Uncertainty quantification in the Importance-truncated No-Core Shell Model

INT program 12-3

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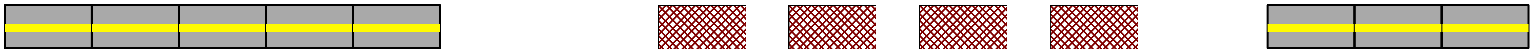
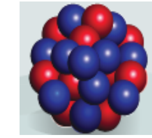
A road-map for the future

QCD





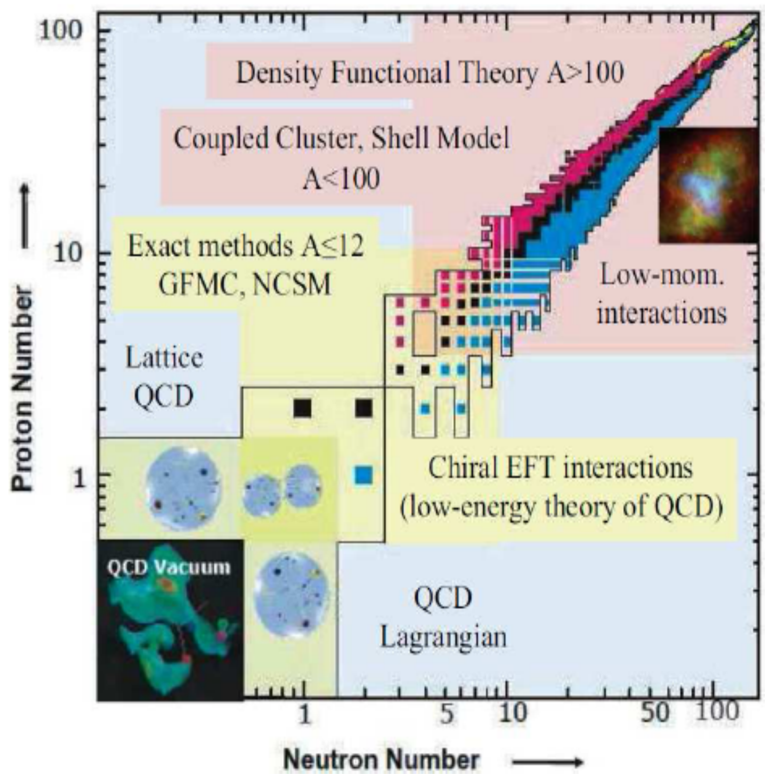
- **From the 2007 Nuclear physics long-range plan**

- What is the nature of the nuclear force that binds protons and neutrons into stable nuclei and rare isotopes?
- What is the origin of simple patterns in complex nuclei?
- What is the nature of neutron stars and dense nuclear matter?
- What is the origin of the elements in the cosmos?
- What are the nuclear reactions that drive stars and stellar explosions?

- **Use realistic interactions to probe nuclear forces in many-body systems.**
- **Can our ab-initio studies provide new insights for nuclear matter? Yes:neutron drops.**
- **Put light-ion reaction theory on a very solid footing (little to no approximations).**

Nuclear physics as seen today

- **Ab-initio techniques, e.g. NCSM and GFMC**
- **Lattice could give us LEC's(?)**
- **QCD coupling constant is small for high energy; but large for low energy.**



- **Repulsive core of nuclear forces makes many-body "difficult".**
- **EFT Lagrangian**

More detail next slide

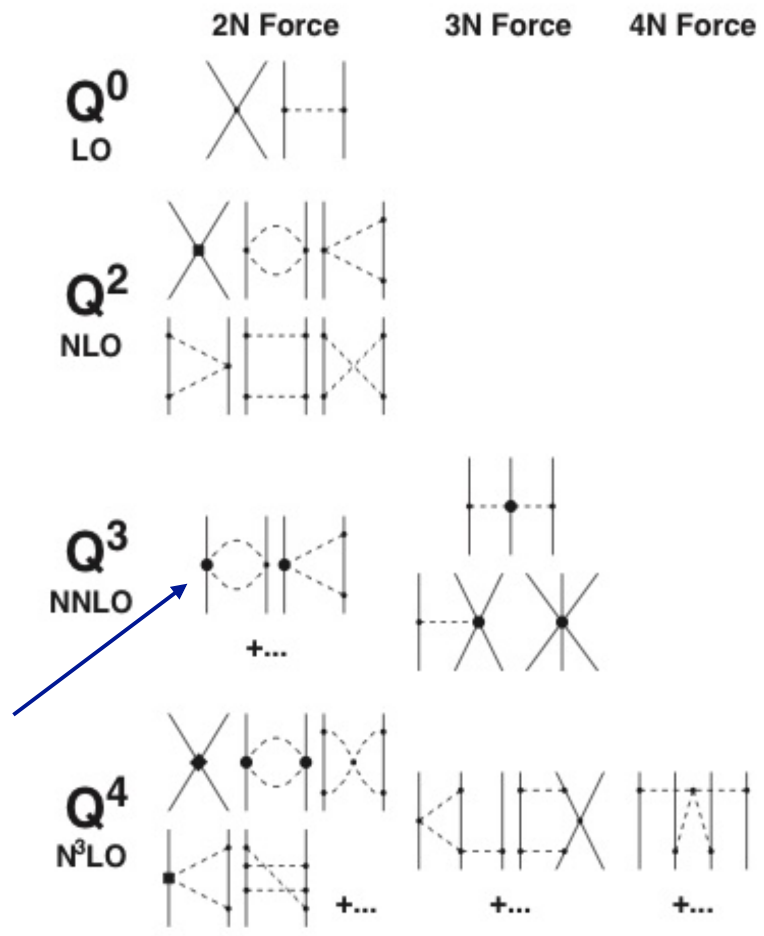
Credit: Achim Schwenk

- **QCD → EFT → Structure → Large CI → Inform DFT models?**

Lattice QCD **Effective interactions**

Chiral Effective Field theory
(Machleidt, Entem, Meissner,…)

- Low-energy theory of QCD, in which the degrees of freedom are now nucleons and pions.
- Based on the symmetries of QCD.
- Systematic power-expansion* (Weinberg), in powers of momentum over "QCD" scale.
- Short-range physics is integrated out, leading to Low-energy constants (LEC's), that need to be determined exp.
- Hierarchy of 2N, 3N and 4N forces.



No-Core structure calculations

PRL 99, 042501 (2007) PHYSICAL REVIEW LETTERS week ending 27 JULY 2007

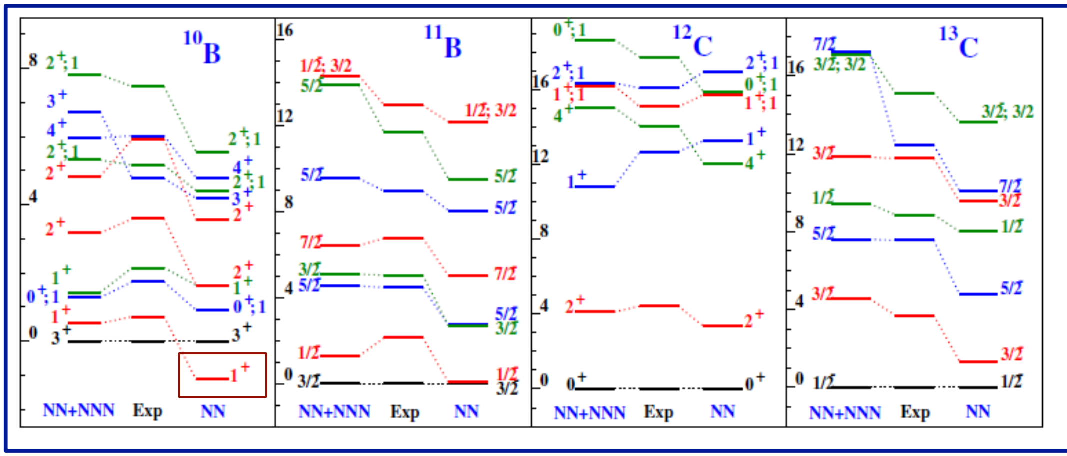
Structure of $A = 10$–13 Nuclei with Two- Plus Three-Nucleon Interactions from Chiral Effective Field Theory

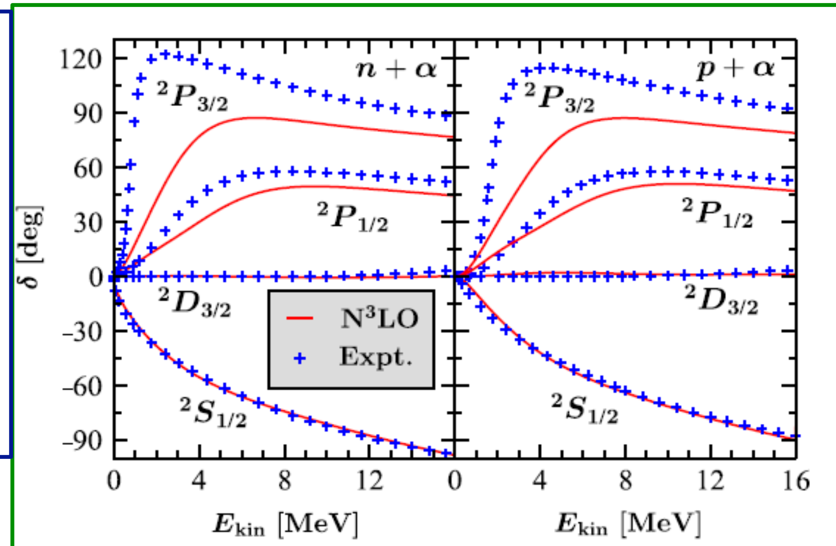
P. Navrátil,[1] V. G. Gueorguiev,[1,*] J. P. Vary,[1,2] W. E. Ormand,[1] and A. Nogga[3]

PRL 101, 092501 (2008) PHYSICAL REVIEW LETTERS week ending 29 AUGUST 2008

***Ab Initio* Many-Body Calculations of n-^{3}H, n-^{4}He, p-^{3,4}He, and n-^{10}Be Scattering**

Sofia Quaglioni* and Petr Navrátil+





- Three-nucleon force is essential to reproduce experimental data.

Where do we go from here?

A<16 gs states fairly well described by NCSM or GFMC calculations.

Beyond A>16, methods become intractable.

- **Bound-state techniques struggle to describe resonances or reactions.**

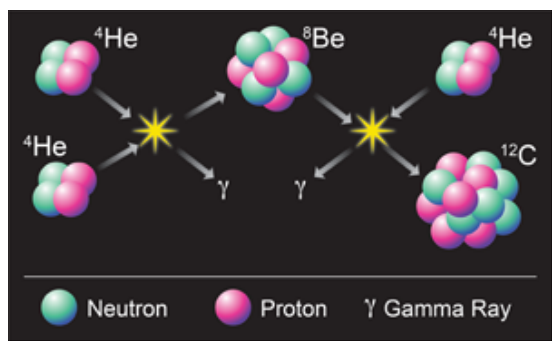
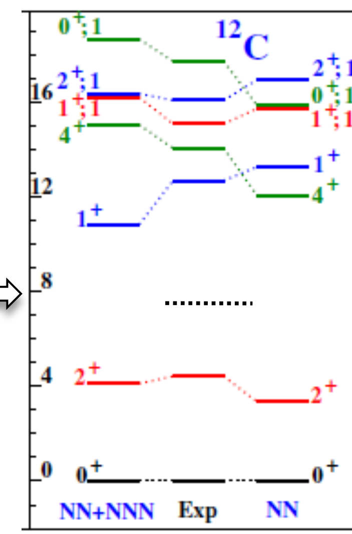


Image credit: Physics 4, 38 (2011)

Hoyle state

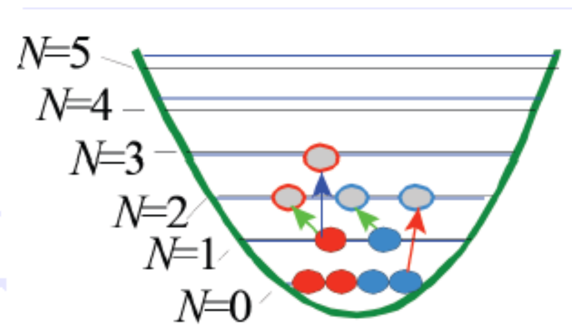


The No-Core Shell Model (NCSM)

Starting Hamiltonian is <u>translationally invariant.</u>

$$H_A = \frac{1}{A}\sum_{i<j}^{A}\frac{(\vec{p_i}-\vec{p_j})^2}{2m} + \sum_{i<j}^{A} V_{\mathrm{NN},ij}$$

NCSM has two parameters: Nmax and Ω



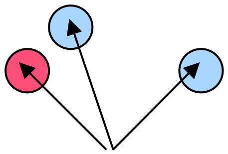
Provided interaction is "soft" we don't need to do any renormalization of interaction,

It's that "simple".

If we now use a single-particle basis, we have to remove the spurious CM states.

Advantage in m-scheme: Antisymmetry is easy to implement.

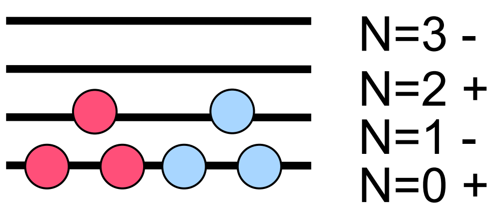
Disadvantage in m-scheme: Number of basis states is much larger than JT basis



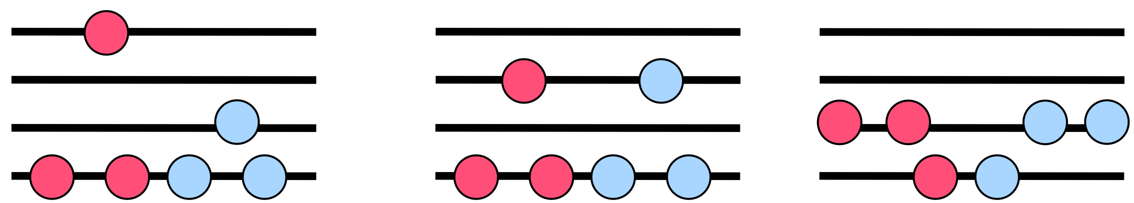
The NCSM basis

- For heavier nuclei (A > 5) we work with Slater determinants → single particle states of Harmonic Oscillator.

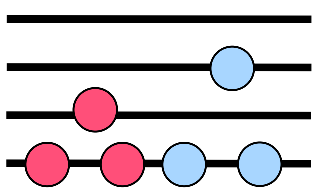
Li-6



Unperturbed cfg.



Valid Nmax=2 cfgs for positive parity states.



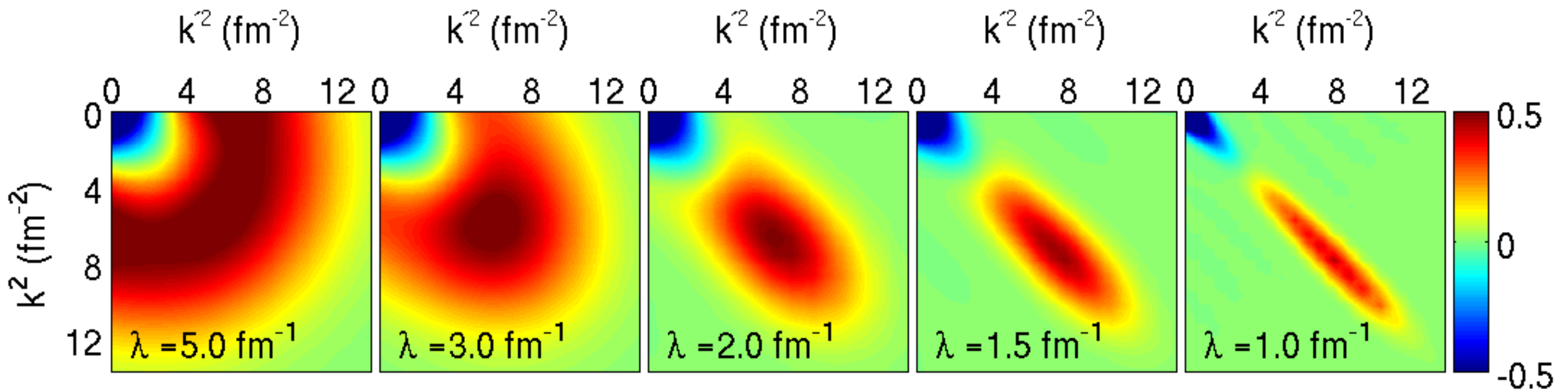
Parity is negative!

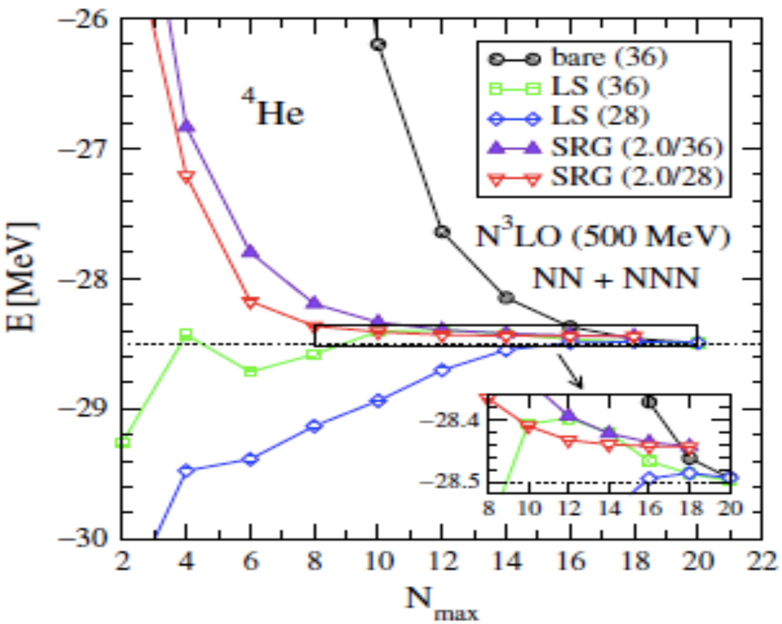
- **The basis is truncated on an 'energy-quanta' level. This is required to have exact factorization of CM and intrinsic states.**
- **Atomic calculations use a different basis truncation. No need to consider CM.**

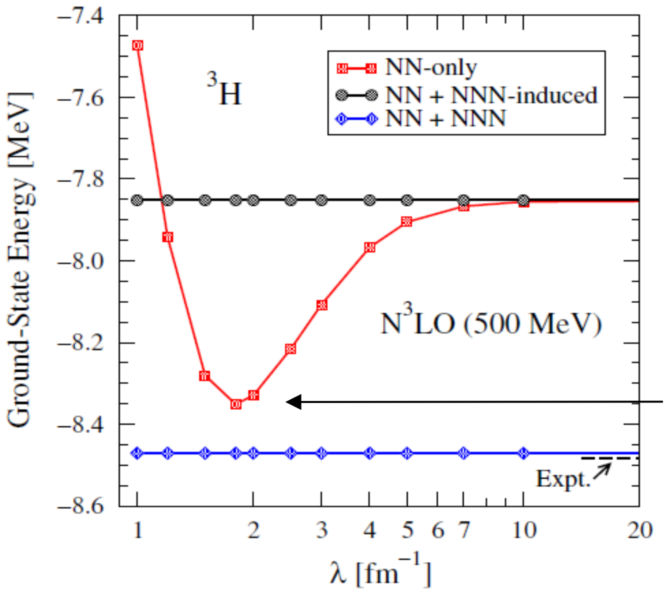
SRG evolved interactions

PRL **103**, 082501 (2009)
Jurgenson et al

$$H_\lambda = U_\lambda H_{\lambda=\infty} U_\lambda^\dagger \qquad \frac{dH_\lambda}{d\lambda} = -\frac{4}{\lambda^5}[[T, H_\lambda], H_\lambda]$$

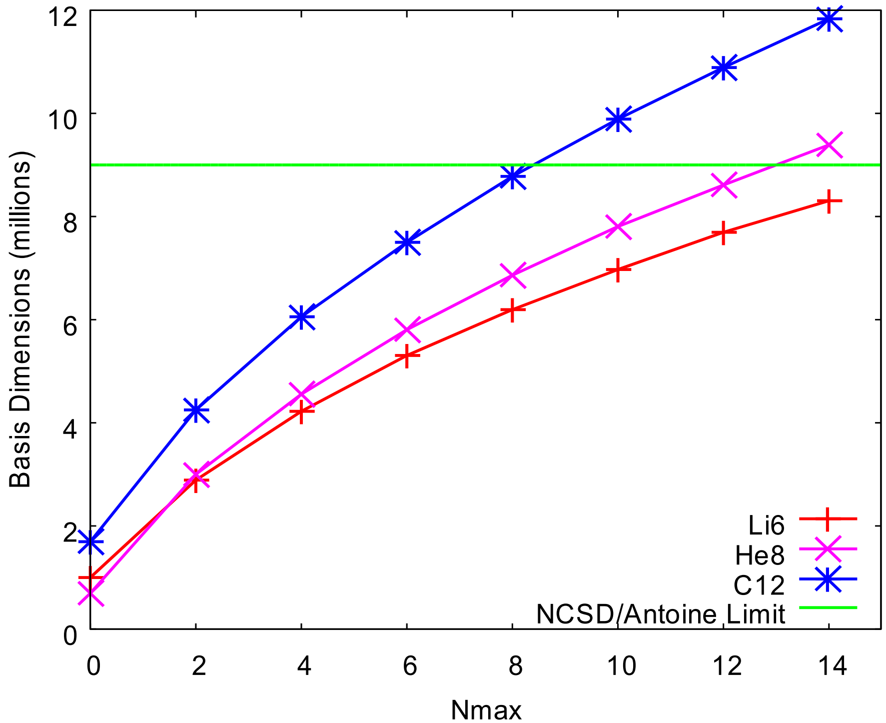






NN force „acts“ as though it is a NNN force. Closest to 3N at about 1.5-2.0/ fm

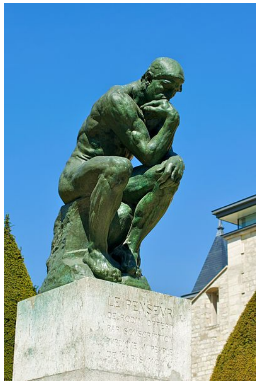
M-scheme basis dimensions



- Size of the m-scheme basis grows rapidly with increasing Nmax.
- Switch to HO JT coupled basis? Possibly, but painful.
- Difficulties with such an approach, e.g. Jacobi co-ordinates or rewrite codes.
- Even if techniques like SRG potentials are used, you still can't perform converged calculations all the time.

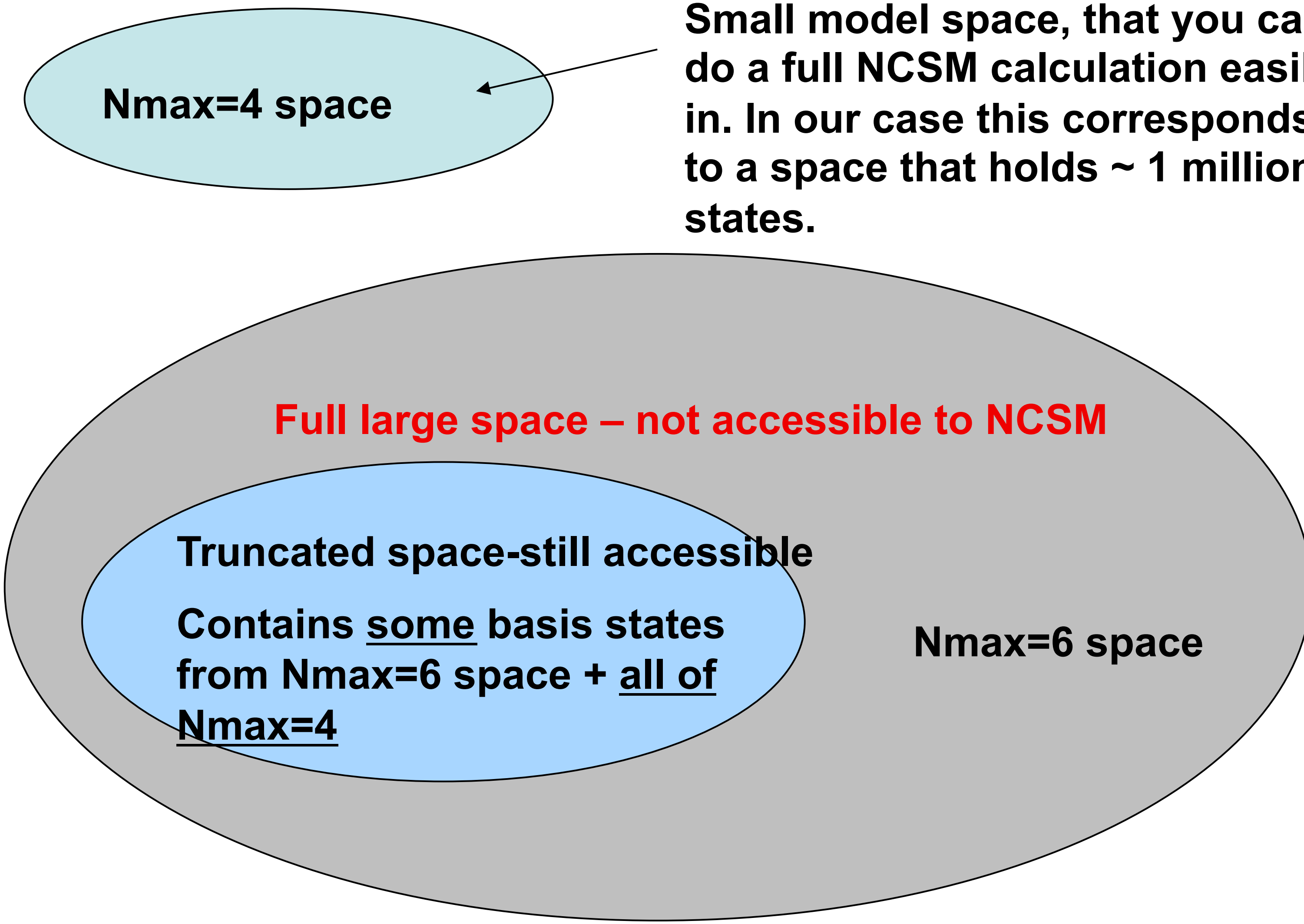
- **But why stick with the HO basis?**
- **Only basis where center of mass and intrinsic states can be completely decoupled.**

Questions?



Importance-truncation in pictures

Small model space, that you can do a full NCSM calculation easily in. In our case this corresponds to a space that holds ~ 1 million states.



Formalism of Importance truncation.

- **First order multi-configurational perturbation theory gives as the correction to the wavefunction,**

$$|\Psi^{(1)}\rangle = -\sum_{\nu \notin \mathcal{M}_{\text{ref}}} \frac{\langle\Phi_\nu|W|\Psi_{\text{ref}}\rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}|\Phi_\nu\rangle$$
$$= -\sum_{\nu \notin \mathcal{M}_{\text{ref}}} \frac{\langle\Phi_\nu|H|\Psi_{\text{ref}}\rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}|\Phi_\nu\rangle.$$

By making the choice that

$$W = H - H_0$$

We find that H_0 only acts on reference state slater determinants, and does not connect you to any Φ.

IT in NP developed by R. Roth: PRC 79, 064324 (2009)

Importance truncation schematically

$\langle \Phi_\nu |$?

Nmax=6
Next-larger space

Nmax=4
Reference space

$$\kappa_\nu = \frac{| \langle \Phi_\nu | H | \Psi_{ref} \rangle |}{\epsilon_\nu - \epsilon_{ref}}$$

Typically choose κ ~ 10^{-5}

$$\Delta_{\text{excl}}(\kappa_{\min}) = -\sum_{\nu \notin \mathcal{M}(\kappa_{\min})} \frac{|\langle \Phi_\nu | H | \Psi_{\text{ref}} \rangle|^2}{\epsilon_\nu - \epsilon_{\text{ref}}}$$

$\langle \Phi_\nu |$

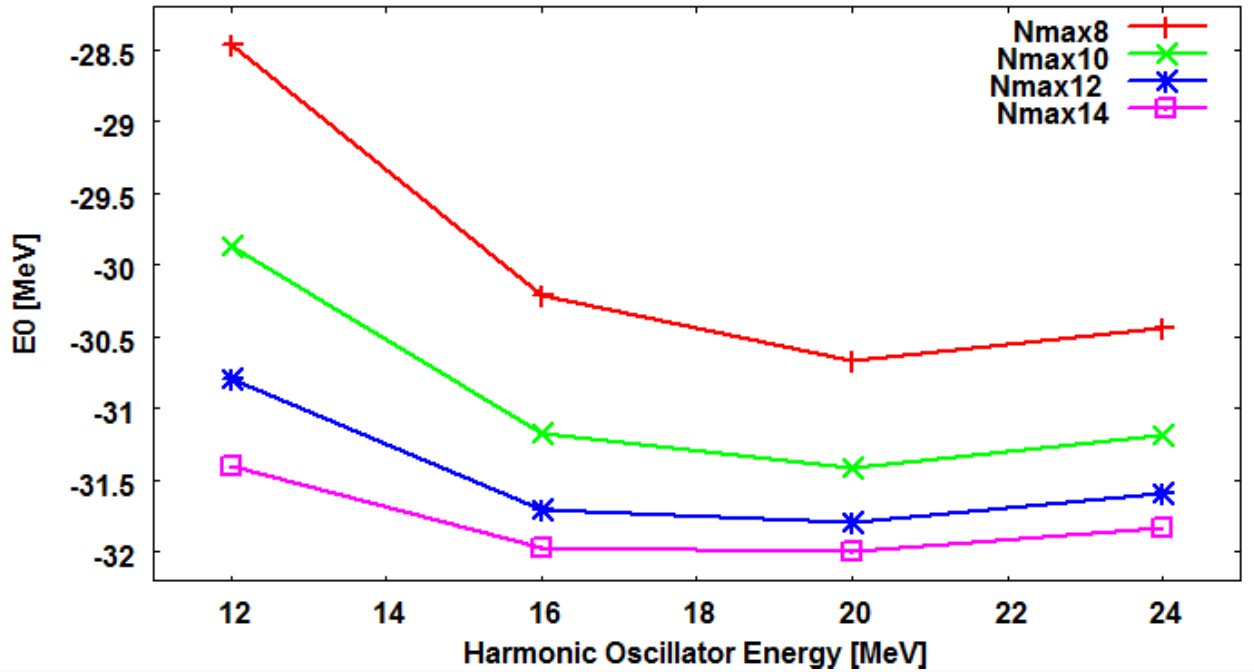
Nmax=6
Kept states

Nmax=4

Test calculations

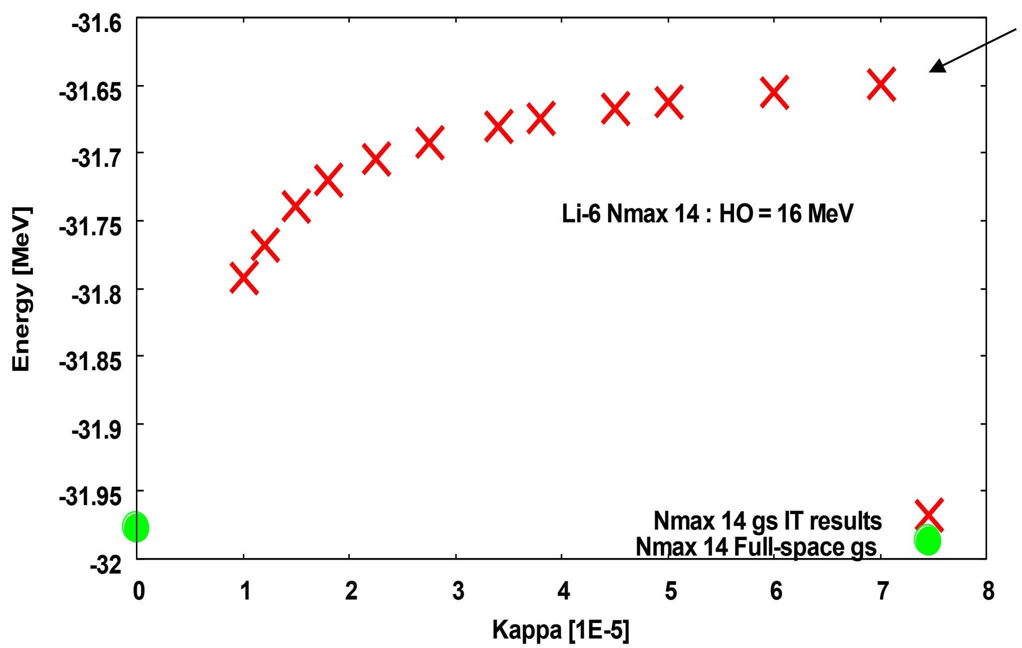
- Use Lithium-6 as a good test case; more complex than He4 but not as challenging as mid p-shell nuclei (exact up to Nmax=14)
- Use SRG N3LO two-body interaction.
- Importance truncation always starts at Nmax=6 and bootstraps up to Nmax=14.
- Determine error from various aspects of the fitting procedure (next few slides).

- **Check dependence on Nmax, HO energy, SRG momentum-decoupling scale and excited states.**



A typical IT-NCSM calculation

- Vary kappa and calculate gs for each value. Later used in extrapolation to kappa=0.



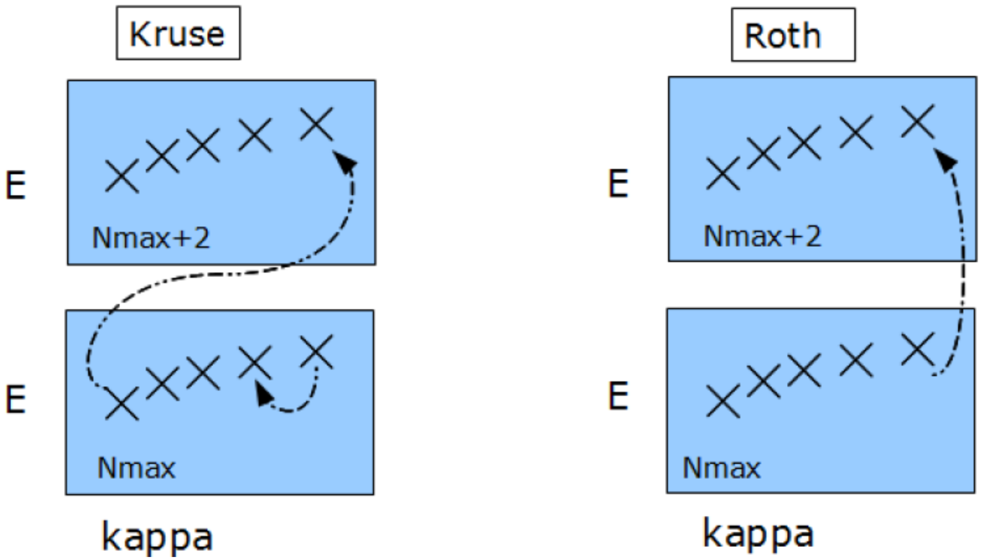
$$\kappa_\nu = \frac{|\langle \Phi_\nu | H | \Psi_{ref} \rangle|}{\epsilon_\nu - \epsilon_{ref}}$$

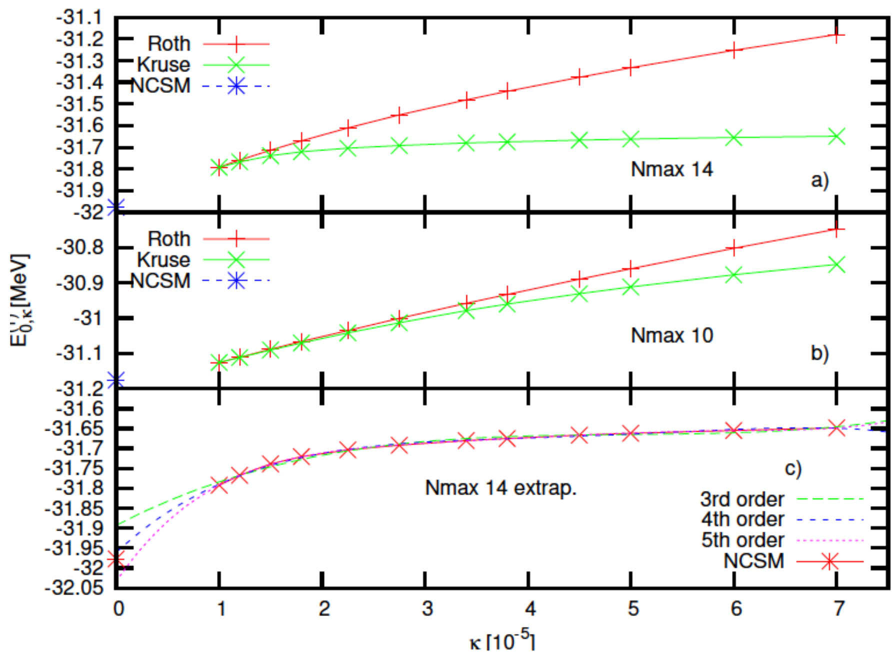
- **When gs is calculated using only the above formula: "1st order".**

- **Obviously, we just fit some polynomial(s) to these points (and pray).**
- **Note: results are preliminary in what is to follow.**

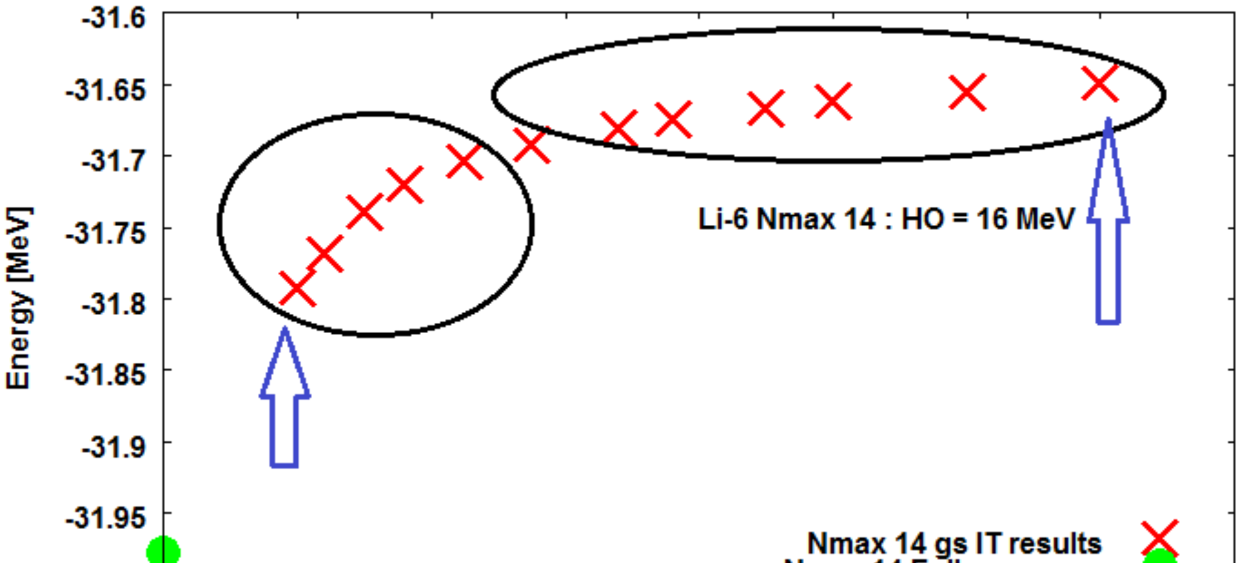
A quick note for the experts:

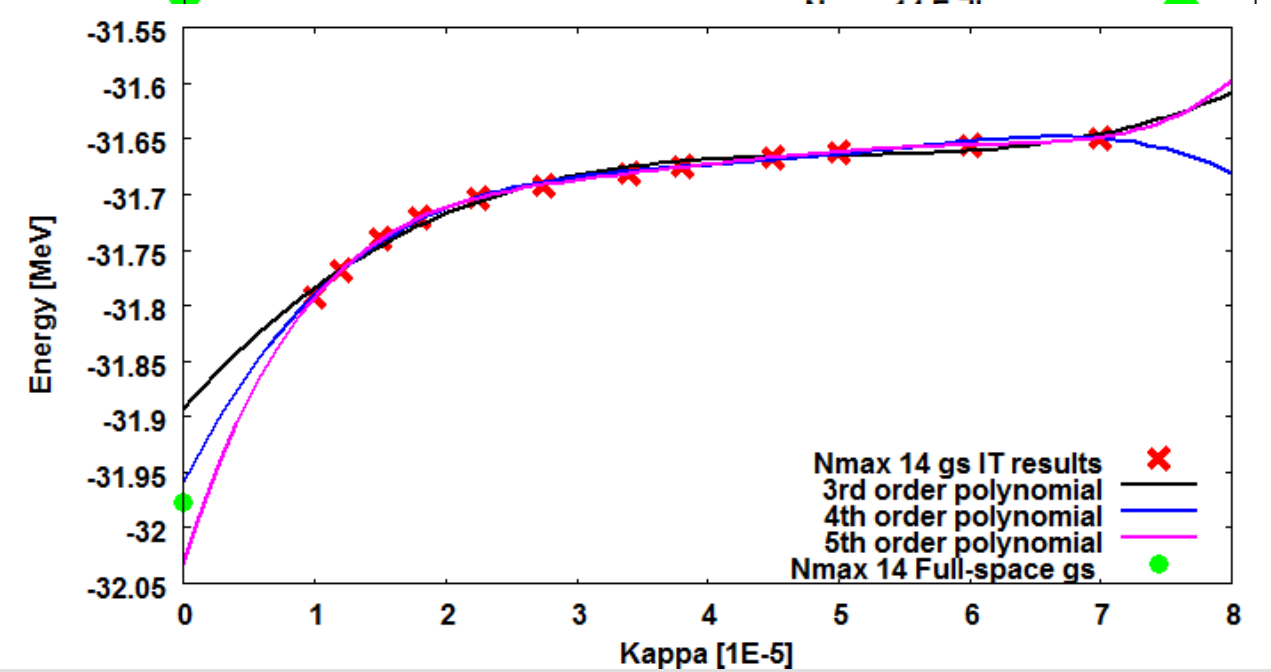
My calculations differ from Robert Roth:
1) The order of operations as shown below,
2) There is no truncation on the reference wavefunctions.





Possible ways to fit points





Fit is sensitive to *range* of kappa and the *spacing* of the points.

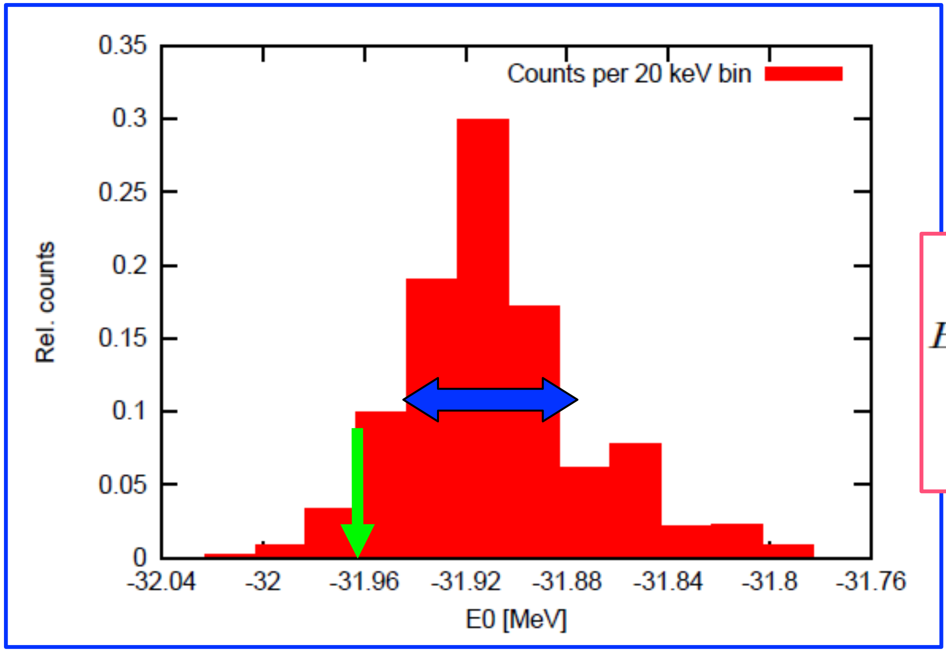
Three *polynomials* were fitted:

Cubic, 4th and 5th.

The spread is about 150 keV between 3rd and 5th order poly.

Characterizing the grid choice

- Do a combinatorial fit (i.e. choose 7/12 of the points), and calculate median and standard deviation. Repeat for 8,9,10 of 12 combinations.



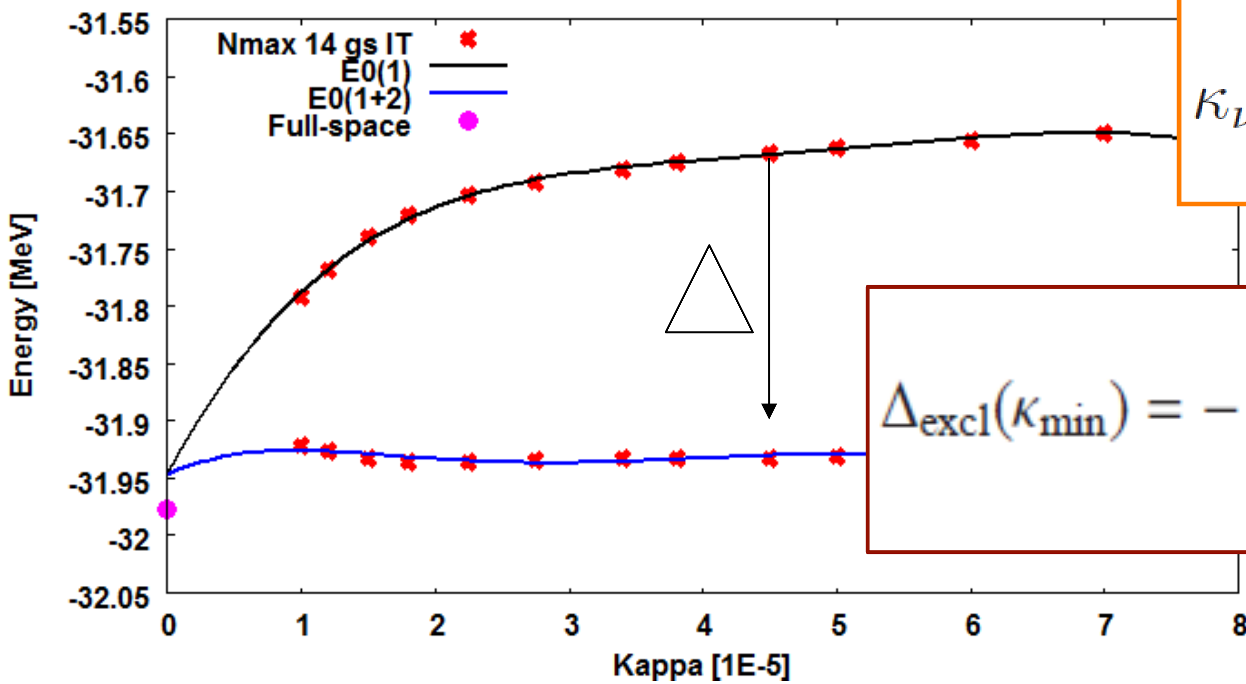
- **Error from fits determined by these two equations.**

$$E_{0,\kappa=0} = \frac{E_{0,\kappa=0}^{\binom{12}{7}} + E_{0,\kappa=0}^{\binom{12}{8}} + E_{0,\kappa=0}^{\binom{12}{9}} + E_{0,\kappa=0}^{\binom{12}{10}}}{4}$$

$$\sigma = \frac{\sigma_{\binom{12}{7}} + \sigma_{\binom{12}{8}} + \sigma_{\binom{12}{9}} + \sigma_{\binom{12}{10}}}{4}$$

- **Above: Distribution of predicted gs energies for Nmax=14 using the cubic polynomial (12 choose 7 points).**
- **Std Dev = 36 keV (blue), exact value = -31.977 MeV (green)**

Constrained fits (2^{nd} order)

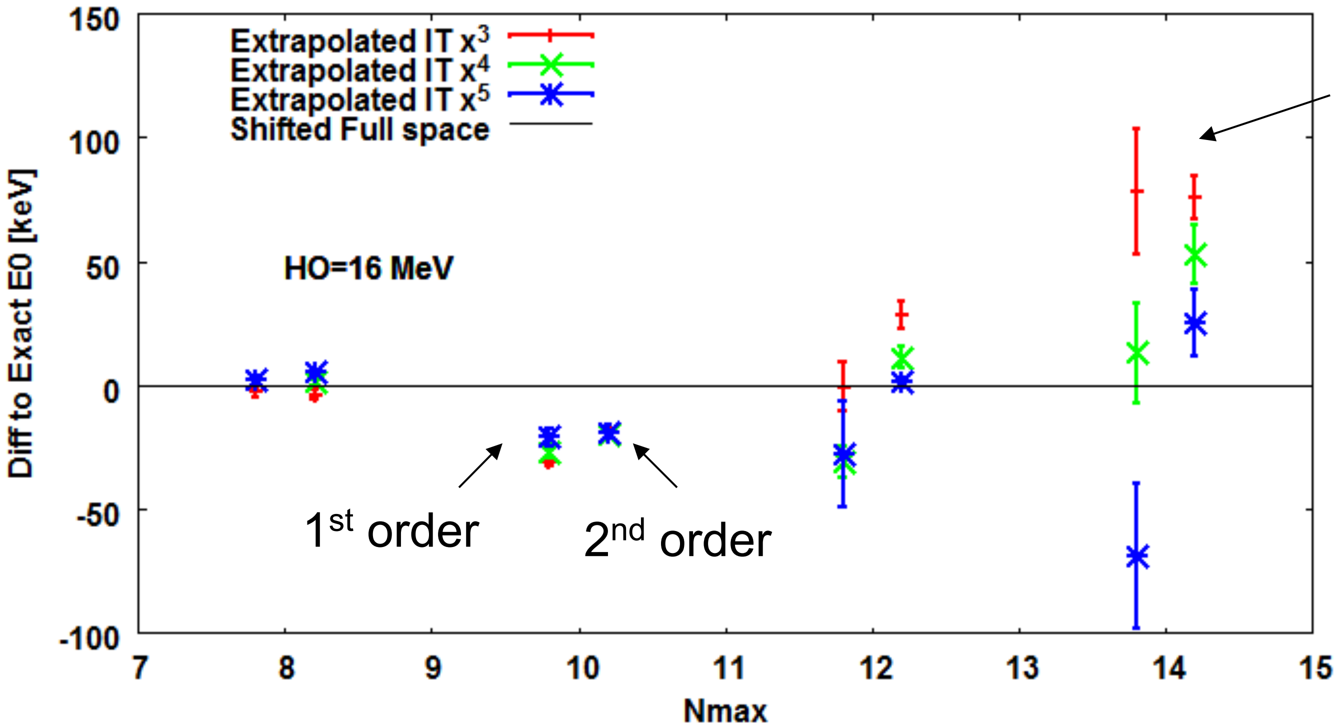


$$\kappa_\nu = \frac{|\langle \Phi_\nu | H | \Psi_{ref} \rangle|}{\epsilon_\nu - \epsilon_{ref}}$$

$$\Delta_{\text{excl}}(\kappa_{\min}) = -\sum_{\nu \notin \mathcal{M}(\kappa_{\min})} \frac{|\langle \Phi_\nu | H | \Psi_{\text{ref}} \rangle|^2}{\epsilon_\nu - \epsilon_{\text{ref}}}$$

- **Constrain the fit in such a way that both curves intercept at k=0. Argument: Makes physical sense, and provides stability.**
- **However, 2^{nd} order curve does not seem variational.**
- **1^{st} order curve *is* variational (thus monotonically decreasing).**

Nmax dependence



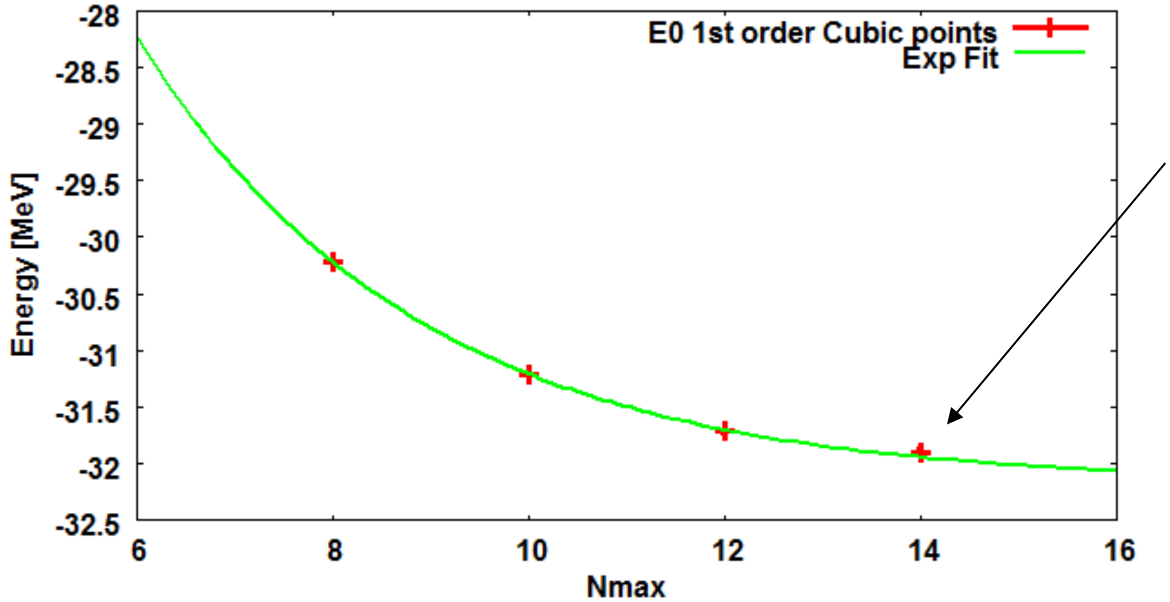
Nmax 14:
IT space ~ 9 mil,
Full space ~ 211 mil.

Exact value (relative)

- Above plot shows the associated error bars from the fitting procedure, for various polynomials. The left points correspond to 1st order results; the right points correspond to 2nd order results.
- The spread is larger for larger Nmax values (expected).

Extrapolating to Nmax infinity

- The final step is to take a series of Nmax gs energies, and extrapolate to Nmax infinity, using an exponential decay.

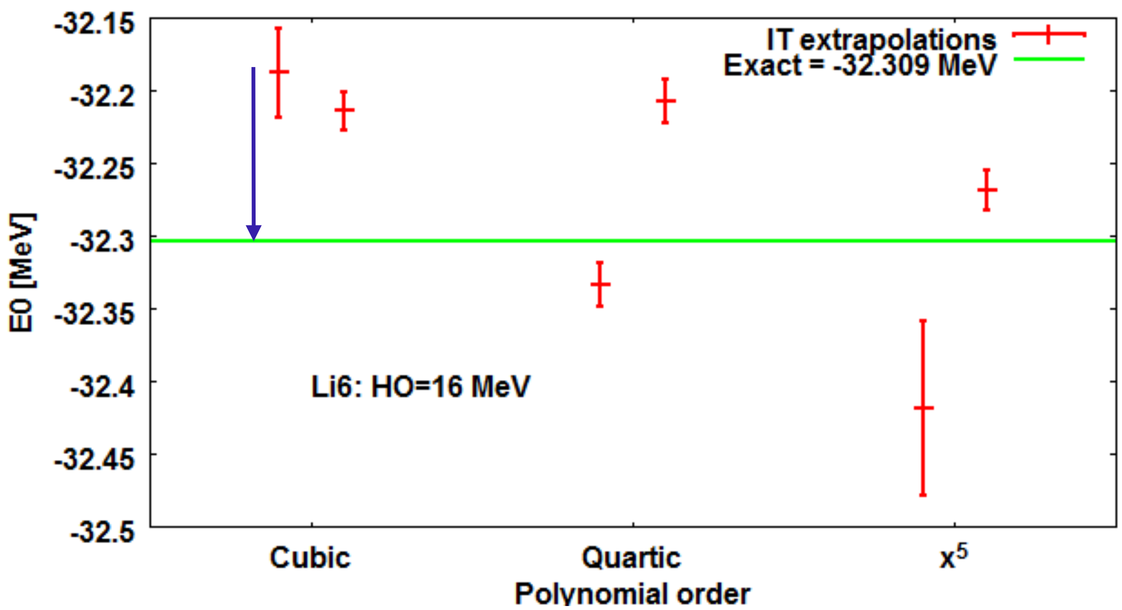


- This fit takes into account the error from the extrapolation procedure.

- Above: Fit is done for 1st order cubic IT-NCSM results.
- Predicted E0 = -32.188 ± 0.031 MeV (31 keV).
- But how does this compare to the "exact" results?

Comparison for all polynomials

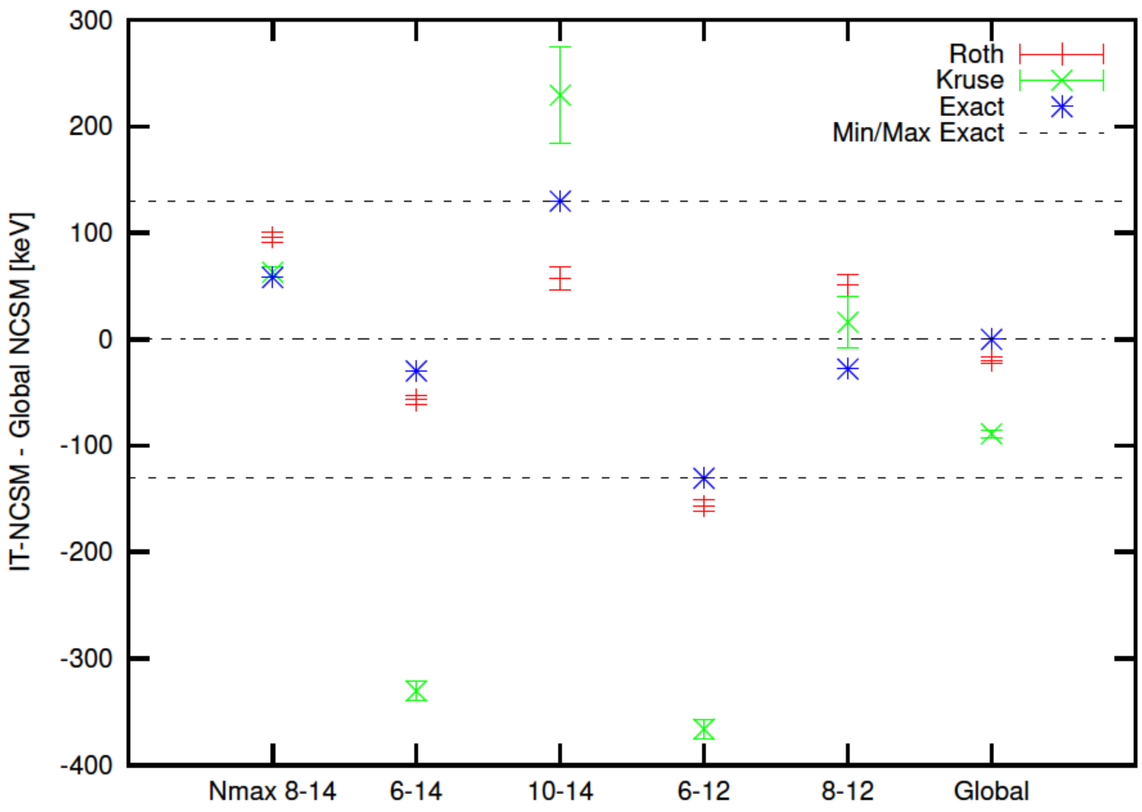
- Extrapolate to Nmax infinity for all polynomials and both 1st and 2nd order data sets.



- **Errors on extrapolations typically 30-50 keV.**
- **"Miss" the exact result by about 100 keV.**

- **100-150 keV total "error" from true result is a good rule of thumb (other results in Li6 confirm this).**
- **Note: Result specific for *one* HO value, and for *this* particular nucleus (Li6).**

Extrapolations to Nmax → infinity.



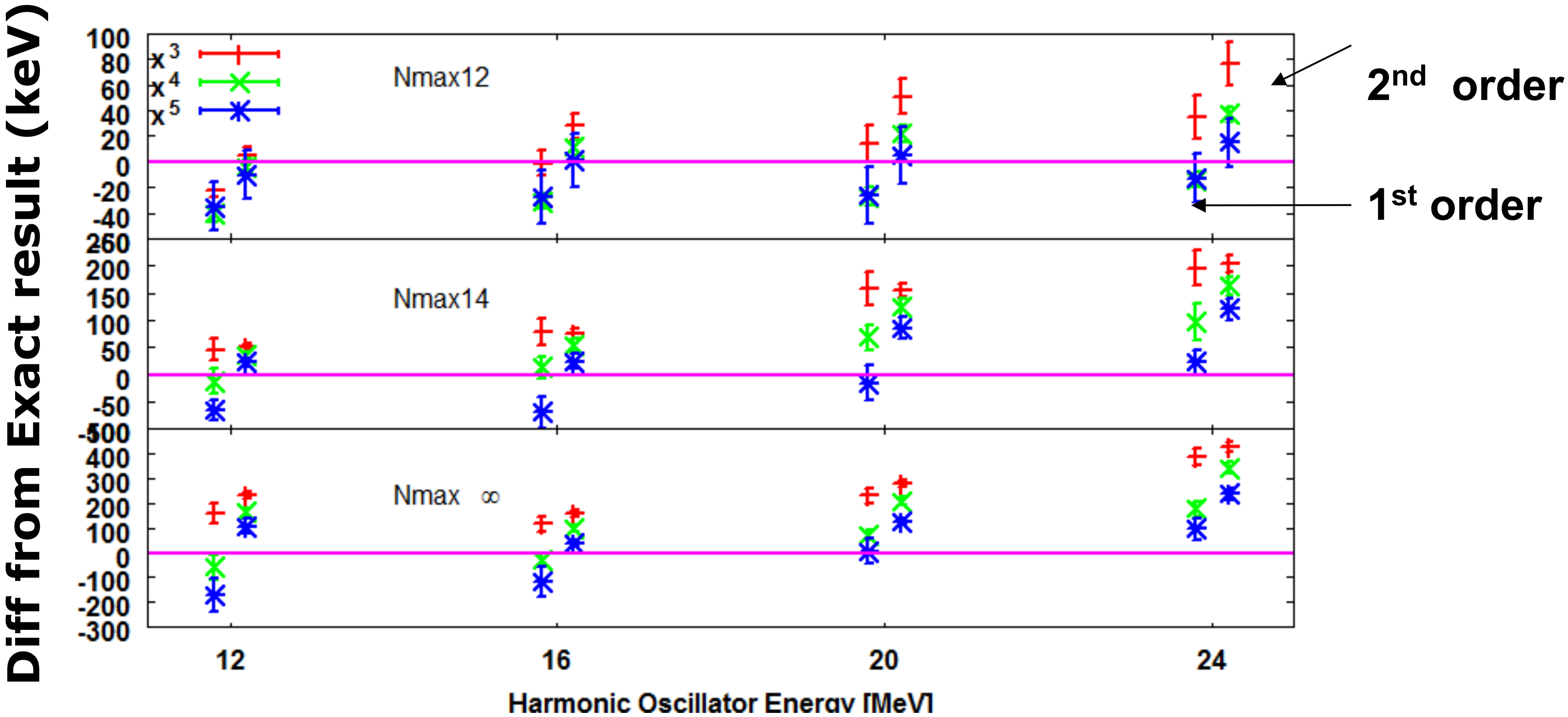
Extrapolations to infinite basis are sensitive to choice of Nmax points.

"Error" in these extrapolations are the largest concern.

We need to think about better ways (or quantify) uncertainties for these extrapolations.

HO Dependence

- Extrapolations to gs for Nmax 12,14 and Nmax infinity.



- **Note there is a systematic drift away from the exact result, indicating a dependence on HO frequency.**
- **The same pattern is seen for SRG λ = 1.5/fm.**

Truncation selection criteria

- Consider how the basis states are selected.

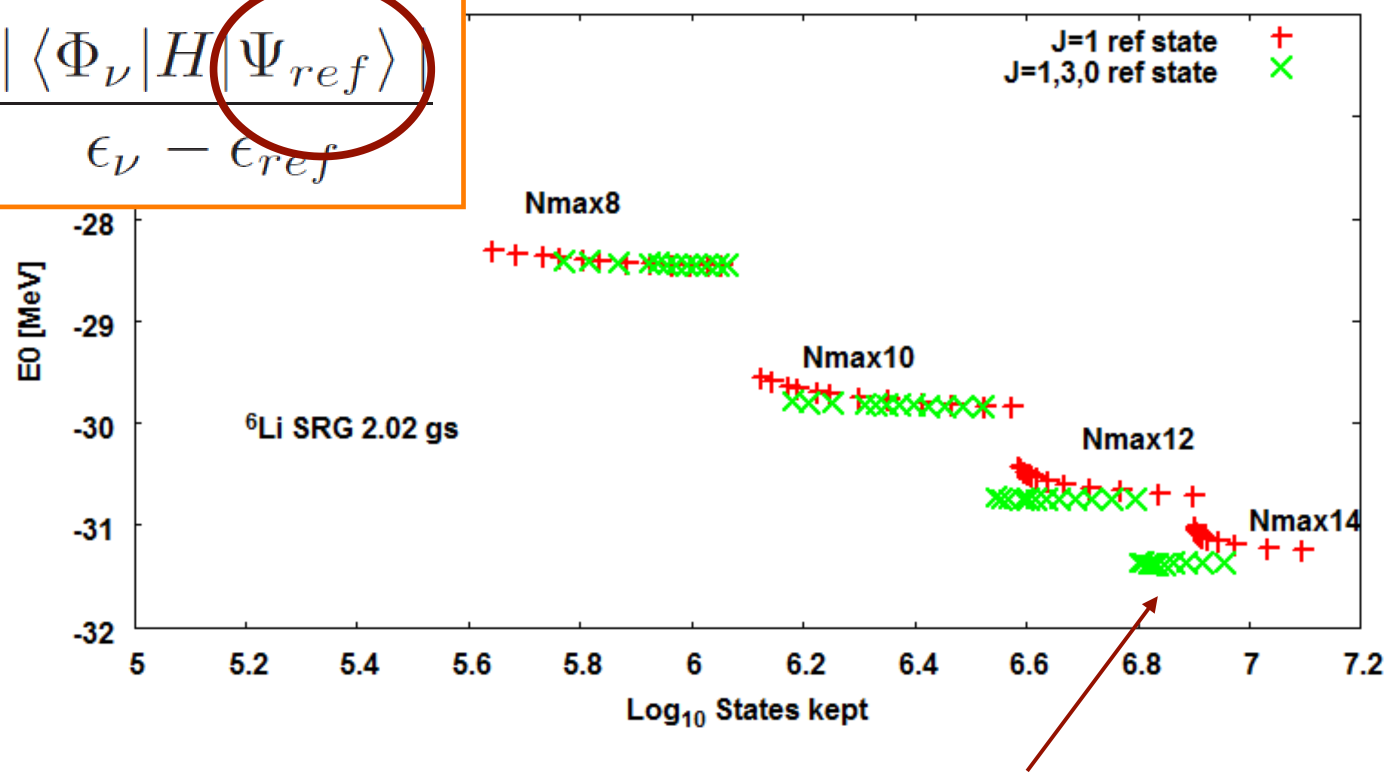
$$\kappa_\nu = \frac{|\langle \Phi_\nu | H | \Psi_{ref} \rangle|}{\epsilon_\nu - \epsilon_{ref}}$$

- **Hamiltonian matrix element has HO dependence. Perhaps has some effect on selection of state?**
- **Energy denominator is proportional to HO value, since the energies are taken at the single-particle level.**
- **E ~ (2n + l)hbar*Omega.**
- **Ref E = Lowest unpertubed cfg**

- **Thus, as HO increases, matrix element in effect needs to become larger to still have the basis state kept.**
- **As Nmax increases, denominator increases, thus less states kept at higher Nmax (reasonable selection criteria).**

Physical effect of using multiple reference states

$$\kappa_\nu = \frac{|\langle \Phi_\nu | H | \Psi_{ref} \rangle|}{\epsilon_\nu - \epsilon_{ref}}$$



- With a larger value of kappa, the multiple reference states seem to select the basis states for the gs much better than using just the gs as a reference state.

Conclusions

- Nuclear structure is calculated from realistic interactions, which can be traced back to the symmetries of QCD.
- First-principles techniques, such as the No-Core Shell model or Green's function Monte Carlo, have shown the importance of 3N forces (amongst other things).
- Modifications of the techniques, such as importance truncation, allow for even larger calculations, *but,* you must provide an error for the calculation.
  - Uncertainty quantification:
  - Make use of data-sets to provide uncertanties based on statistical estimates.
  - Dependence on HO energy.
  - Multiple reference states improve basis state selection.
  - Nmax → infinity extrapolations could have large error (250+ keV).

People I am in debt to

- **Bruce Barrett**

- **Petr Navratil**

- **Sid Coon**

- **Eric Jurgenson**

- **Erich Ormand**

- **Bira van Kolck**

- **Hank Miller**

- **Sofia Quaglioni**