Importance-truncation:
A discussion for workshop participants

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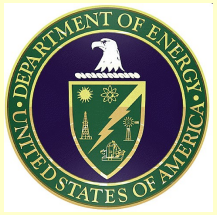


No Core Shell Model

Starting Hamiltonian

$$H = \sum_{i=1}^{A} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j}^{A} V_{NN}(\vec{r}_i - \vec{r}_j) + \left(+ \sum_{i<j<k}^{A} V_{ijk}^{3b} \right)$$

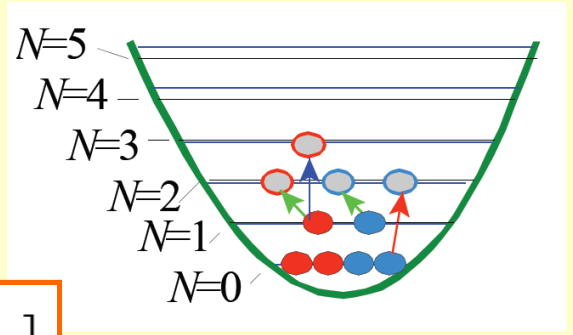
Realistic NN and NNN potentials

Coordinate space – Argonne V18, AV18', CD-Bonn, chiral N^{3}LO,

Momentum space – NNN Tucson - Melbourne, NNN chiral N^{2}LO

Binding center-of-mass HO potential (Lipkin 1958)

$$\frac{1}{2} Am\Omega^2 \vec{R}^2 = \sum_{i=1}^{A} \frac{1}{2} m\Omega^2 \vec{r}_i^{\,2} - \sum_{i<j}^{A} \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2$$



$$H^{\Omega} = \sum_{i=1}^{A} \left[\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2} m\Omega^2 \vec{r}_i^{\,2} \right] + \sum_{i<j}^{A} \left[V_{NN}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right]$$

<HO|$V_{NN}(\Omega,A)$|HO>

Two-body cluster approximation

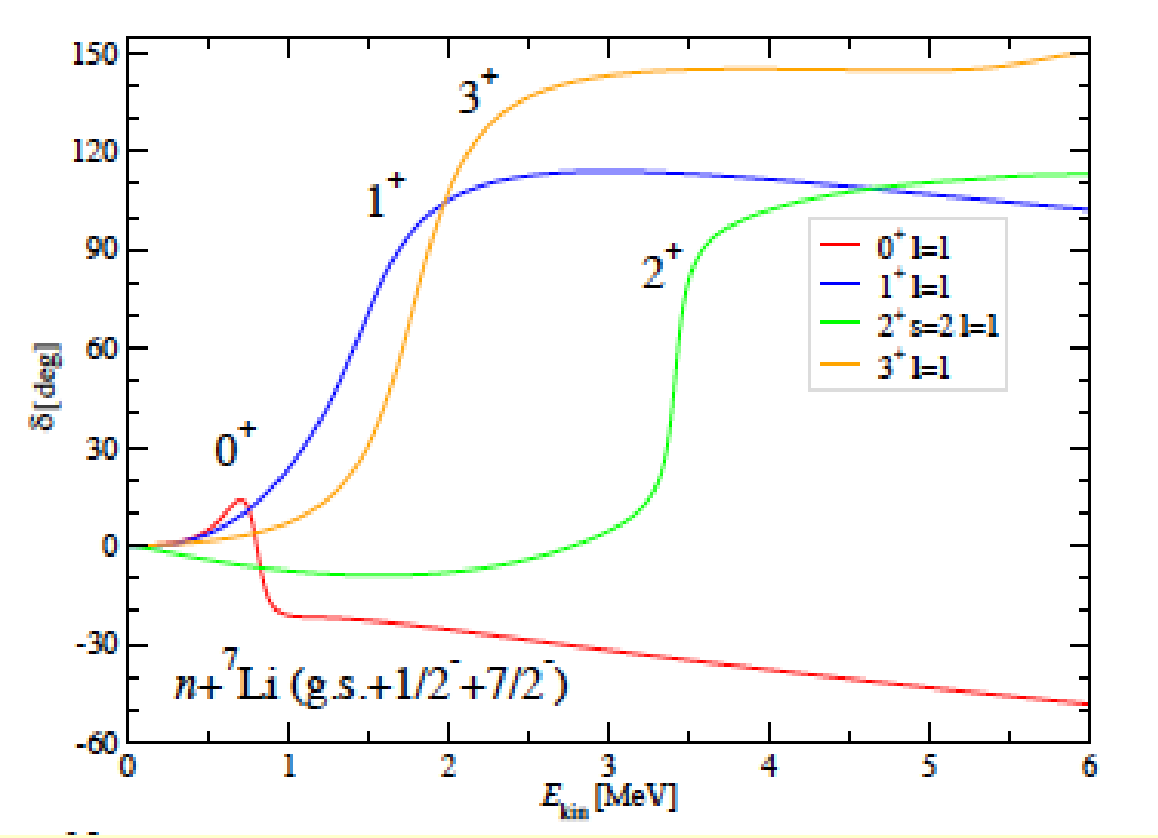
$$H_2^{\Omega} = \sum_{i=1}^{2} \left[\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2} m\Omega^2 \vec{r}_i^{\,2} \right] + \sum_{i<j}^{2} \left[V_{NN}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right]$$

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

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

NCSM/RGM reaction studies

- **Great interest in extended or halo systems. Role of 3-body forces etc.**
- **Nucleon-Nucleus reactions and extensions have recently been done, although, with some help from SRG potentials and Importance truncation calculations.**
- **However, basis size limitations is a problem and requires more work.**



P. Navratil, R. Roth, S. Quaglioni
Phys. Rev. C 82, 034609 (2010)

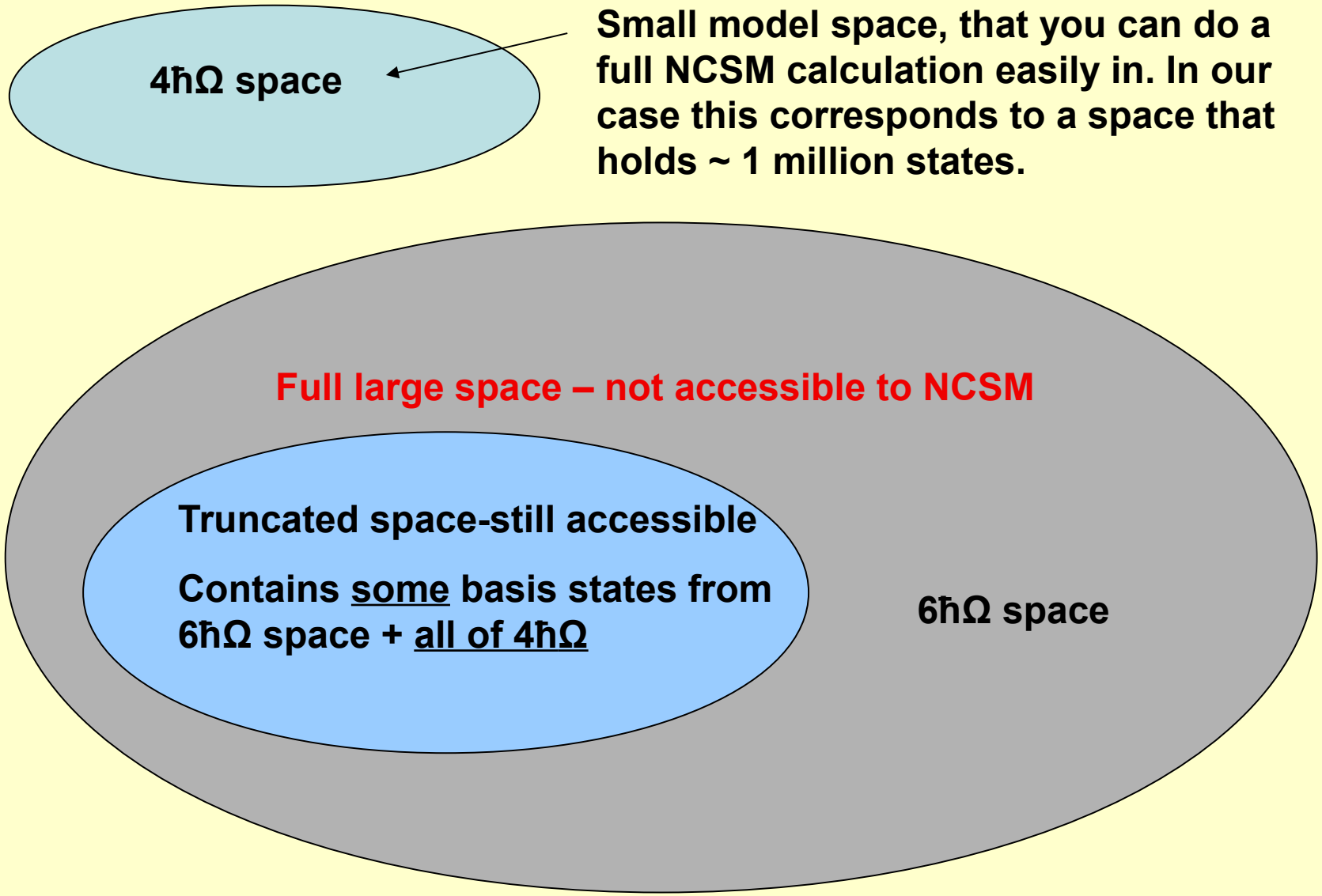
Two recent achievements aids NCSM/RGM calculations.

- The main problem is exponential growth in the basis size, in order to reach converged results. Current technology allows for a basis size on the order of 10^9 (m-scheme), although 50 million is already difficult (with our code).

- "Softened" phase shift equivalent potentials: Improve the convergence rate over previous methods (i.e. smaller model spaces).

- Importance truncation: Select only those basis states that are most relevant to finding the "optimal" state wavefunction, be it for the ground or excited states.

The idea of Importance Truncation



Formalism of Importance truncation.

- First order multi-configurational perturbation theory gives...

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

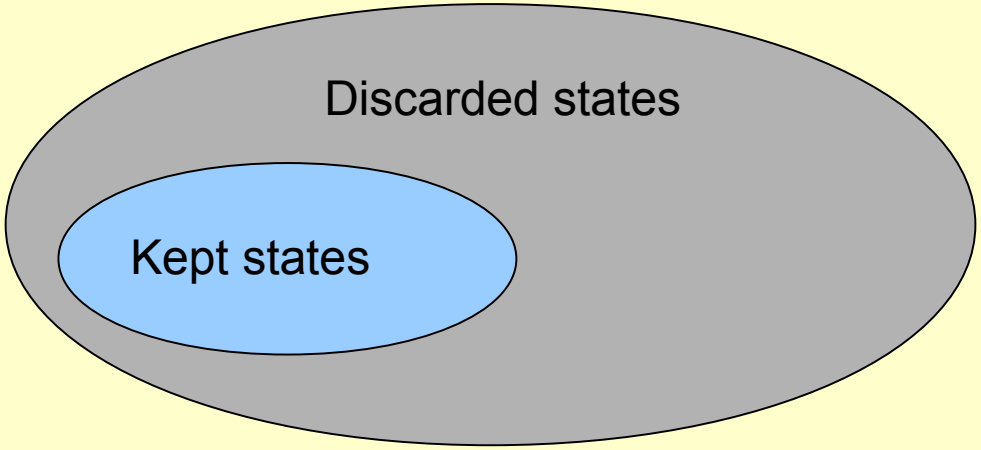
By making the choice that $W = H - H_0$

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

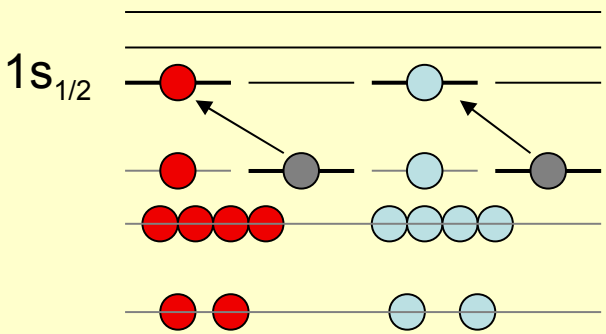
Importance truncation schematically

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

Typically we choose $\kappa \sim 10^{-5}$



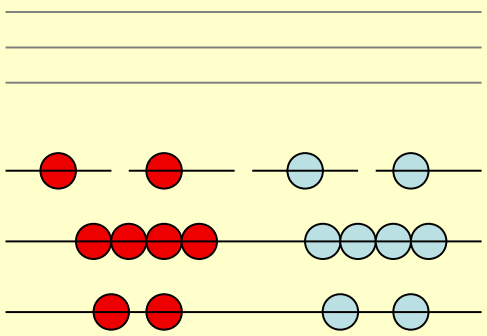
$\langle \Phi_\nu |$



O16 – one possible 2ħΩ configuration

H

$|\Psi_{ref}\rangle$



O16 - 0ħΩ configuration

N=2 (sd-shell)

M_z = -1/2, 1/2, -1/2, 1/2

N=1 (p-shell) → $0p_{3/2}$ $0p_{1/2}$

N=0 (s-shell)

Extension to excited states

- There is no conceptual difficulty in extending this idea to excited states.
- The reference state now becomes which ever state you care about (like excited states).

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

Extension to excited states

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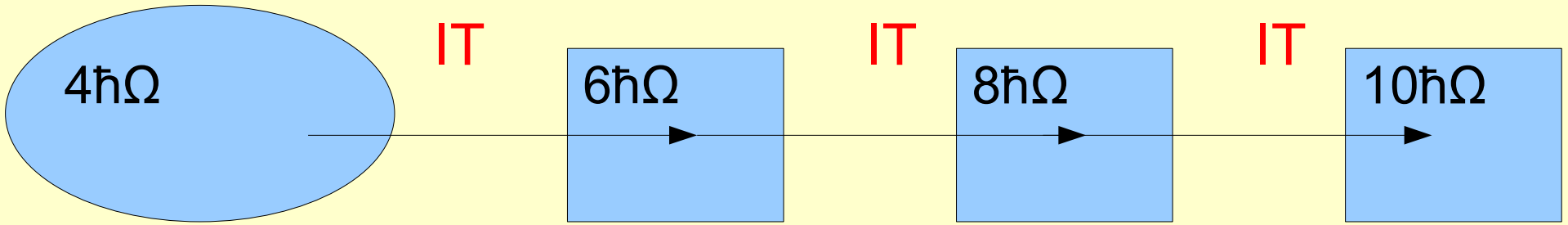
$$\kappa_\nu = \frac{|\langle \Phi_\nu | H | \Psi_{ref} \rangle|}{\epsilon_\nu - \epsilon_{ref}}$$

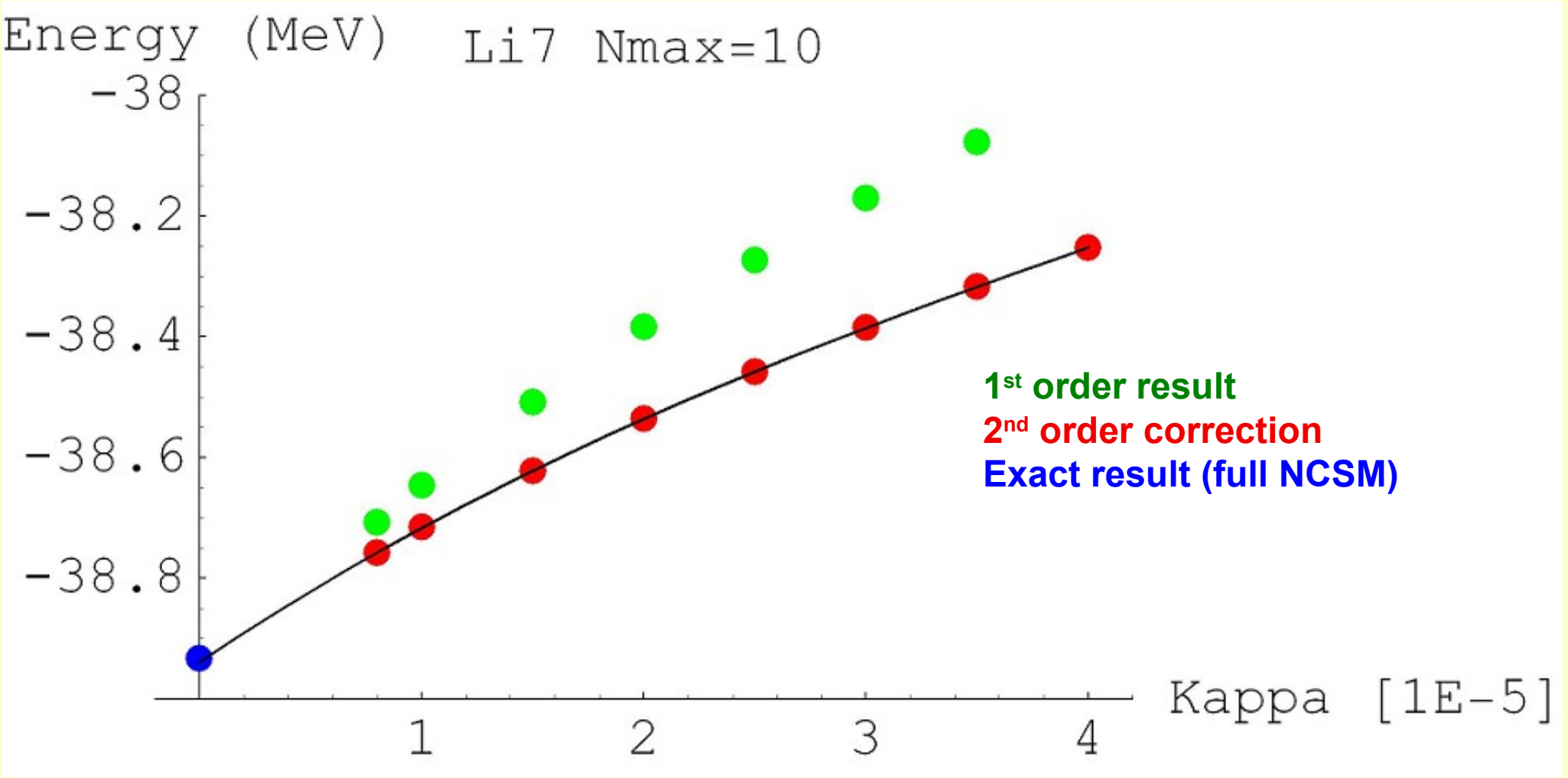
Comment for James Vary: What about excited states with the same angular momentum assignment as the ground state?

A typical calculation is as follows

- We begin with a complete N_{max} = 4ħΩ space, using the ground state as the reference state.
- All of the 6ħΩ basis states are created, then each basis state is evaluated (kept/discarded?).
- The NCSM calculation is then done in this truncated space, producing a new ground state.
- The "truncated" ground state becomes the reference state for the next calculation.
- The process repeats up to desired $N_{max.}$



^{7}Li: Truncation starts at N_{max} = 6, final space is N_{max} = 10



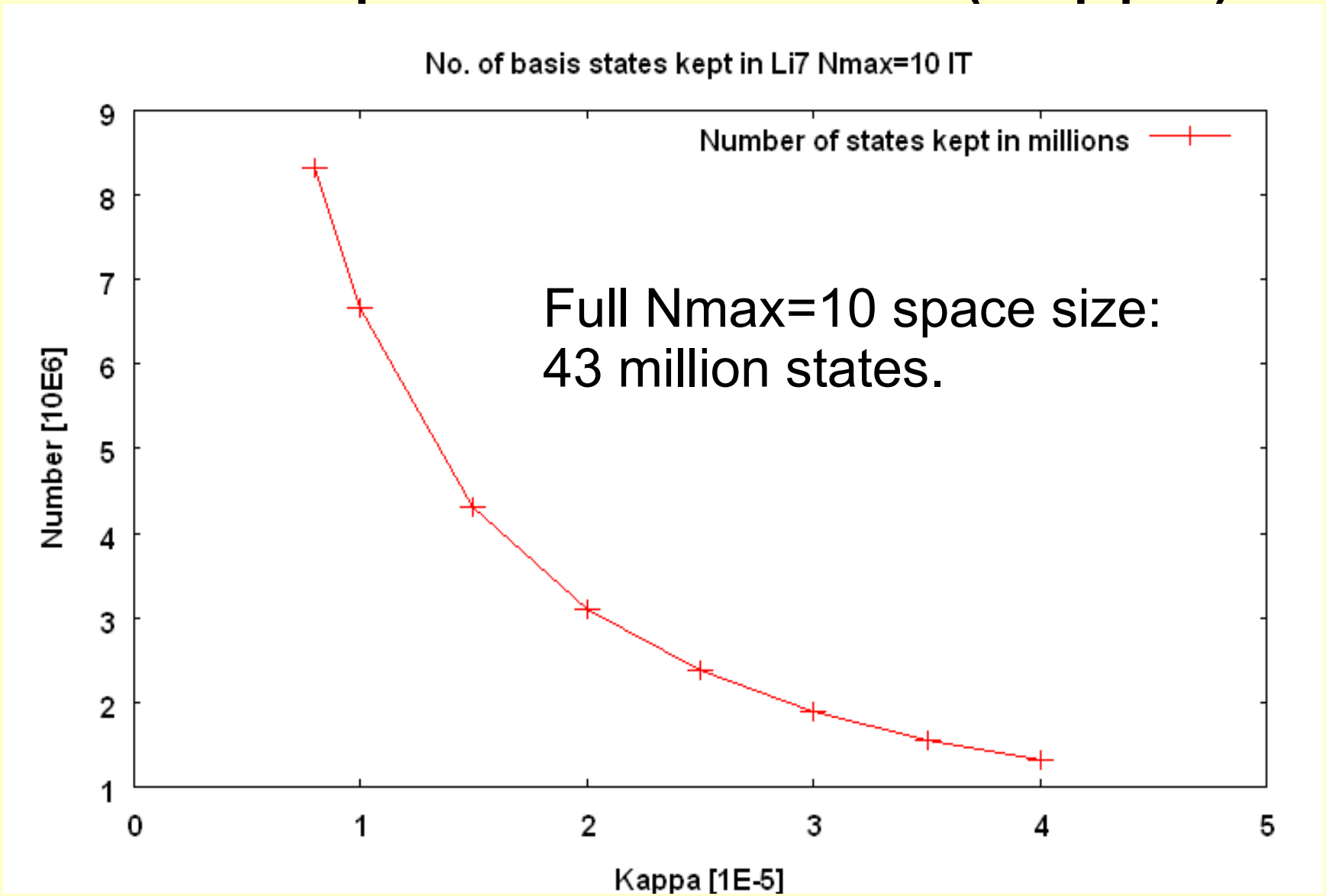
Interaction: ^{7}Li SRG N3LO λ=2.02/fm, N_{max} = 10

Definitions of "1st order" and "2nd order" results

- 1st order result refers to the ground state energy found, only by keeping the states, as per your importance criteria value (kappa).
- 2nd order result is the contribution from excluded states (those that were discarded) and is added energies of the 1st order result, giving the red dots on the previous slide.

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

The basis size depends on the value of the importance criteria (kappa).

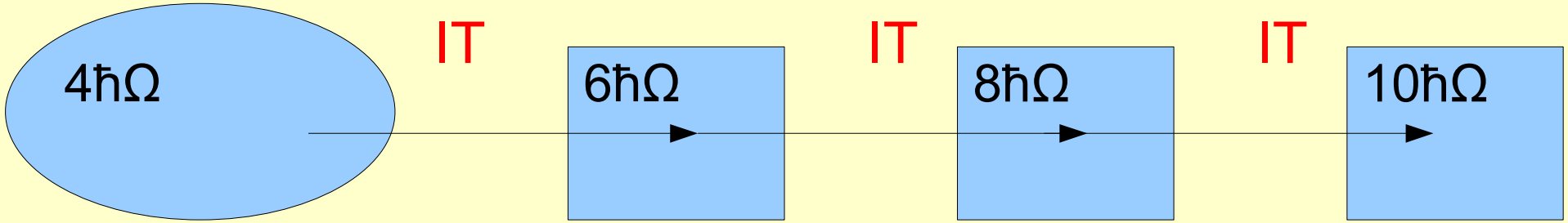


The finer details of my work on importance truncation.

- The next few slides will describe how I have performed my importance truncation calculations.
- I will highlight some of the differences from Robert's calculation – interesting to discuss?
- My calculations have the benefit of hindsight, e.g. Range of kappa to use, how many states are discarded, extrapolation techniques etc.
- Beneficial for us, since Robert and me can compare results; very useful for finding mistakes.

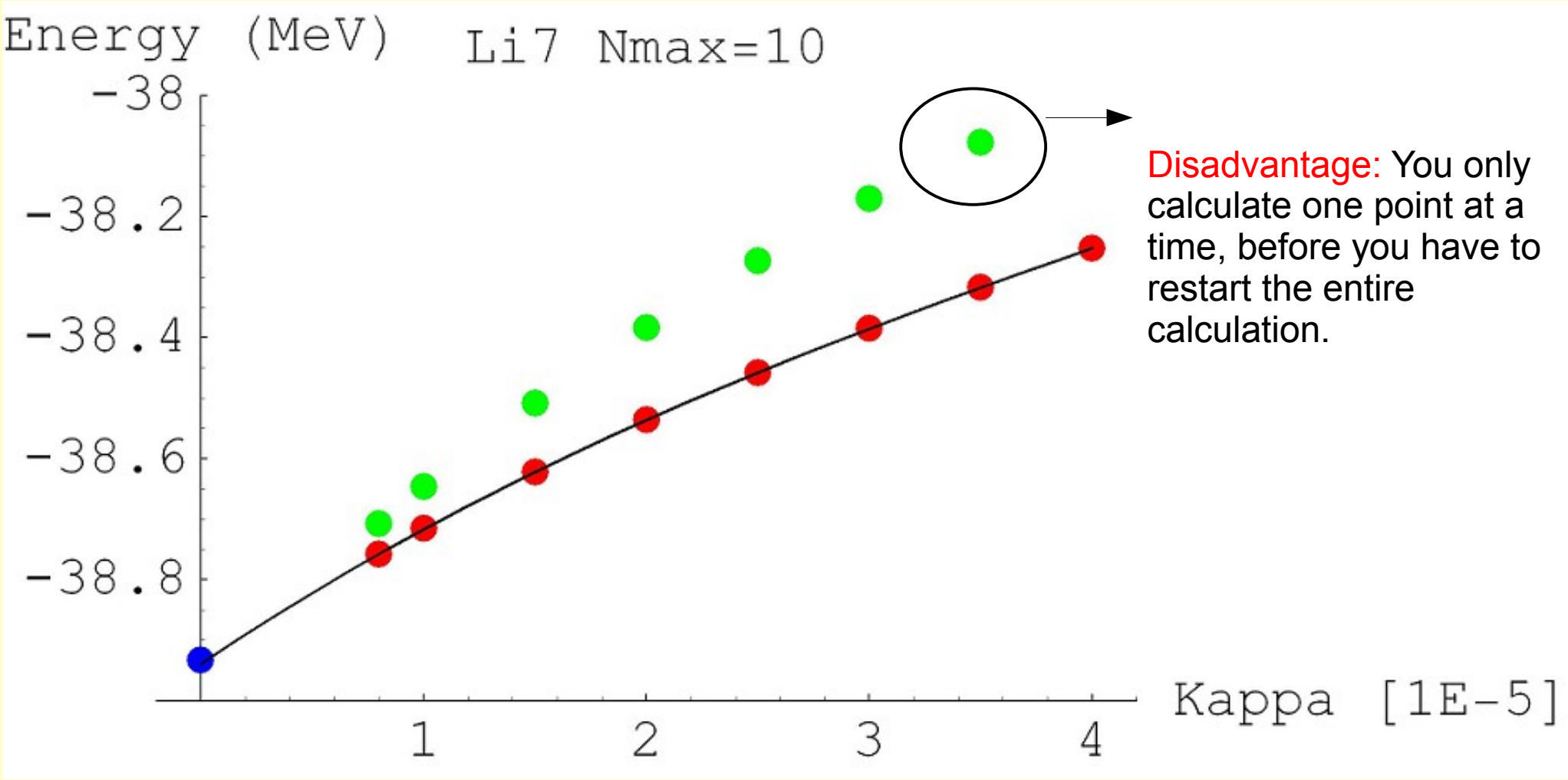
Progression through Nmax
Bootstrapping your way up in Nmax

- Option 1: Fix the importance criteria and work your way up in Nmax.



Example: Fix k=3x10E-5.

Progression through Nmax (case 1)

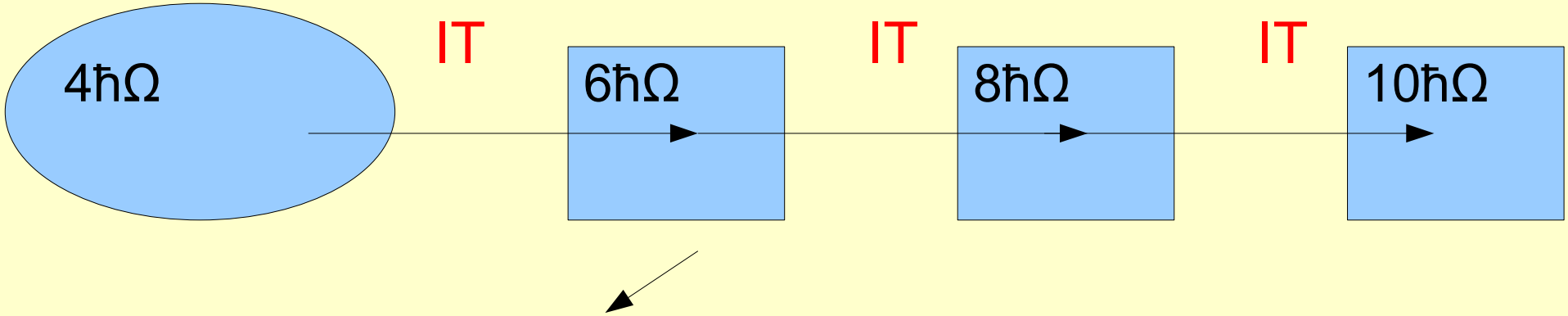


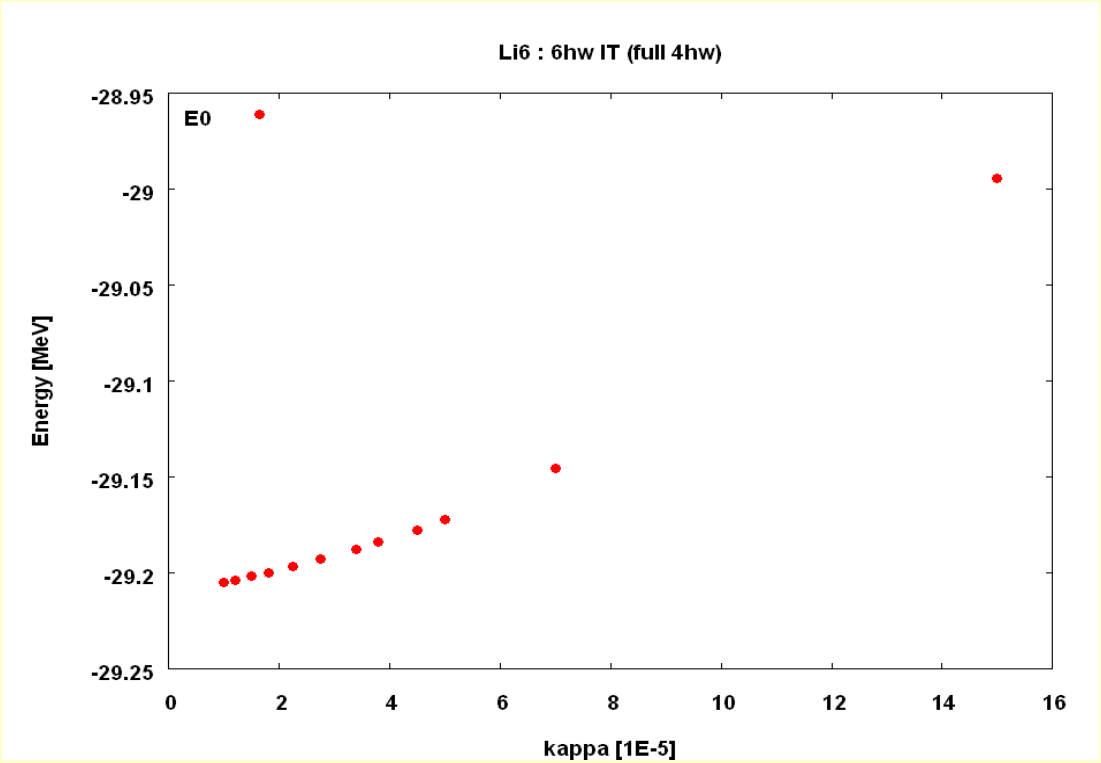
Disadvantage: You only calculate one point at a time, before you have to restart the entire calculation.

Progression through Nmax
A different approach

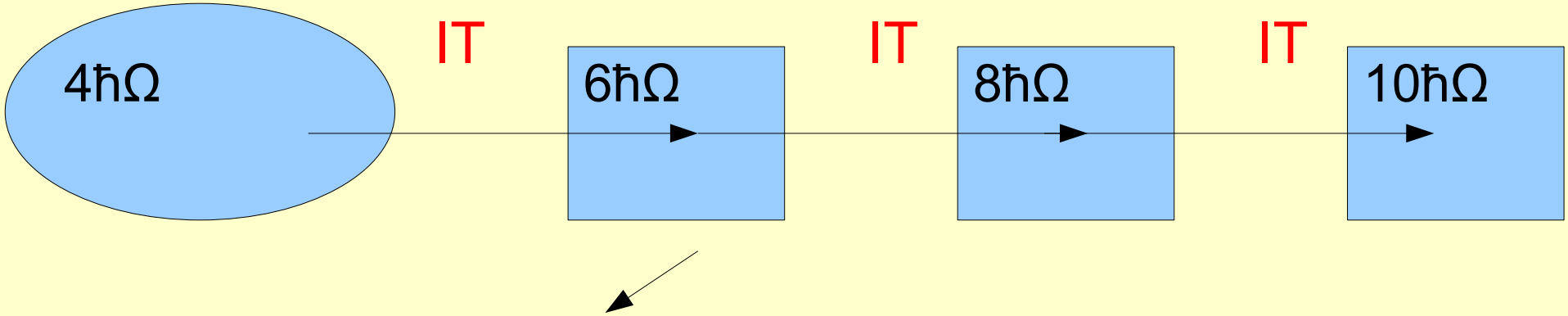
- Instead of calculating only one point at a time (fixed kappa)...
- Do the entire Nmax space at once, then continue to the next Nmax space.
- The next slide has a picture...

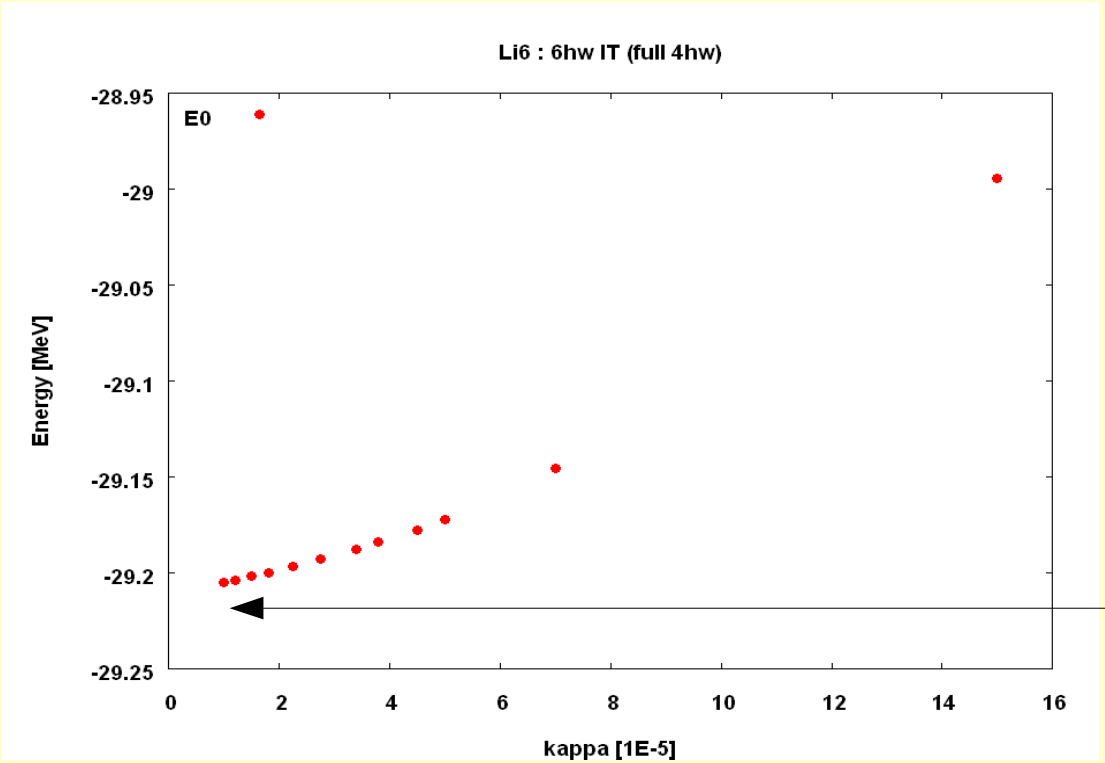
Progression through Nmax
A different approach





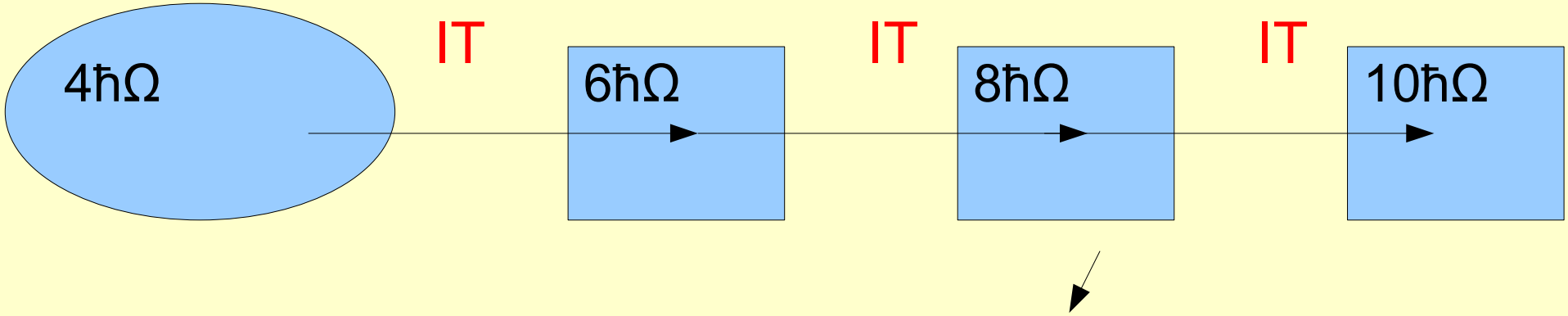
Progression through Nmax
A different approach

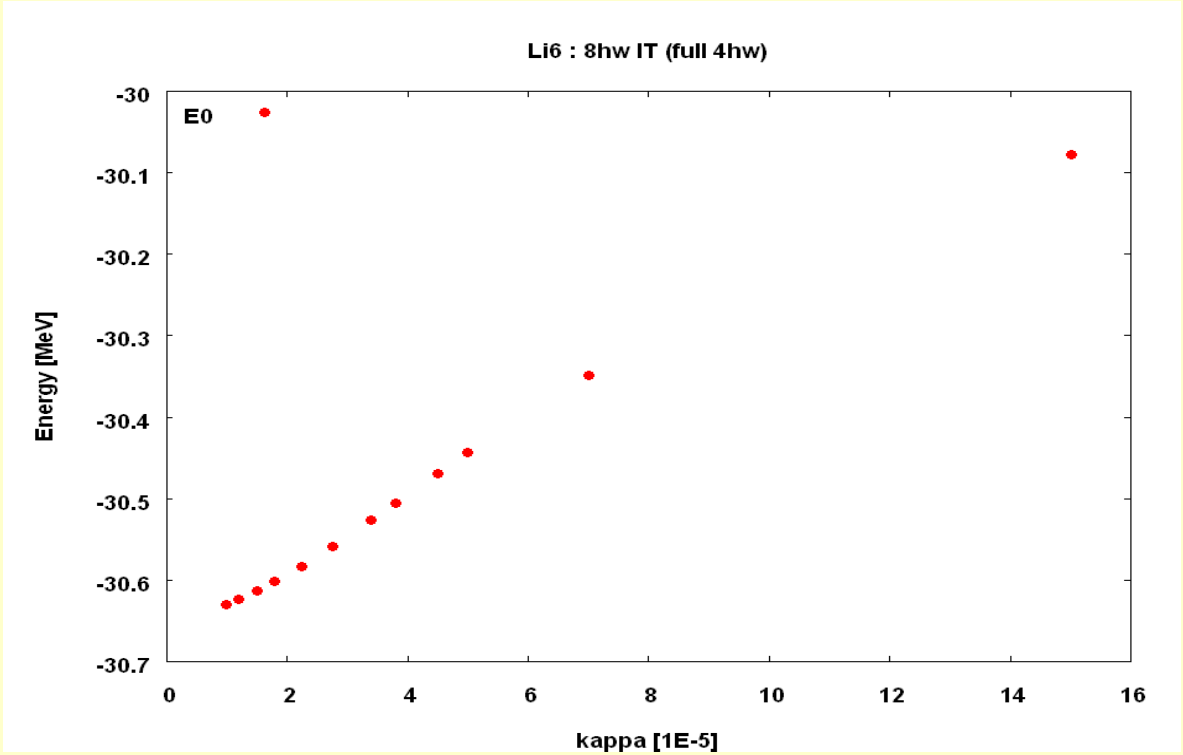




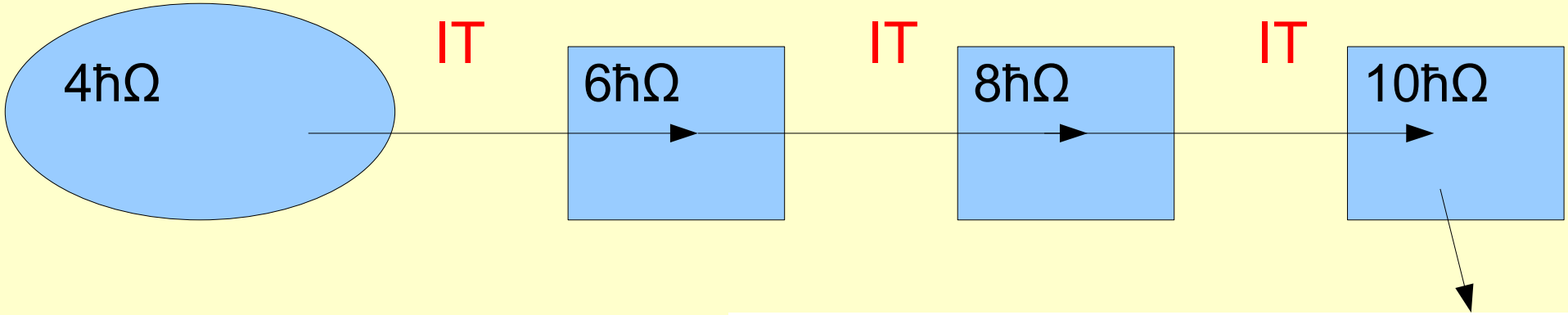
The last point calculated, becomes the reference state for evaluating which basis states in Nmax=8, should be kept.

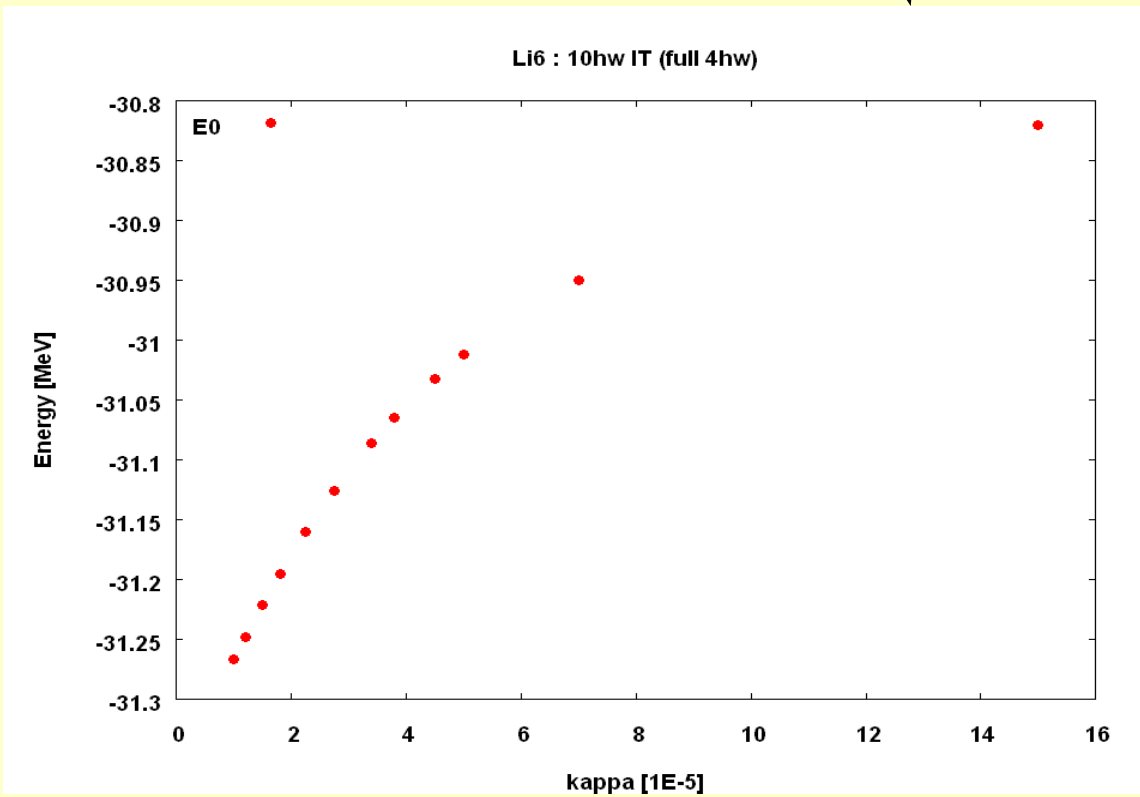
Progression through Nmax
A different approach





Progression through Nmax
A different approach





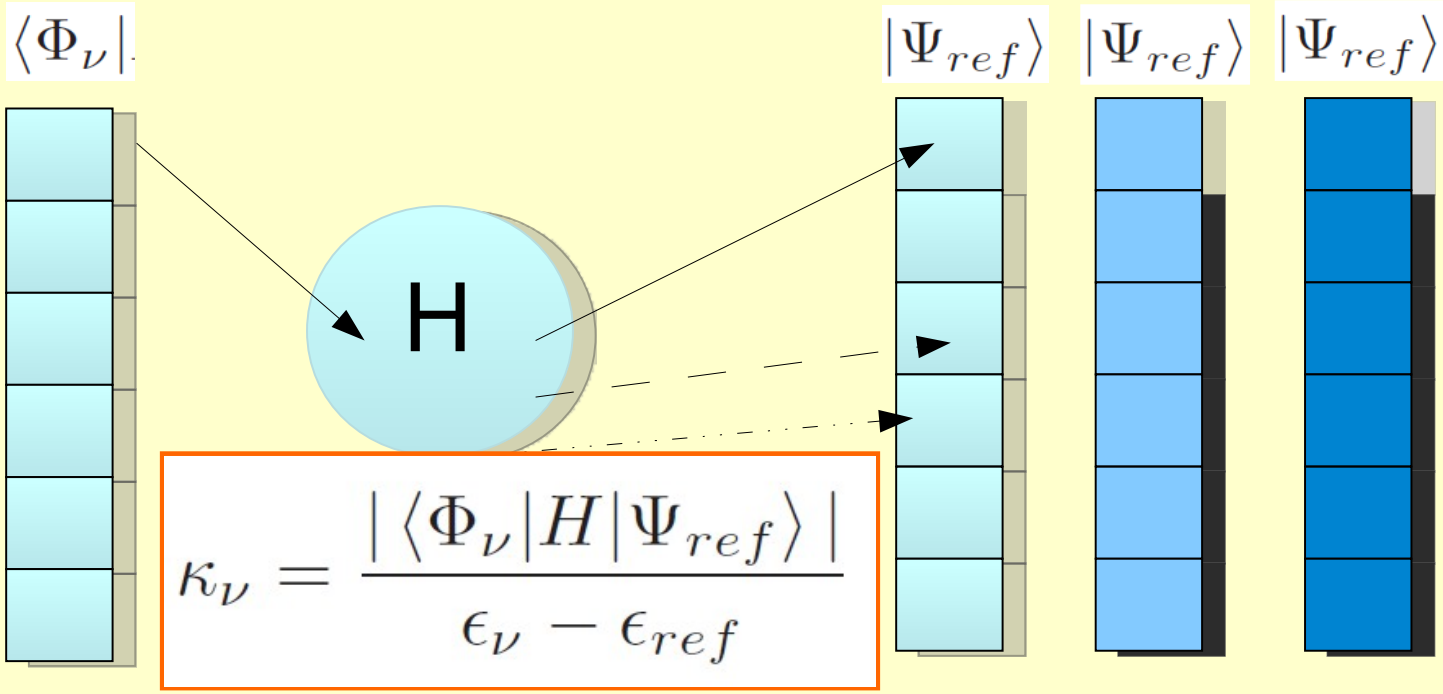
Progression through Nmax
A different approach conclusions

- Consequence: Keep *more* states at larger kappa values, but keep *same* at smallest value.
- Recall that these values of kappa, are only used to extrapolate to the full space results.
- The smallest kappa value would be used for other calculations (NCSM/RGM), since you store that wavefunction for later use.

The wavefunction is kept intact.

- We don't perform the "c_{min}" cut at any stage.
- Conceptually, the c_{min} cut is easy to do, but programming it was tough, so I left it for "later".
- Perhaps this is not a "bad" thing to do, since you should do as little harm as possible.
- Price to pay: Calculate kappa for every basis state in the "large" space*.
- * Ok, this is not entirely neccessary, but it turned out this way in the program.

Our calculation of kappa, for each basis state in the "large" space



- Advantage: Only need to store one 'large' basis state in memory at a time, instead of a large array of numbers.

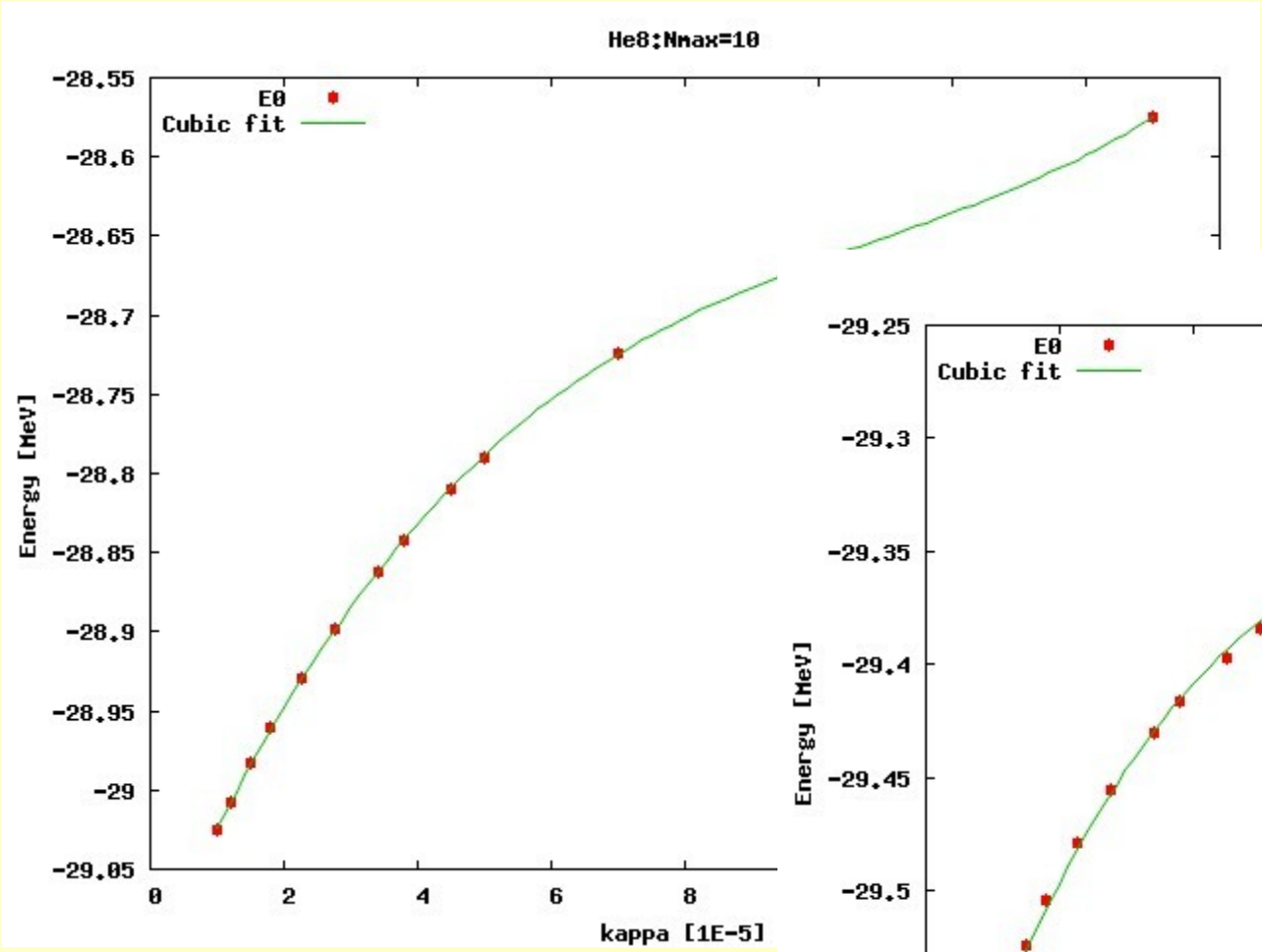
- Disadvantage: Must evaluate each basis state $\langle \Phi_\nu |$ in the next Nmax space – ultimately this limits us to a few billion states (?).

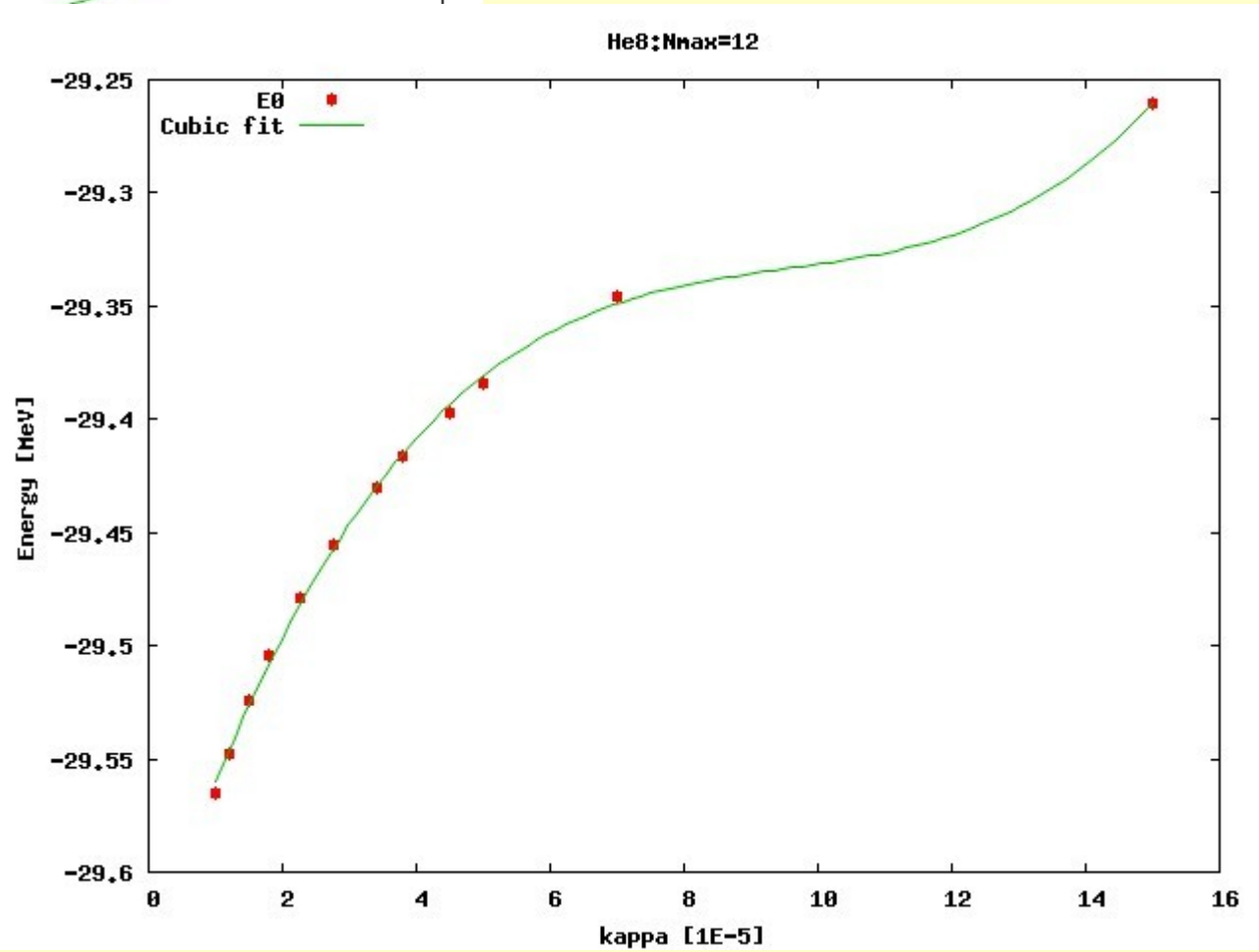
Helium 8 calculation Details

- Calculate the positive parity J_z=0 states

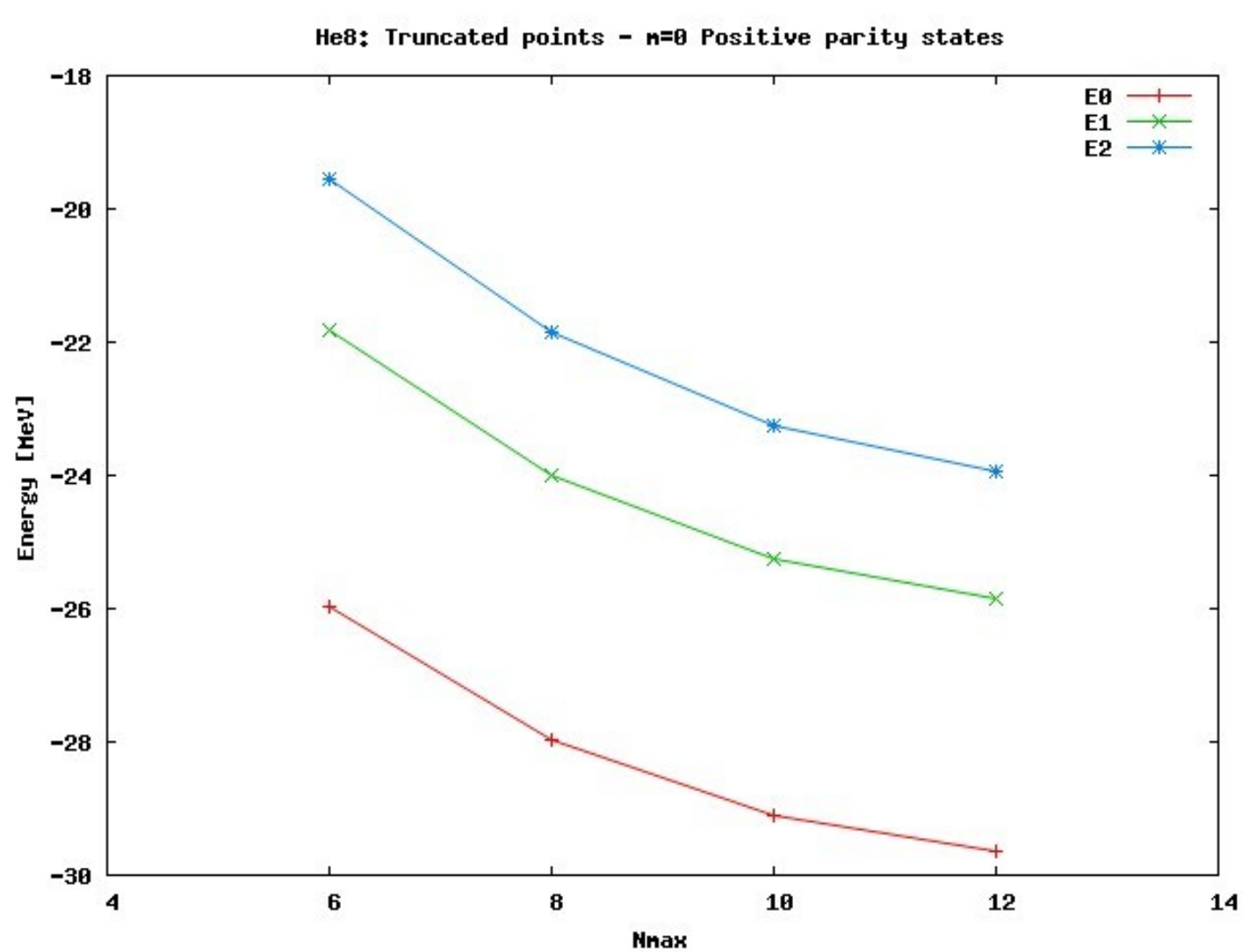
  - ground state + two excited (J=0,J=2,J=1)
- Also calculate the wavefunctions for the same set of states, for J_z=1. Required for transition densities.
- Calculate the negative parity state (J=1).
- Wavefunctions ultimately to be used in n+He8 reaction NCSM/RGM calculation.

Helium 8: 1st order results (illustrative)





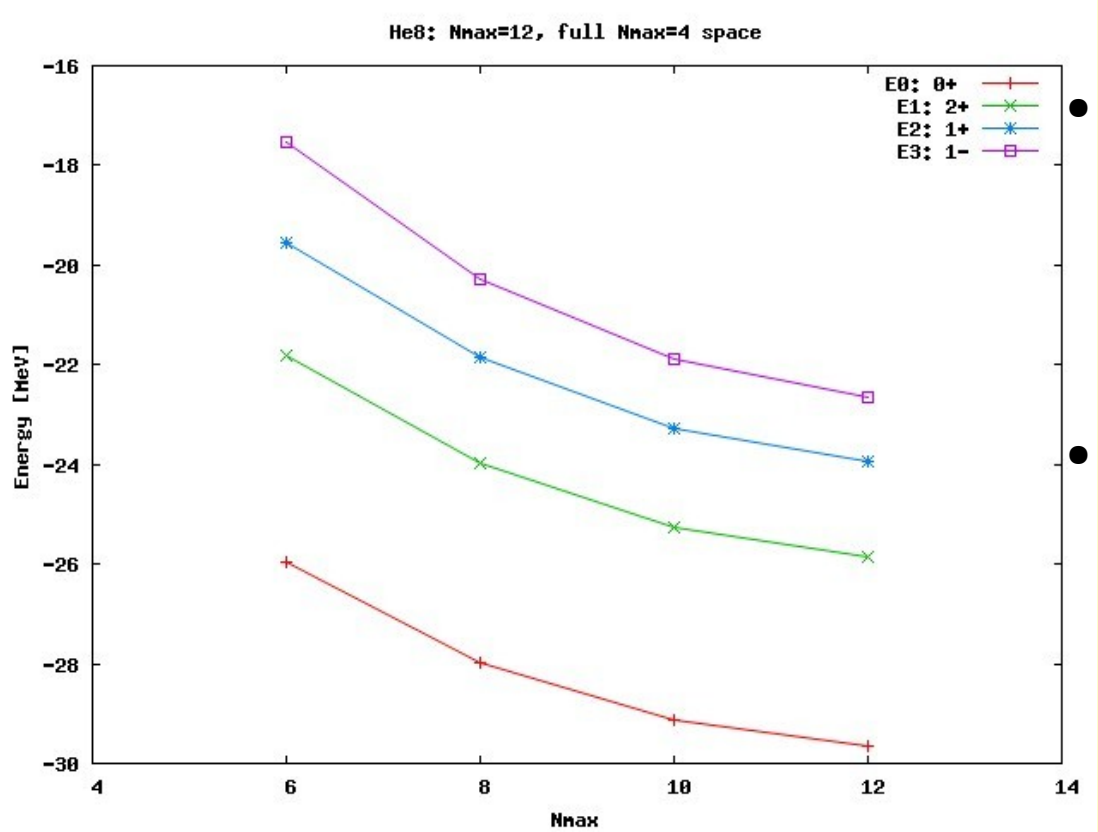
Helium 8: Nmax=12 (J_z=0 states)



Nmax	E0 (MeV)	E1 (MeV)	E2 (MeV)
12	-29.604	-25.854	-23.951

Nmax	Full space	IT space (k=1E-5)
12	~ 428 million	~ 13.65 million

Helium 8: Inclusion of 1^- state



- Negative parity state has to be calculated using a larger Nmax value (Nmax+1).
- Final space (Nmax=13) has 1 billion states, although we only had to evaluate ~ 850 million, and only kept ~14 million.

Nmax	E0 (MeV)	E1 (MeV)	E2 (MeV)	E3 (MeV)
12	-29.604	-25.854	-23.951	-22.664

Lessons Learned from Helium 8

- SRG potentials are key to reaching Nmax convergence.
- Checking 1 billion states is possible (256 processors); seems likely that we can go up to 2 billion states, but then we are stuck (?).
- Excited states increase the basis, but most CPU time is spent on waiting for convergence.
- Technical refinements needed with the code

  - basis evaluation?

More comments on importance truncation and its implementation

- Does it matter where you start the truncation?

  - In principle, one would expect that you should keep as many complete Nmax spaces as possible.

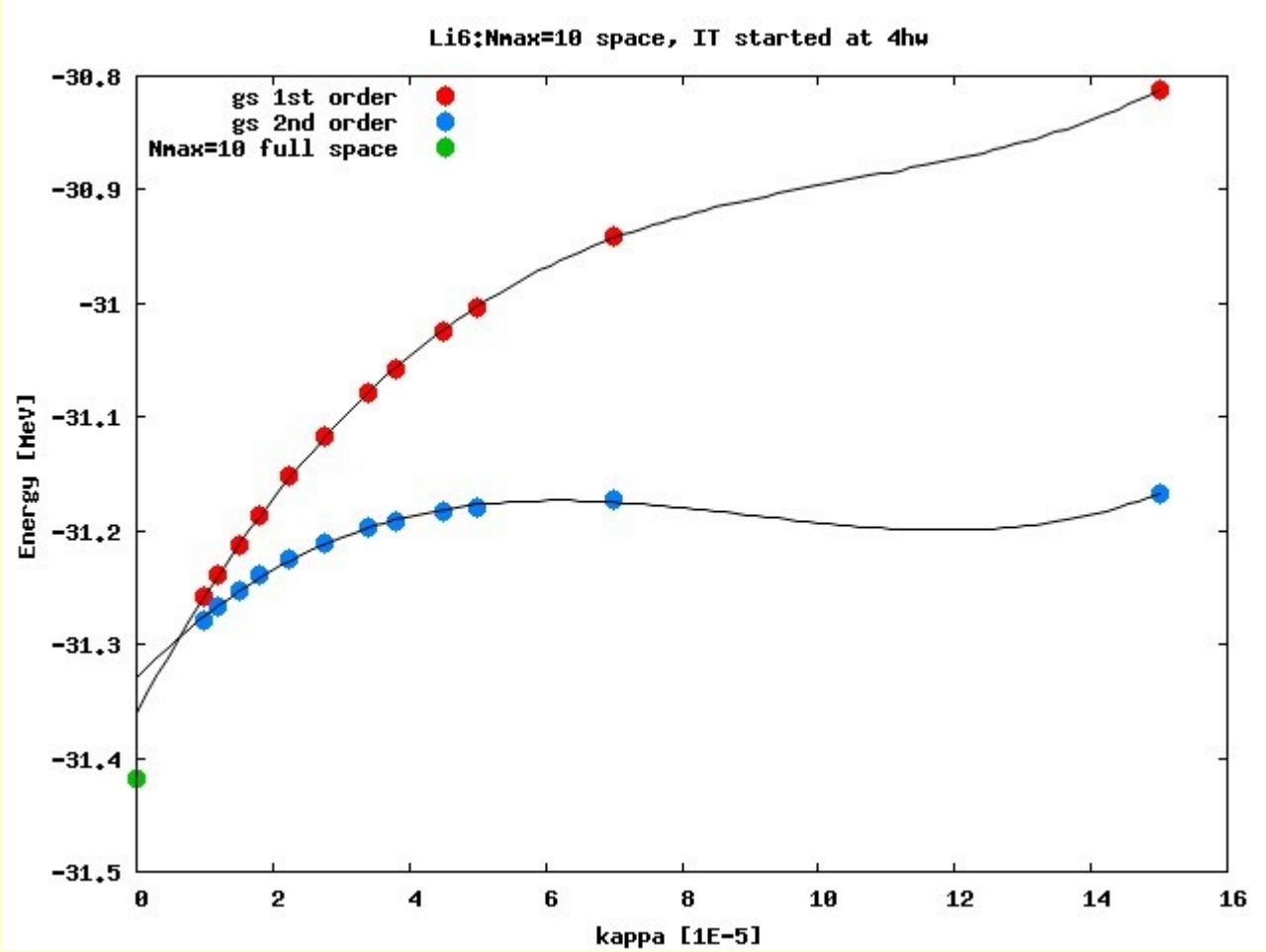
- The selection criteria works for energies and wavefunctions, but what about other operators?
- Extrapolations?

  - 1^{st} order fits vs 2^{nd} order corrections.

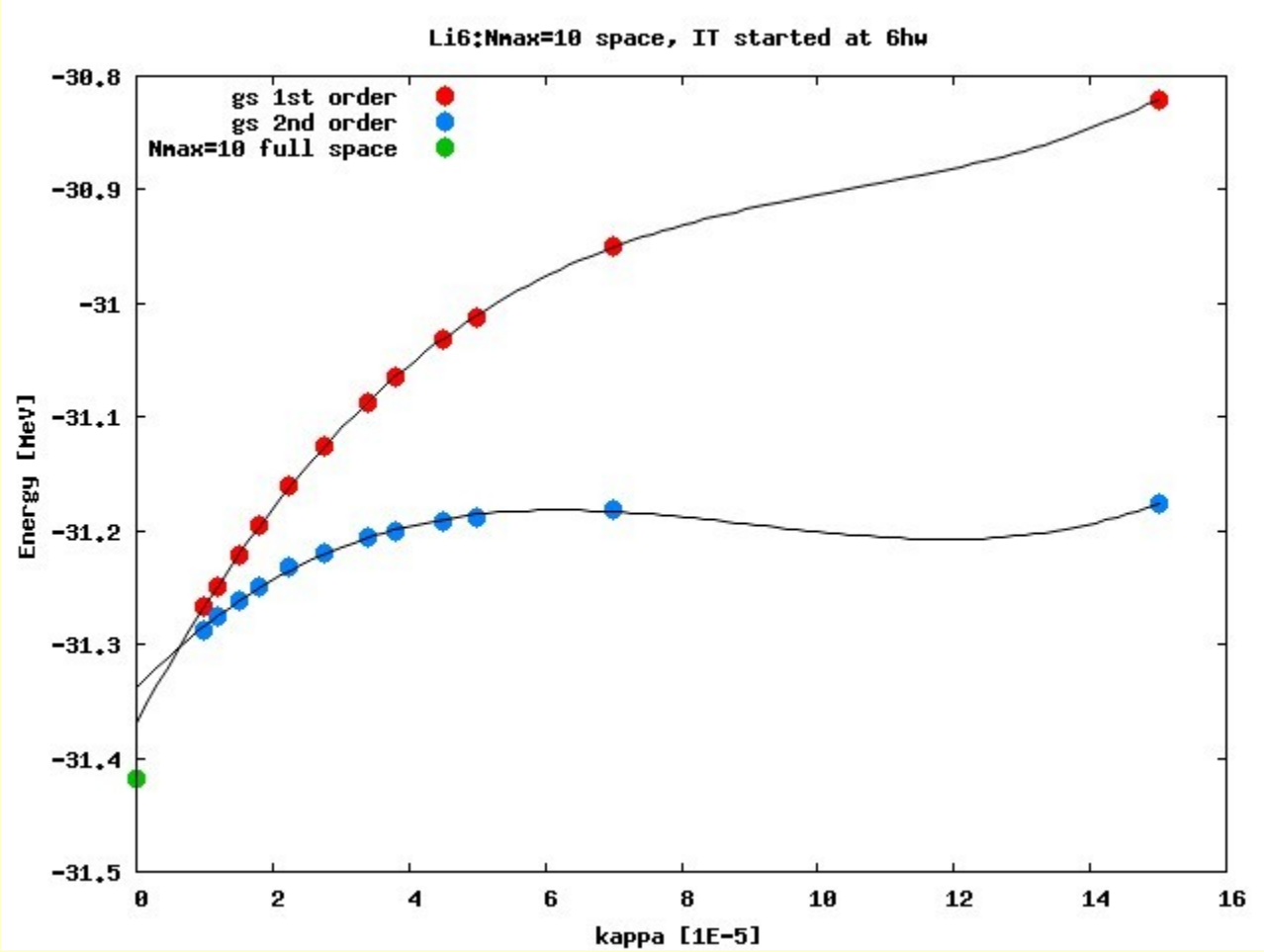
A quick investigation of these questions

- We will use Lithium-6 as our "test-bed".
- The basis is fairly small, up to Nmax=10, which has about 10 million states.
- The Quadropole moment is used to investigate another operator, besides the Hamiltonian.
- We use an SRG interaction (N3LO run-down to 2.02/fm) specific for the Nmax=10 space, but this is not too important for our illustrations.

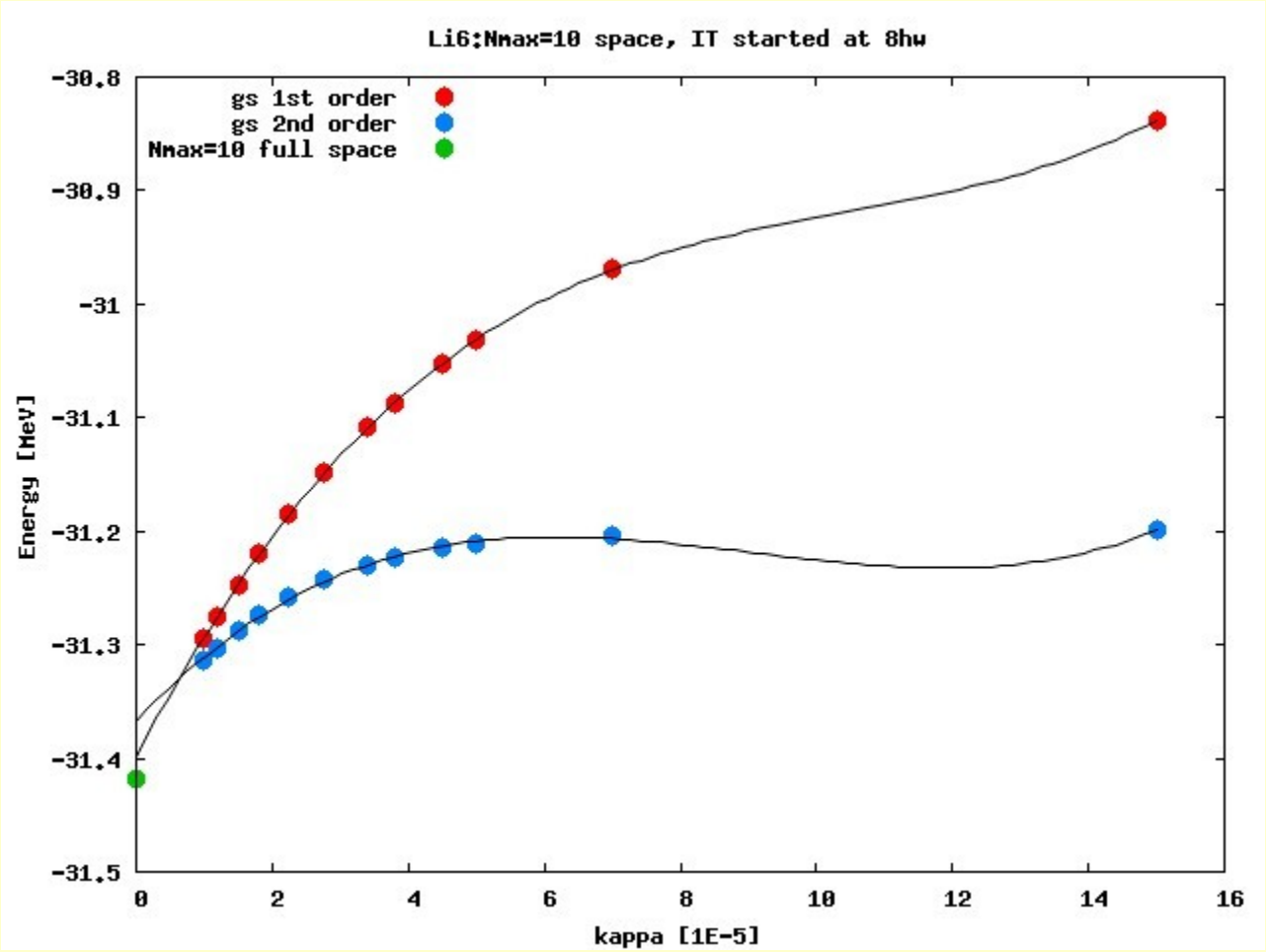
Truncation started at Nmax=4



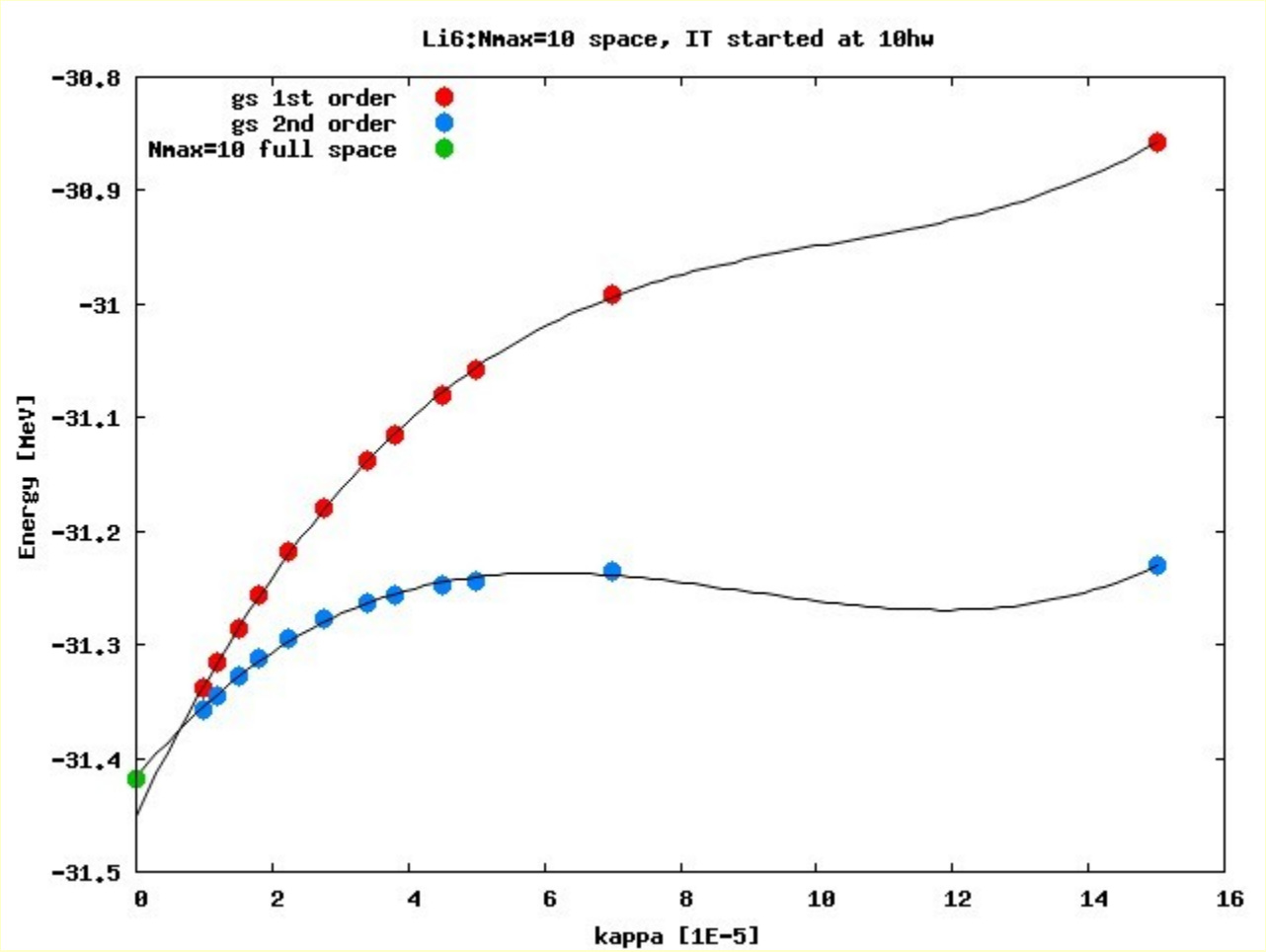
Truncation started at Nmax=6



Truncation started at Nmax=8

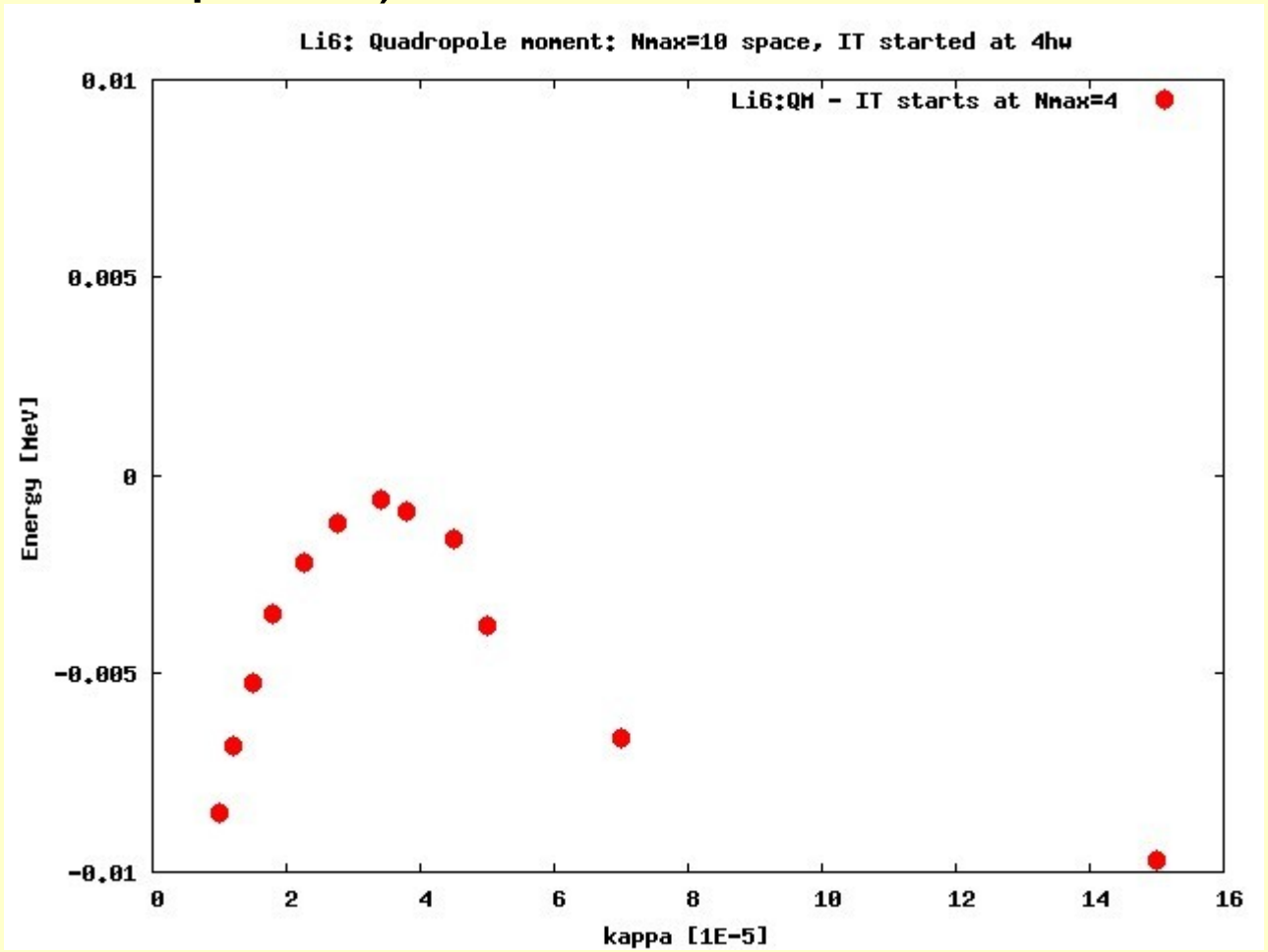


Truncation started at Nmax=10

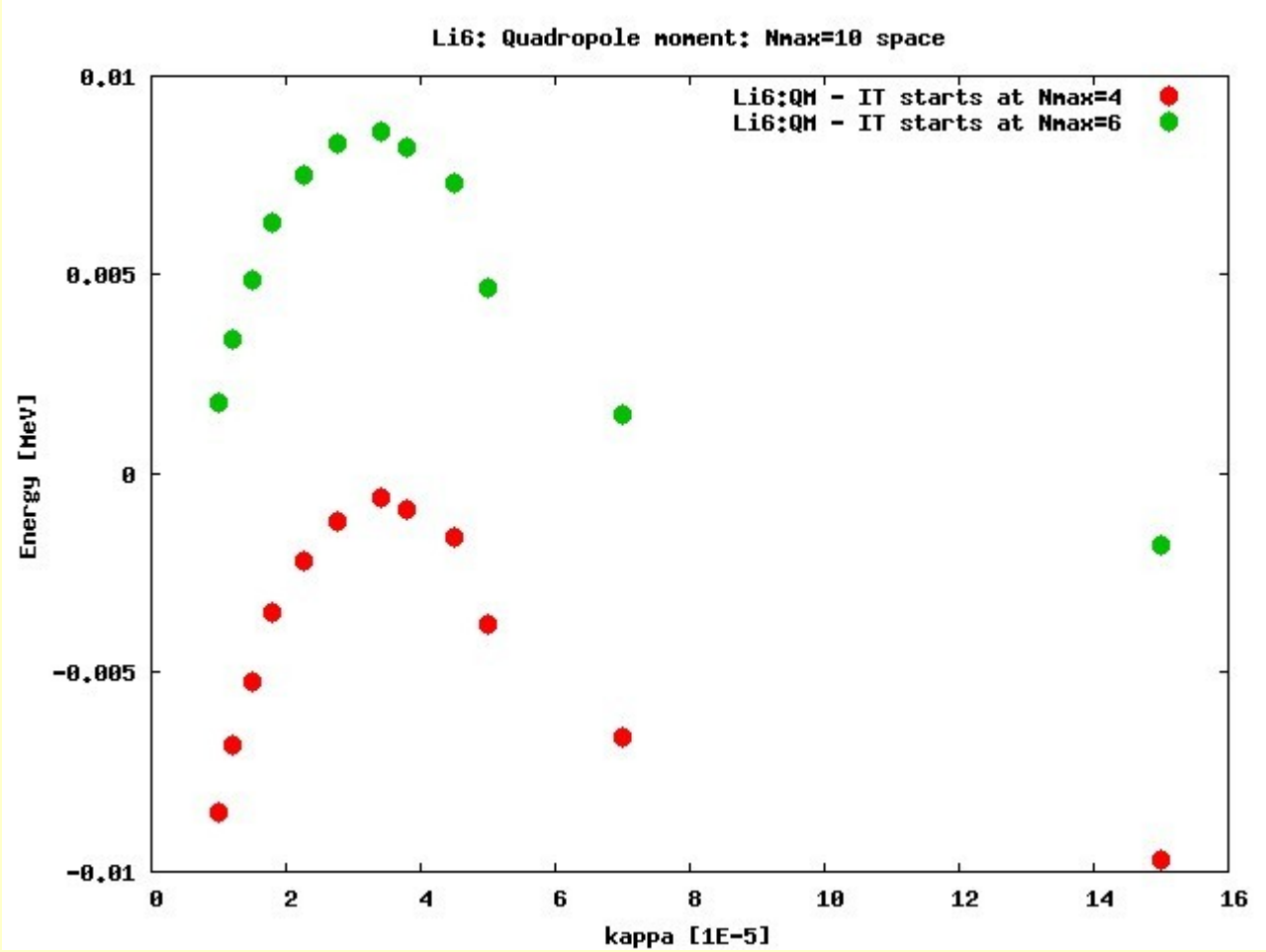


The quadropole moment (Li-6:gs)

- Calculation started importance truncation at Nmax=4, the results shown are the QM in the Nmax=10 space (where one would extrapolate).

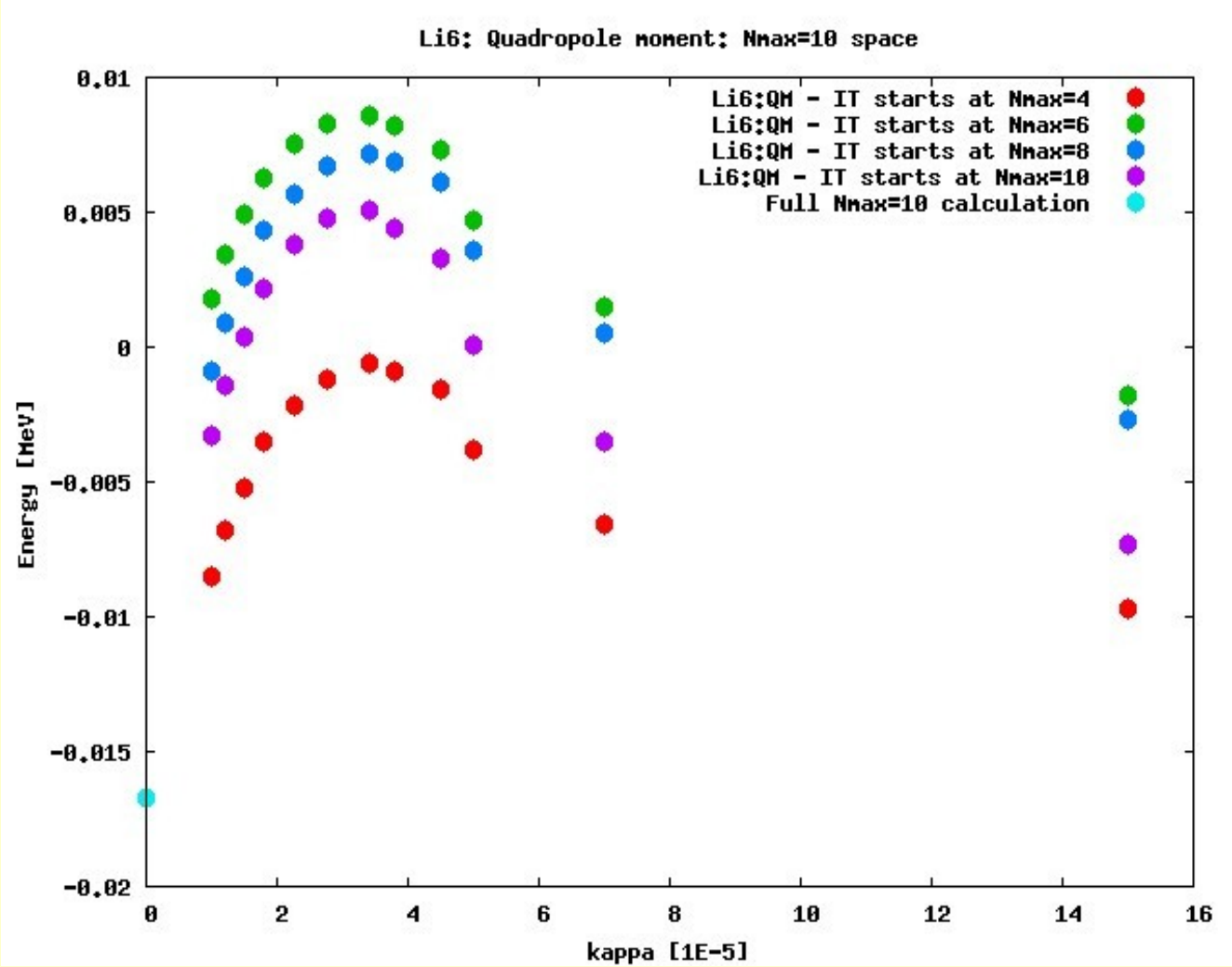


The quadropole moment (Li-6:gs)



Overall behaviour is the same, but the points are shifted vertically. Seems to suggest that starting at a larger Nmax value will make the QM more positive...

The quadropole moment (Li6:gs)
All starting truncations



A final comment on extrapolations

- Extrapolating the energies on a 1st order result, is variational in nature, by construction (add more basis states, get a lower energy).
- Extrapolating on the 2nd order result can be dangerous, since you no longer have a variational principle to work with. The fit is perhaps more stable, but is it the correct thing to do?

Thanks to the following people

- Bruce Barrett
- Petr Navratil
- Eric Jurgenson
- Sid Coon