Towards the driplines with the ab initio no-core shell model

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Outline

- Physics output of ab initio nuclear theory
- Uncertainty quantification
  - Converging sequences in the no-core shell model
- Continuum and correlations
  - Many-body correlations
    (Example: The C isotopic chain)
  - Continuum couplings - an outlook

Physics output

- Our claim of connecting nuclear structure with first principles has had some resonance in the nuclear physics community
- There is an increasing number of joint theory/experiment ventures.
- *"How to capitalise on the predictive power and achieve full physics potential"* (JPV)

Towards the exotics

- Interesting physics is taking place at the limits of nuclear existence.
- Realm where many-body correlations and short-range physics meet long-range correlations and the continuum.
- In a microscopic theory we will have to face convergence issues head on and try to quantify them.

Strategy

- Testing the many-body scheme using realistic interactions rather than the details of the interaction.
- For convergence issues we will deal only with NN interactions.
  - CD-Bonn (LSO renorm.), for good convergence
  - INOY (LSO renorm.) to indicate possible 3NF effects
- Uncertainty quantification based on method uncertainties rather than physics uncertainties.

The no-core shell model

- Many-body Schrödinger equation
  - A-nucleon wave function
  - Non-relativistic, point nucleons
- Hamiltonian: $$H_A = \frac{1}{A}\sum_{i<j}^{A}\frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j}^{A} V_{NN,ij} + \sum_{i<j<k}^{A} V_{NNN,ijk}$$
  - Realistic NN interactions (high-precision fit to NN phase shifts up to 350 MeV)
  - Realistic NNN interactions include terms related to two-pion exchange
- Many-body basis: Slater determinants composed of harmonic oscillator single-particle states

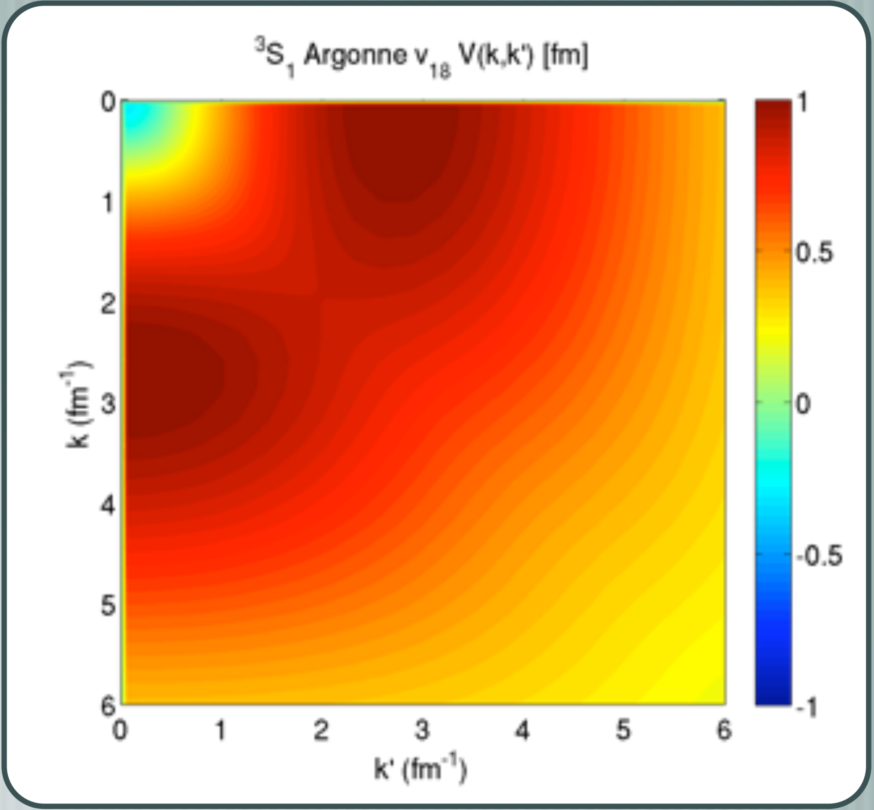
Coordinates, basis and model space

Bound states (and narrow resonances)	Square-integrable A-nucleon basis
NN (and NNN) interactions depend on relative coordinates and/or momenta	Harmonic-oscillator (HO) basis allows easy Fourier transformation and also the choice of using either Jacobi or Cartesian coordinates
Translational invariance and anti-symmetrization	With a complete N_{max} $\hbar\Omega$ model space we are guaranteed translational invariance even when finite SD basis in Cartesian coordinates is used.
Nuclear problems typically require very large model spaces	HO basis allows to take advantage of powerful second-quantization shell model technique
Short- and long-range correlations	Disadvantage: Gaussian asymptotic behaviour

The nuclear interaction

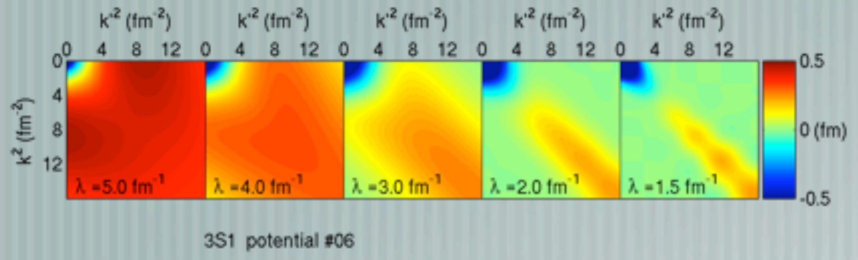
- High-momentum components of realistic NN (+NNN) forces introduce strong short-range correlations.

- Enormously large model spaces required to accomodate these correlations.

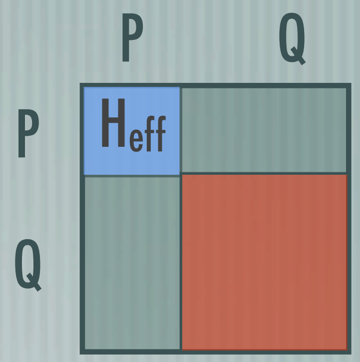


Effective-interaction approaches

... instead: renormalize the interaction using a unitary transformation.



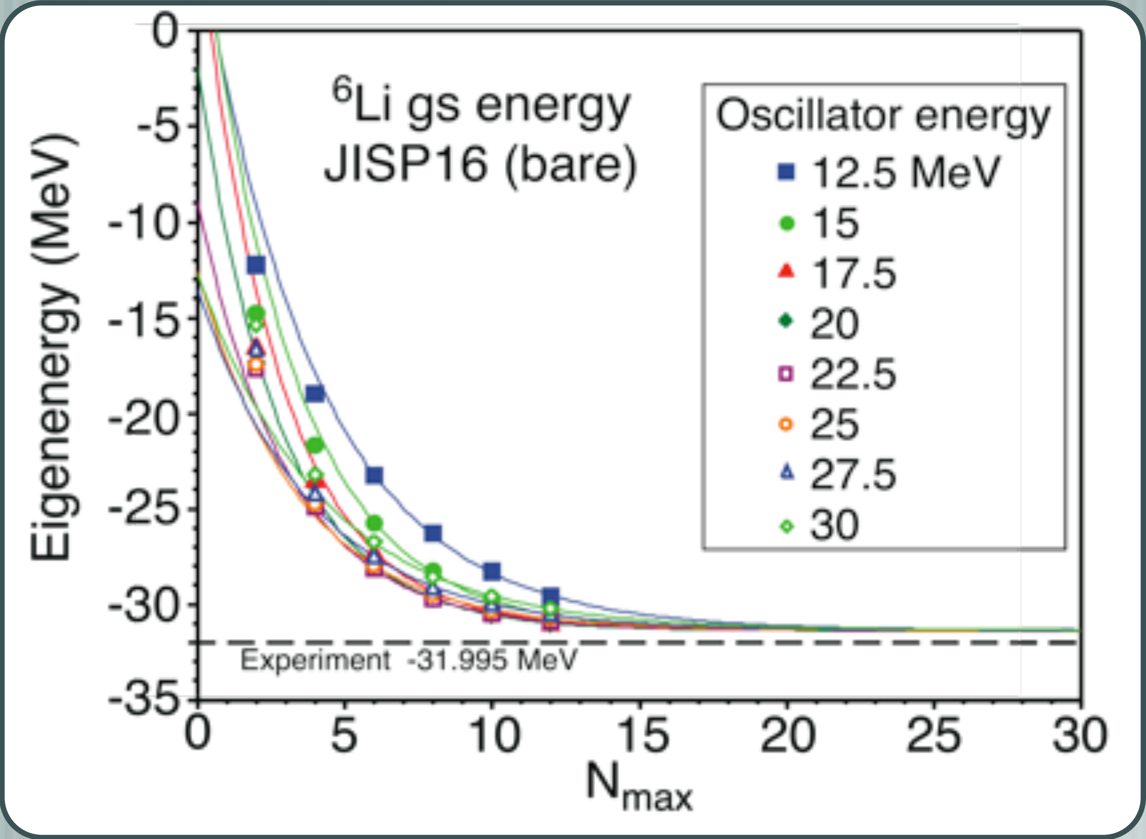
- SRG, V-UCOM, V-lowk.
- H_{eff} is independent of model space.
- Variational calculation
(but without A-body terms the converged result typically depends on the flow parameter)



- Lee-Suzuki-Okamoto
- H_{eff} is model-space dependent.
- Not variational
(but even with only 2-body terms it will converge to exact result)

Converging sequences

Different choices of HO frequency

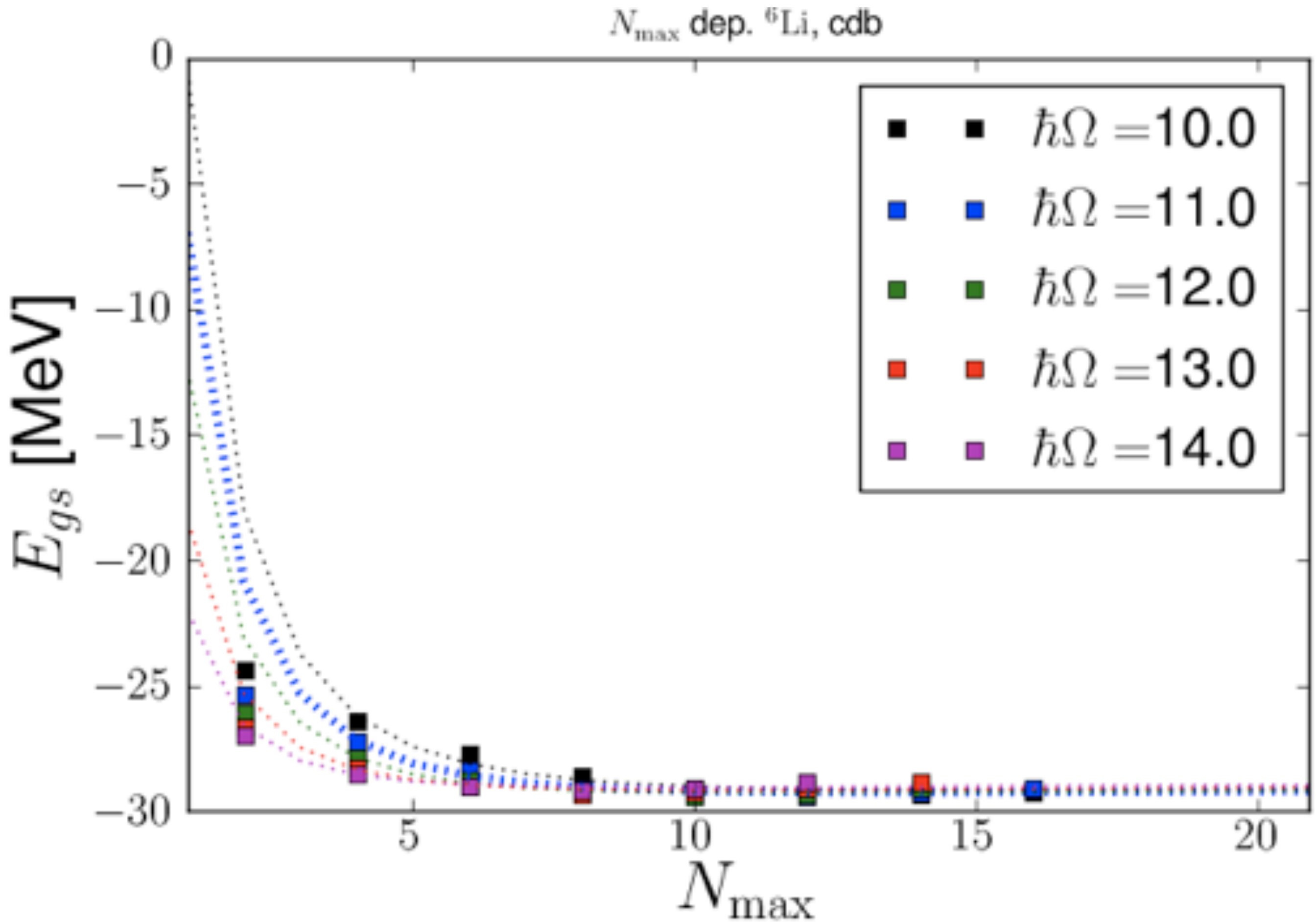


Powerful property

Any sequence that returns the bare Hamiltonian as the model space is increased will converge to the exact result.

CF, J. Vary, E. Caurier, P. Navrátil, Phys. Rev. C **77** (2008) 024301

Converging sequences: eff. interactions



Constrained extrapolations

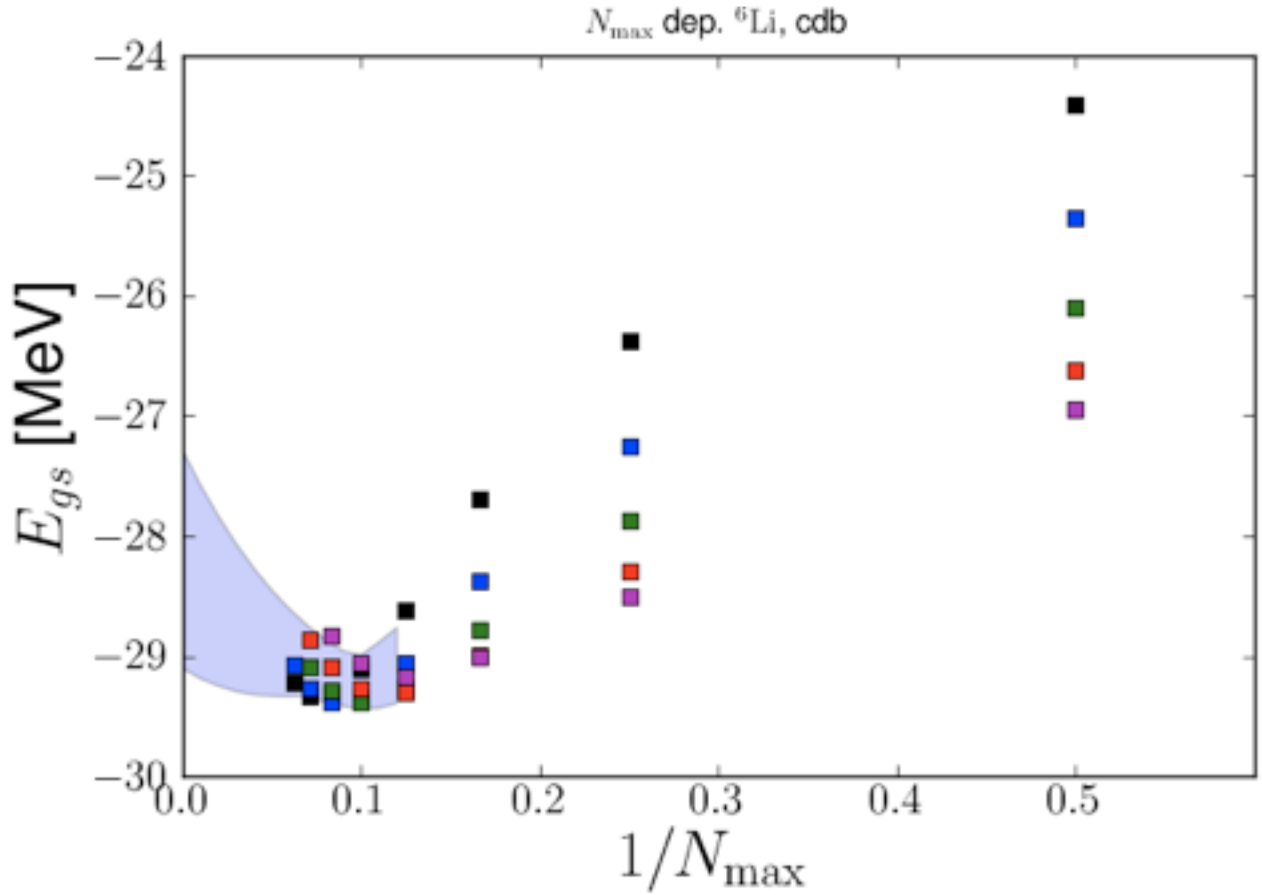
$$\text{Option 1}: \quad y(N_{\max}) = y_\infty + c_0 \exp(-c_1 N_{\max})$$

$$\text{Option 2}: \quad y(N_{\max}) = y_\infty + \frac{c_0}{(N_{\max}+3/2)} + \frac{c_1}{(N_{\max}+3/2)^2} + \ldots$$

$$\text{Option 3}: \quad y(N_{\max}) = y_\infty + \exp(-c_0 N_{\max}) \left[\frac{c_1}{(N_{\max}+3/2)} + \ldots \right]$$

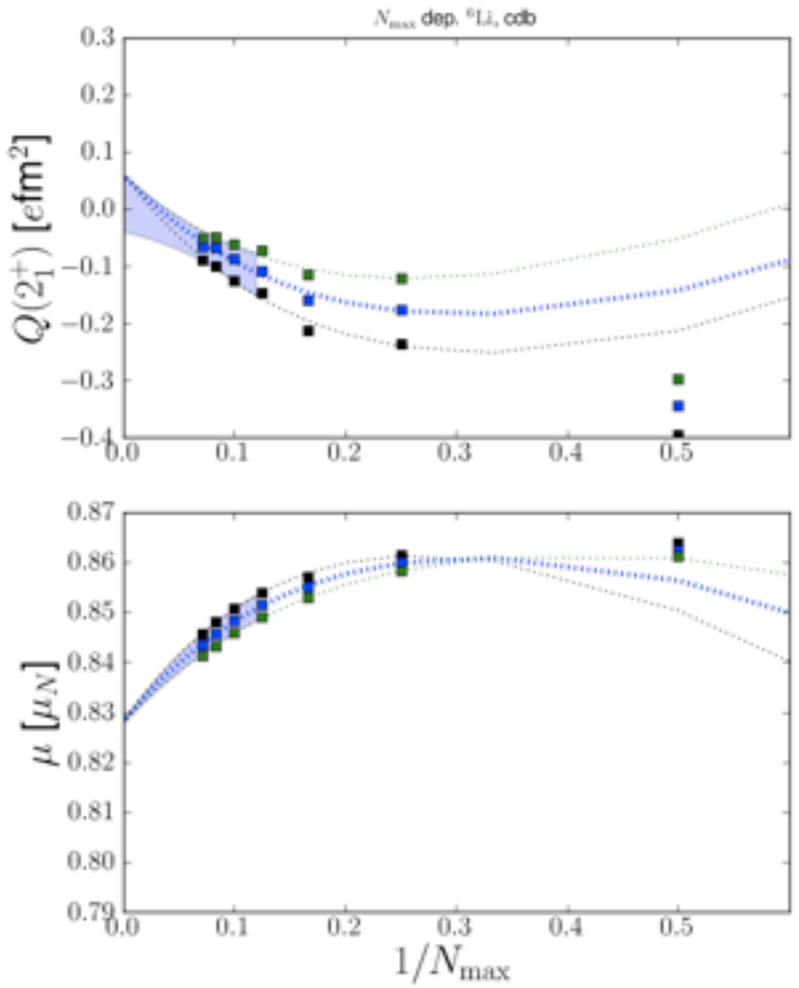
Usually the second and third options provide the best fit

Converging sequences: eff. interactions



- Multiple N_{max} sequences
- Constrained extrapolation to $1/N_{max} \rightarrow 0$
- Error estimates determined by varying the included ħΩ sets

Converging sequences: EM observables



NCSM (CD-Bonn)

- $Q(^6\text{Li}; 1^+) = 0.06(10)$
- $\mu(^6\text{Li}; 1^+) = 0.828(1)$

Exp.

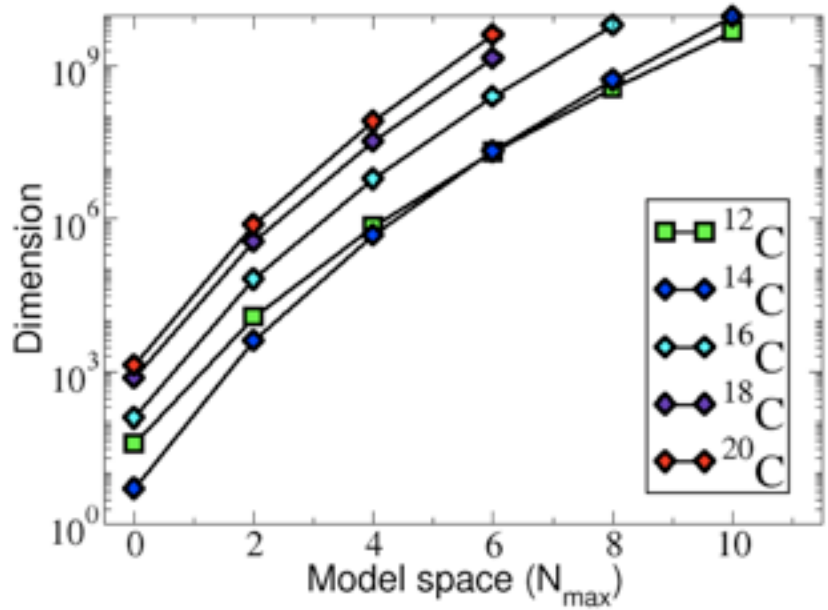
- $Q(^6\text{Li}; 1^+) = -0.0806(6)$
- $\mu(^6\text{Li}; 1^+) = 0.822$

The Carbon isotopic chain

Many-body correlations: C isotopes

- The isotopic C chain traverses the p- / sd-shell boundary
- Possible “decoupling” of protons and neutrons
- Sensitive probe: $B(E2; 2^+ \rightarrow 0^+)$
- Recent experimental lifetime data from RIKEN, LBNL, NSCL
- Challenge for ab initio methods to reproduce data from stable isotopes towards the driplines

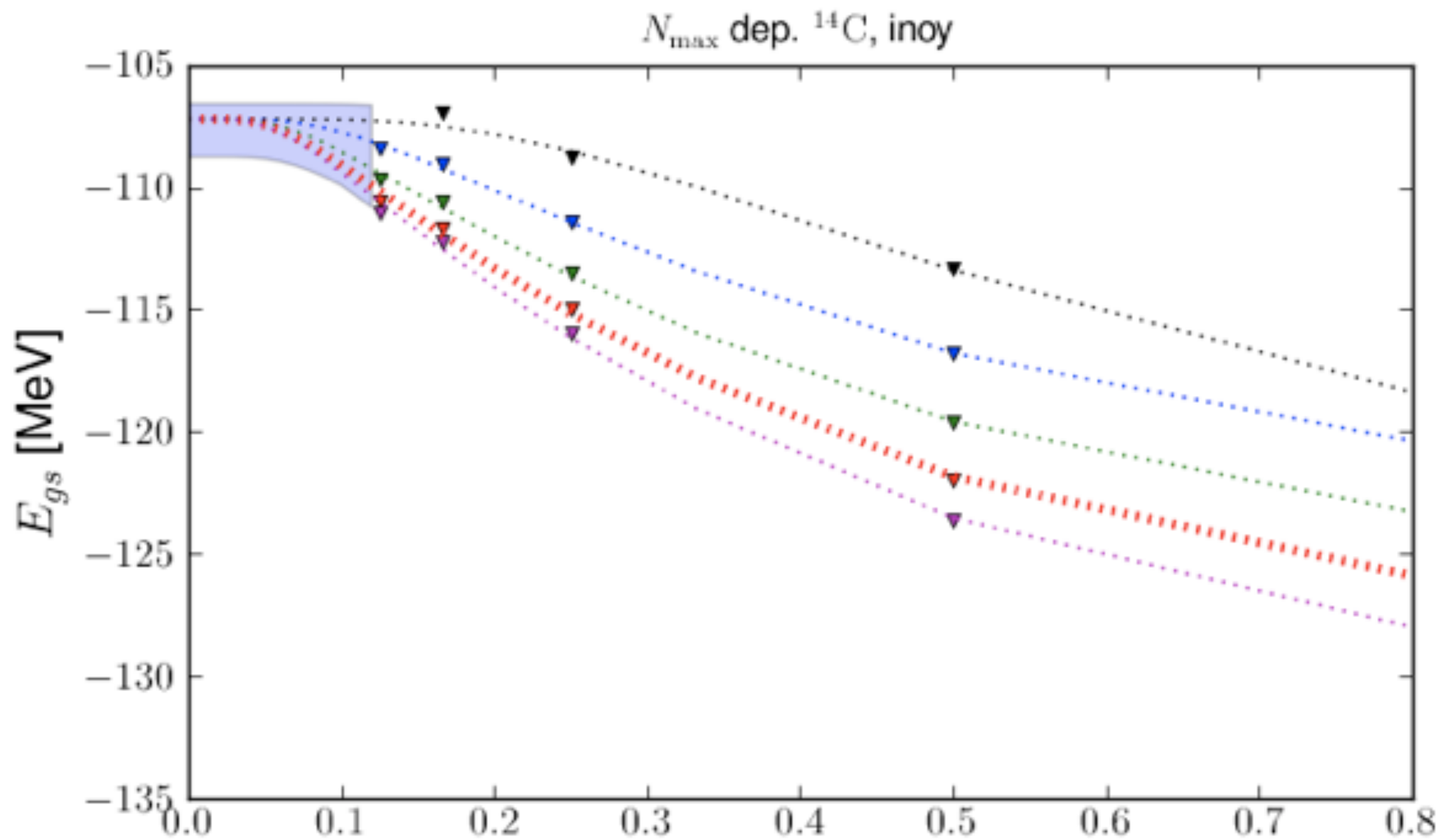
Scale explosion



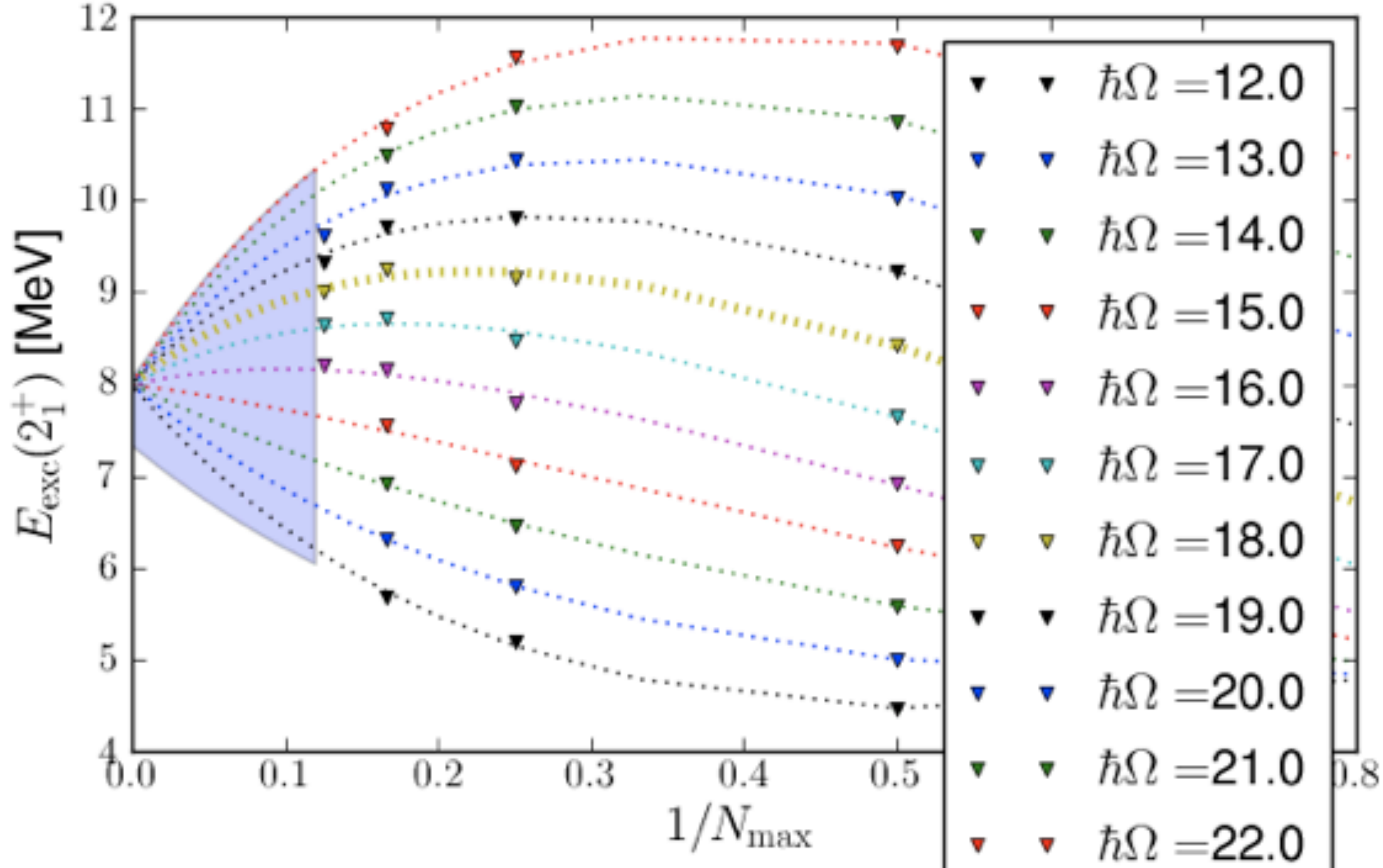
M-scheme (M=0)

Number of non-zero MEs grows approx. as $D^{4/3}$ (NN) or $D^{3/2}$ (NN+NNN)

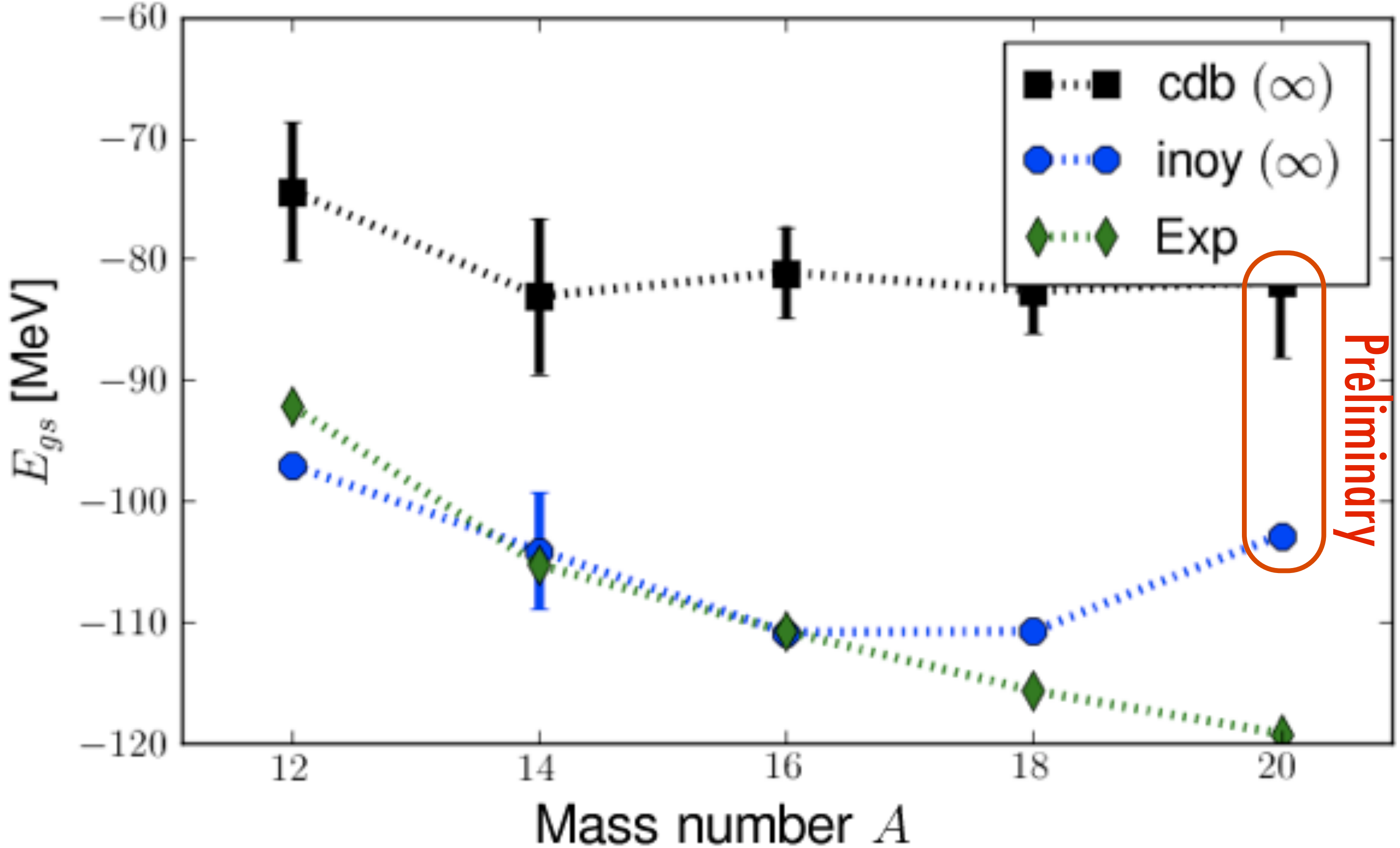
Binding energy convergence (^{14}C w. INOY)



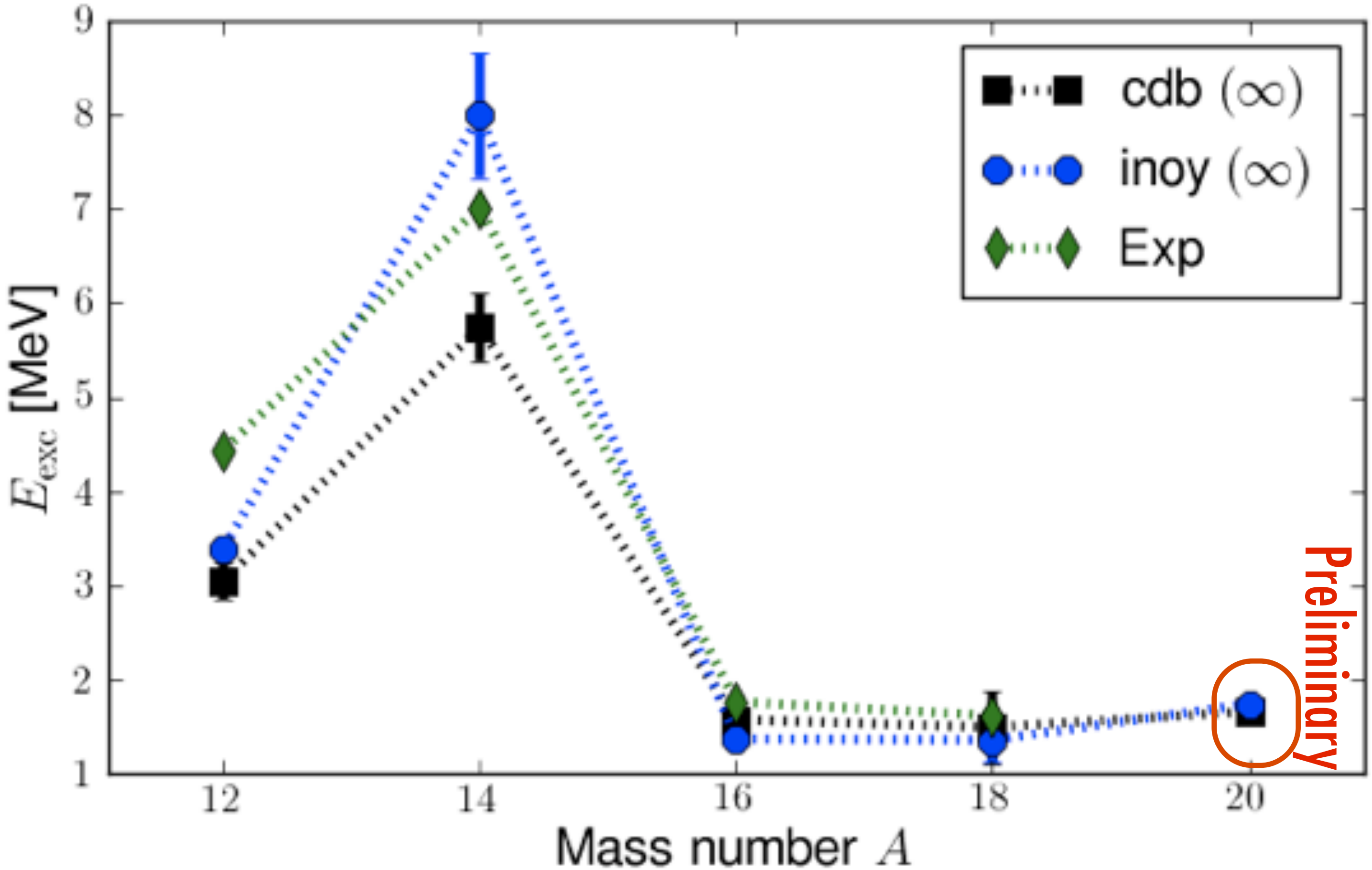
2^+ energy convergence (^{14}C w. INOY)



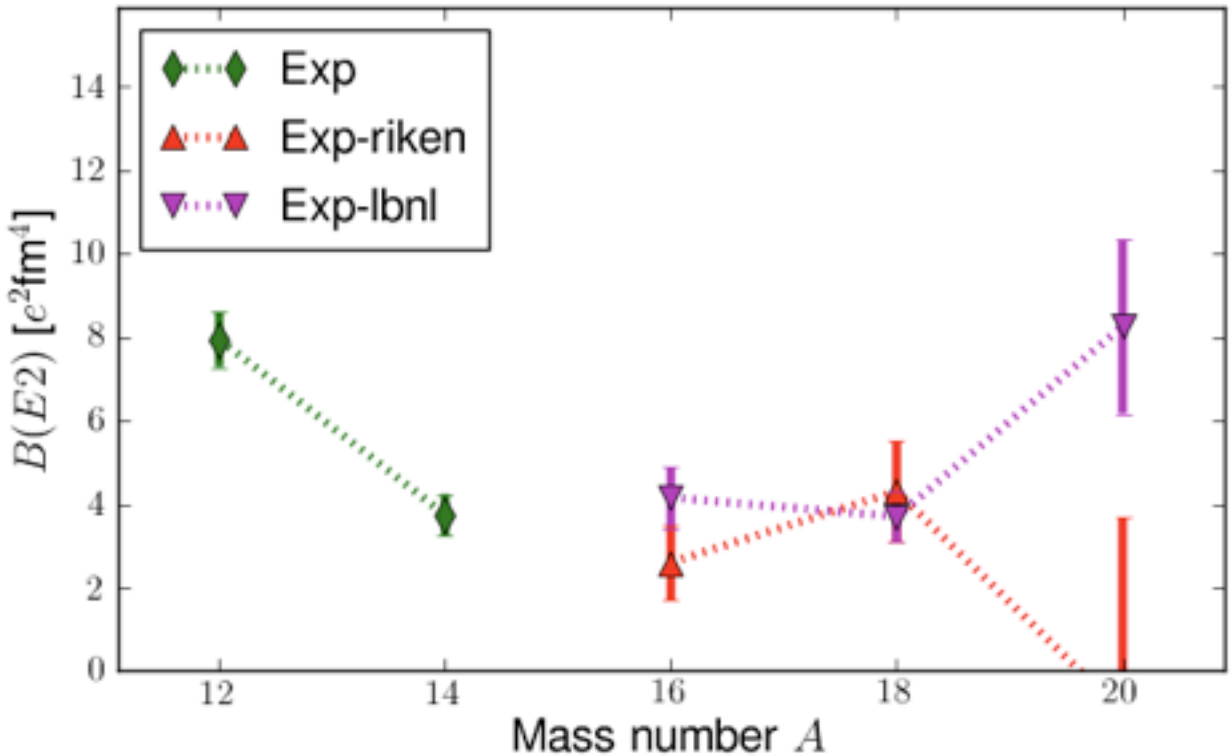
C isotopes: Binding energies



C isotopes: 2^+ excitation energies



Exp. campaigns: $^{16\text{-}20}$C B(E2; $2^+ \rightarrow 0^+$)

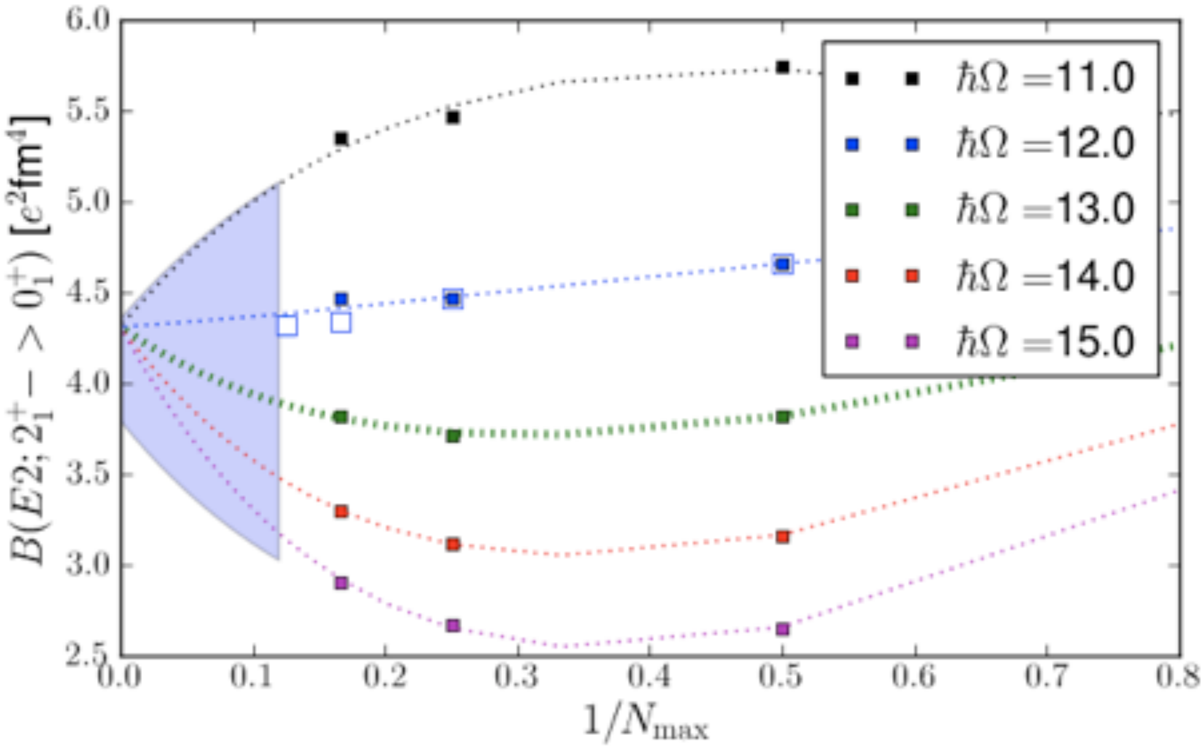


Experimental lifetime data from RIKEN, LBNL, NSCL

H.J. Ong et al., PRC78(2008)014308
Z. Elekas et al., PRC79(2009)011302(R)

M. Wiedeking et al., PRL100(2008) 152501
P. Voss et al., unpub.
M. Petri et al., unpub

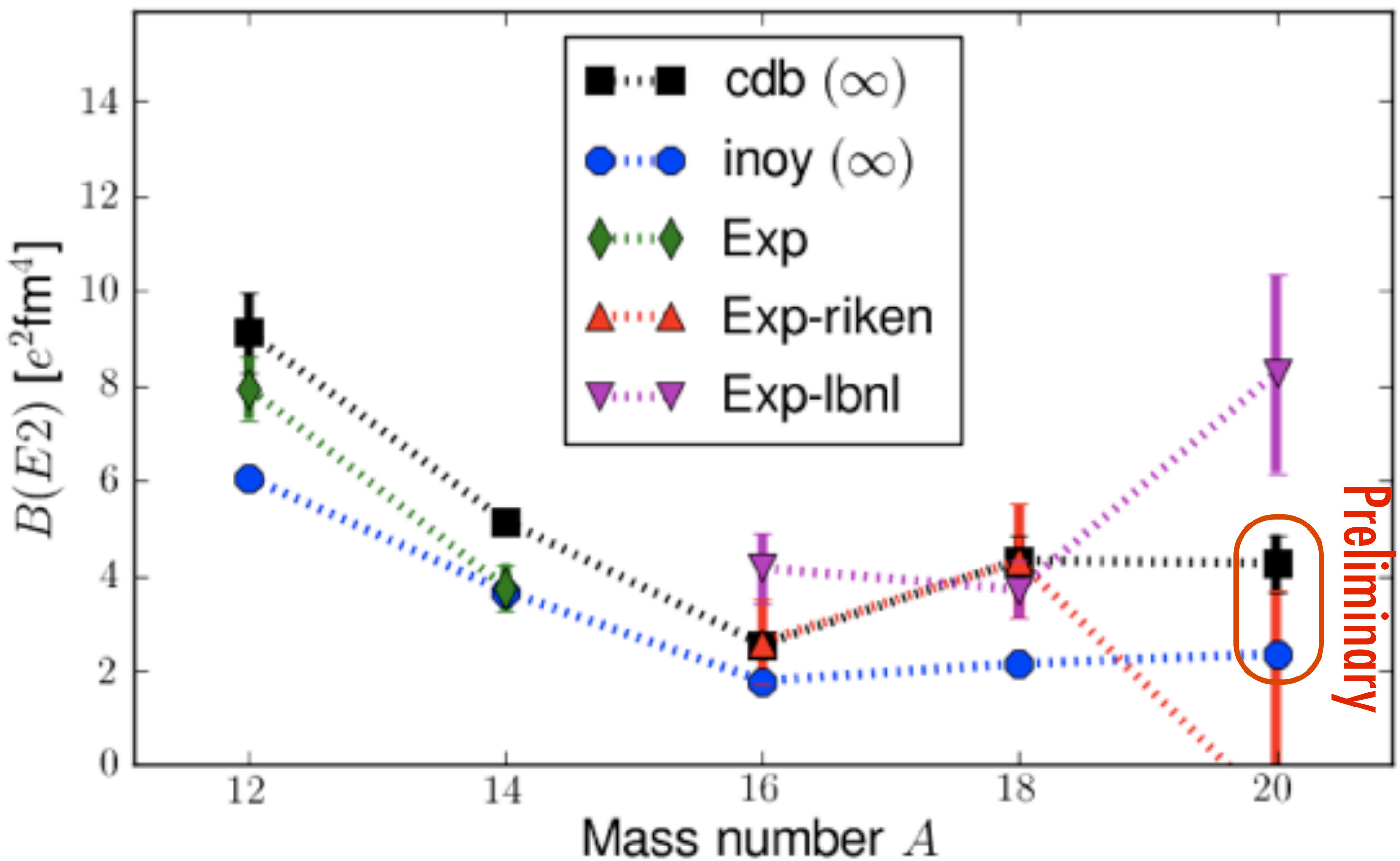
Theory (NCSM/NCSM-IT) campaign: $^{12\text{-}20}$C



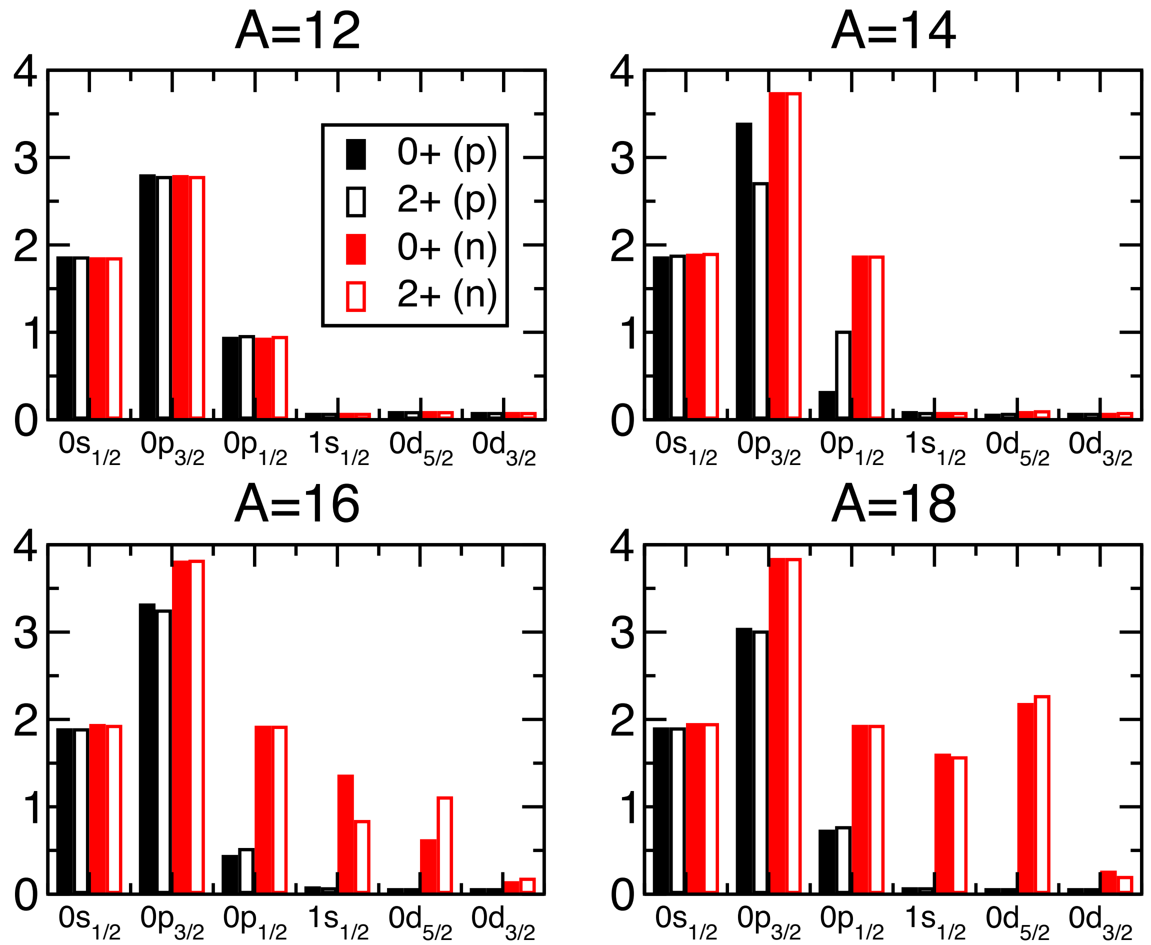
18C with CD-Bonn 2000. NCSM (filled) and IT-NCSM (open) results.

- $^{12\text{-}20}$C with NN interactions
- Full-space NCSM and IT-NCSM results
- Lee-Suzuki eff. int.
- Extrapolation scheme with multiple converging sequences

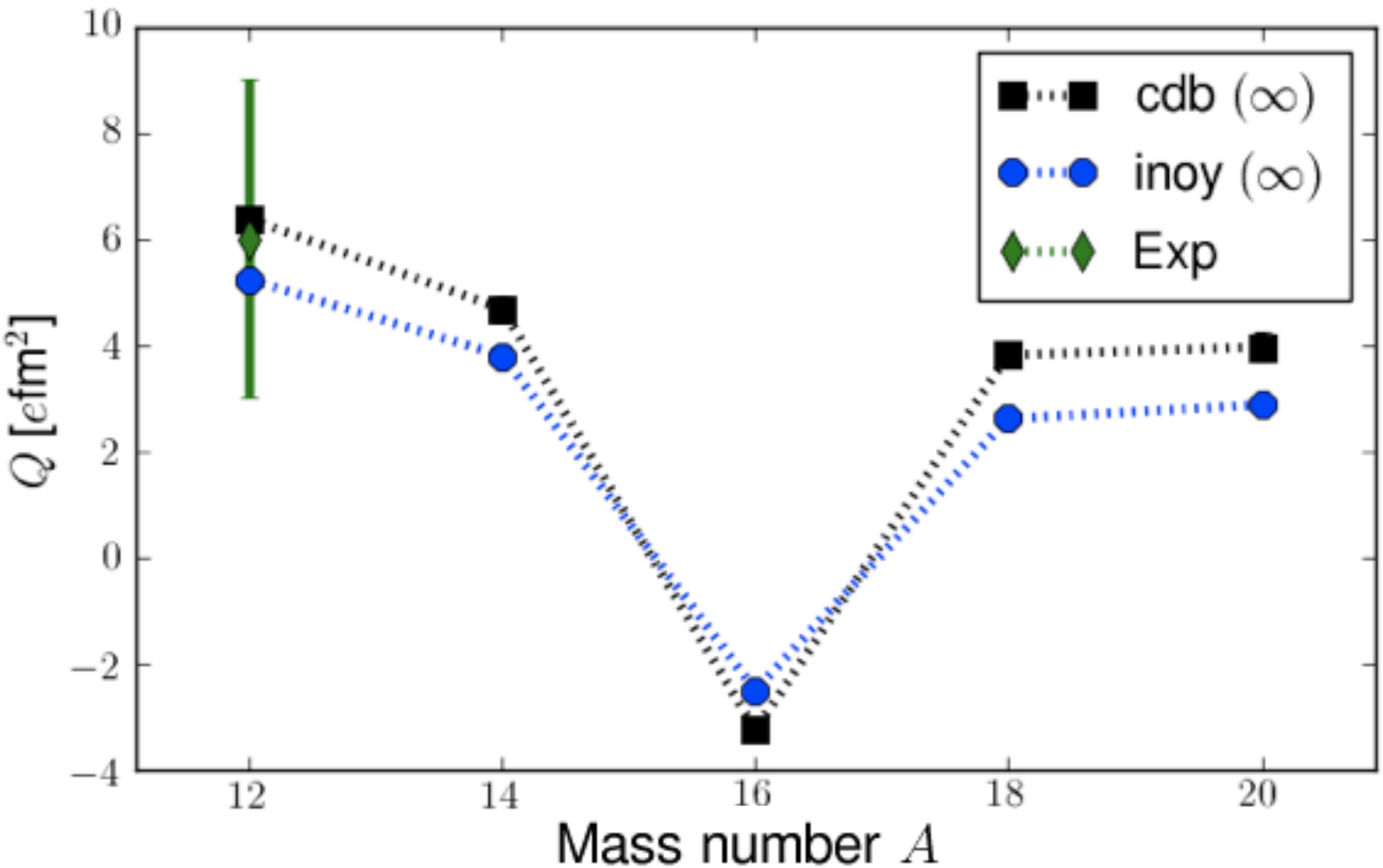
C isotopes: EM observables



Carbon occupation numbers



Carbon quadrupole moments



C isotopes: EM observables

- Overall, we find a consistent NCSM description of the $B(E2; 2^+_1 \rightarrow 0^+_1)$ dependence on the mass number for the whole Carbon isotopic chain.
- Predict sign changes of $Q(2^+_1)$ between different Carbon isotopes
- Predict differences up to an order of magnitude between the B(E2) transition strengths from the 0+ ground state to 2^+_1 and 2^+_2 states, respectively.

The continuum and correlations

Separation of scales

Despite the complexity of the many-body nuclear system we know the form and structure of the wave function at two limiting cases:

1. *When all relative distances are small the wave function can be well described with bound-state techniques. Many-body correlations are more important than cluster structures at small distances.*
2. *When the average distance between nucleons is large the wave function will only contain terms describing the relative motion of the fragments into which the nucleus can decay (real or virtual decay).*

Correlations and the continuum

- Change the many-body basis (Woods-Saxon s.p. states, Berggren basis,...)?
- Augment the many-body basis with a cluster basis to treat explicitly the relevant degrees of freedom (will have to deal with an overcomplete basis)?
- Use bound-state techniques to extract scattering information?
- For these studies there is a strong sensitivity to separation energies. Should we stay "realistic"?

Collaborators and sponsors

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