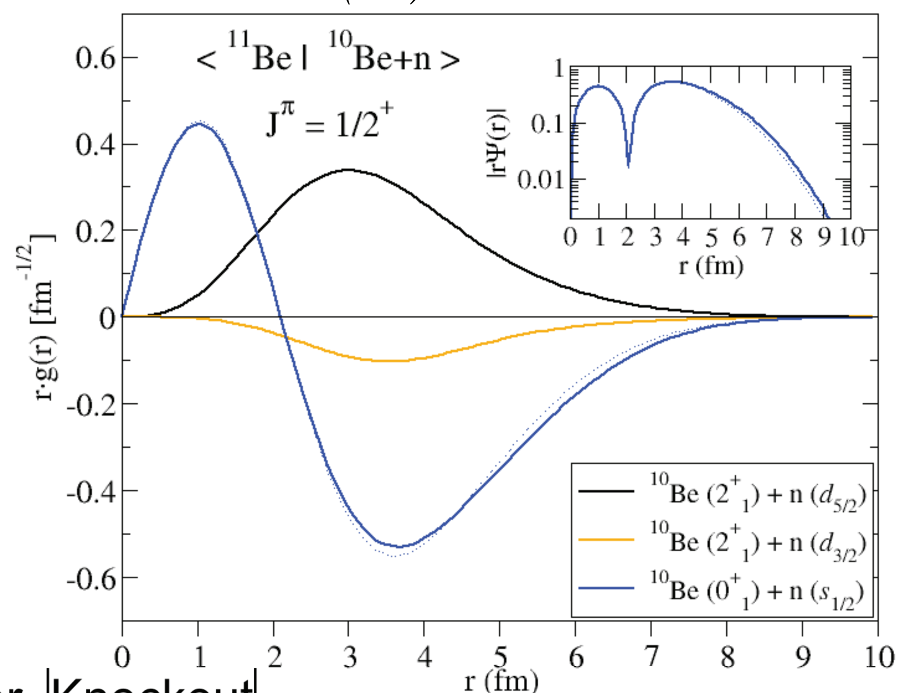
Cluster overlaps from NCSM eigenstates

$$g(r) = \langle \Psi^{(A)} | \mathcal{A} \Phi^{(A-a)} \Phi^{(a)} \delta_{r, r_{A-a,a}} \rangle$$

P. Navrátil, Phys. Rev. C. **70**(2004)054324



- Pauli principle inherent
- Converged spectroscopic factor
- Converged interior
- Non-converged asymptotics



Spectroscopic factors for ^{11}Be($1/2^+$):

	NCSM	Transfer	Knockout
$^{10}Be(0_1^+) \otimes n(s_{1/2})$	0.82	0.67-0.80	0.78
$^{10}Be(2_1^+) \otimes n(d_{3/2})$	0.02		
$^{10}Be(2_1^+) \otimes n(d_{5/2})$	0.26	0.09-0.16	
		J.S. Winfield et al NPA**683**(2001)48	T. Aumann et al PRL**84**(2000)35

CD-Bonn 2000
$\hbar\Omega = 14$ MeV
$(4-5)$, $(6-7)\hbar\Omega$

Correcting the asymptotics of the overlap function

- **Asymptotic behaviour:**

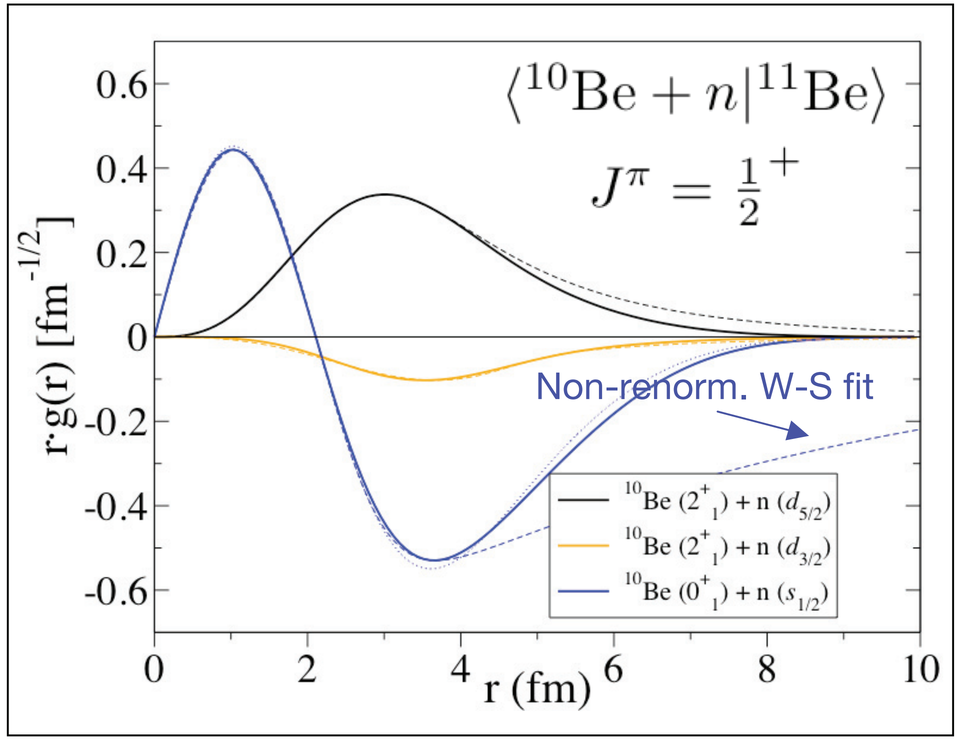
HO single-particle basis states

$$\varphi_{nlm}(r) \sim \exp\left(-r^2/b^2\right)$$

Physical bound-state wave function

$$u(r) \sim \exp\left(-\kappa_0 r\right)/r$$

where $\kappa_0 \propto \sqrt{E_0}$



$\mathrm{CD-Bonn\ 2000}$
$\hbar\Omega = 14\ \mathrm{MeV}$
$(6-7)\hbar\Omega$

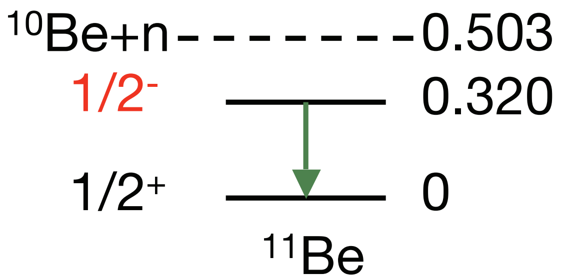
- **Construct effective inter-fragment potentials *$V_{eff}(r)$***

$$\boxed{\left[T + V_{\mathrm{eff}} - E_0\right] u(r) = 0}$$

Exp. treshold energy

- **Renormalize the solution by NCSM spectroscopic factor**

Strong E1 transition in ^{11}Be revisited



Experimental:

B(E1) = 0.116(12) e^{2}fm^2

NCSM (8-9)hΩ result:

B(E1) = 0.0065 e^{2}fm^2

$$\langle \Psi_f^{(A)} | \hat{O}_{E1} | \Psi_i^{(A)} \rangle$$

We know that this transition has a strong s.p. character

<u>Step 1:</u>

- Insert:
  $\Sigma | \mathcal{A}\Phi^{(A-1)}\Phi^{(1)}\delta_{r,r_{A-1,1}} \rangle \langle \mathcal{A}\Phi^{(A-1)}\Phi^{(1)}\delta_{r,r_{A-1,1}} |$
  and calculate E1 transition between (^{10}Be + n) cluster states
- Include only a few (dominant) cluster overlaps

B(E1) = 0.0024 e^{2}fm^2

<u>Step 2:</u>

- Use corrected NCSM cluster overlaps by constructing WS potentials, $V_{eff}(r)$, as described

B(E1) = 0.033 e^{2}fm^2

Summary and outlook

- The no-core shell model provides a microscopic understanding of light nuclei, based on the properties of the *NN+NNN* interactions.

- Today you have seen results from large-scale calculations of A=9-11 isotopes.

- Some particular challenges emerge as we apply the method to study exotic nuclei.

- We have the ability to study cluster structures of NCSM wave functions in a translational invariant approach.

- The development of this ability is the first step in a dedicated effort to achieve a truly fundamental description of nuclear reactions.