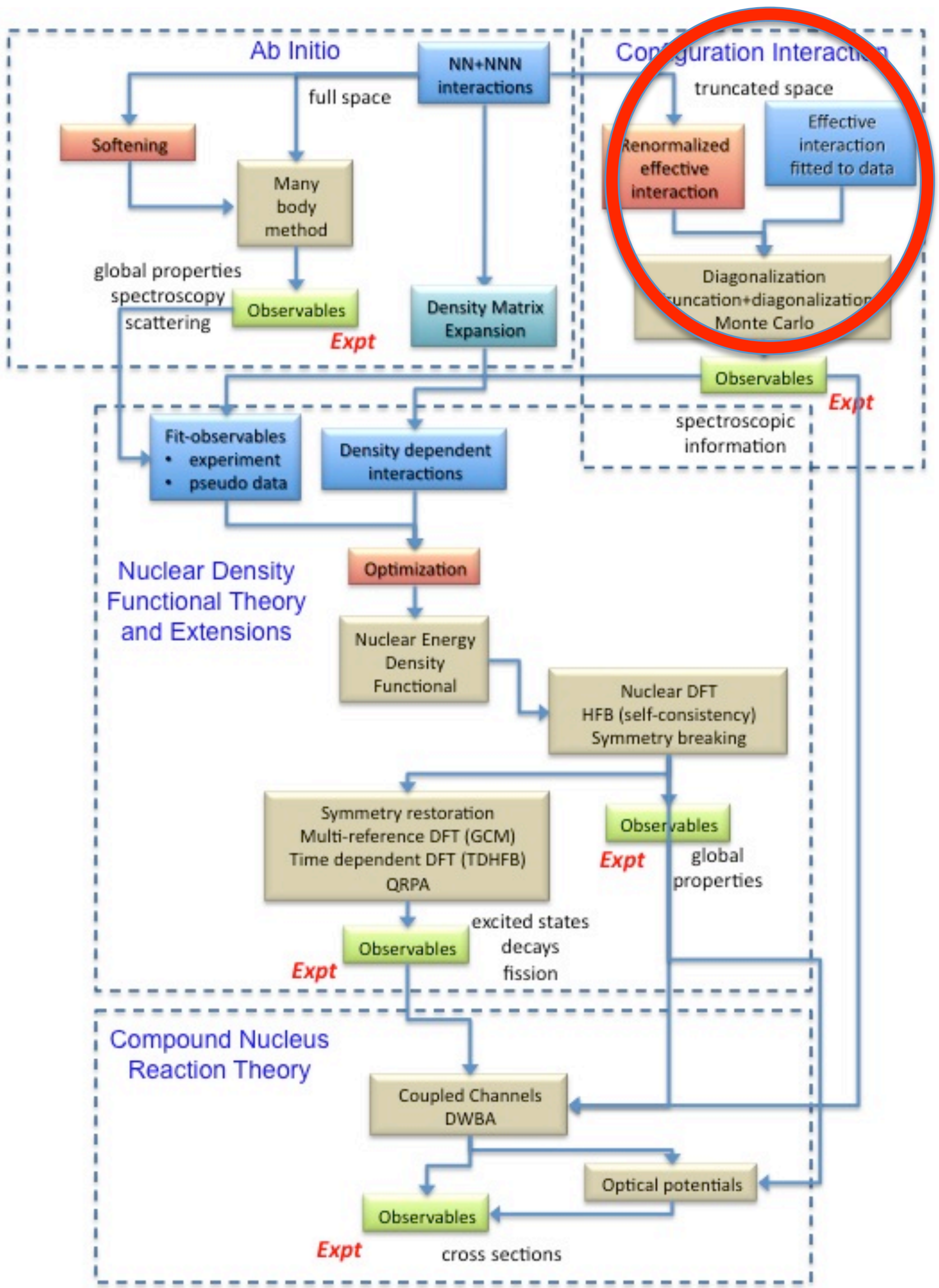
UNEDF Annual Meeting 2010

Making Effective Interactions More Effective

Applications of the `BIGSTICK` CI code to 2-species (up/down) fermions at unitarity:

(1) General effective interaction

(2) Center of mass without exact factorization



Ab Initio
NN+NNN interactions
full space
Softening
Many body method
global properties
spectroscopy
scattering
Observables
Expt
Density Matrix Expansion
Con guration Interact n
truncated space
Renormalized effective interaction
Effective interaction fitted to data
Diagonalization
truncation+diagonalization
Monte Carlo
Observables
Expt
spectroscopic information
Fit-observables
• experiment
• pseudo data
Density dependent interactions
Optimization
Nuclear Density Functional Theory and Extensions
Nuclear Energy Density Functional
Nuclear DFT
HFB (self-consistency)
Symmetry breaking
Symmetry restoration
Multi-reference DFT (GCM)
Time dependent DFT (TDHFB)
QRPA
Observables
Expt
global properties
Observables
Expt
excited states
decays
fission
Compound Nucleus Reaction Theory
Coupled Channels
DWBA
Optical potentials
Observables
Expt
cross sections

What goes into a shell-model CI calculation

Configuration-interaction (CI) calculations in a shell-model basis:

Solve $\hat{H}|\Psi\rangle = E|\Psi\rangle$ in a Slater determinant basis: $|\Psi\rangle = \sum_{\alpha} c_{\alpha}|\alpha\rangle$

where each Slater determinant is built from single-particle states with good angular momentum j,m (but arbitrary radial wavefunction).

The Hamiltonian is input in second quantization:

$$\hat{H} = \sum \varepsilon_a \hat{n}_a + \frac{1}{4}\sum V_{abcd}\hat{a}_a^+\hat{a}_b^+\hat{a}_d\hat{a}_c$$

The single-particle energies and two-body matrix elements are computed externally to the CI code and read in as **a file of numbers.**

The BIG QUESTION:

What are these numbers? How do we get them?

Introduction: Conquering Empirical Interactions

Naive use of *ab initio* interactions fail to describe data.

1. "Hard core" makes calculations troublesome.

2. Tractable model space is too small.

3. Need 3 body forces, but only use 2-body forces.

Introduction: Conquering Empirical Interactions

One creates a renormalized *effective interaction*
which implicitly account for the sums to high-momentum states,

e.g., Brueckner G-matrices.

Modern approaches use unitary transformations

A renormalized effective interaction is numerically more tractable, but still doesn't give the right spectrum.

Therefore one often tweaks a renormalized realistic interaction in order to make it agree better with data.

cf Brussaard and Glaudemans, Ch.7
more recent: Brown and Richter, PRC **74** 034315 (2006) ("USDA", "USDB")
and others...

Introduction: Conquering Empirical Interactions

Therefore one often tweaks a renormalized realistic interaction in order to make it agree better with data.

Given a Hamiltonian ***H***, compute some set of levels (over many nuclei) $\{|\alpha\rangle\}$ with energies E_α ; let E_α^0 be the experimental (target) energies.

Want to minimize $\chi^2 = \sum_\alpha \left(E_\alpha^0 - E_\alpha\right)^2$

Let $\hat{H} \to \hat{H} + \sum_i \delta c_i \hat{H}_i$

and $E_\alpha \to E_\alpha + \sum_i \delta c_i \frac{\partial E_\alpha}{\partial c_i}$

Hellmann-Feynman theorem:

$$\frac{\partial E_\alpha}{\partial c_i} = \langle \alpha | \hat{H}_i | \alpha \rangle$$

Introduction: Conquering Empirical Interactions

$$\frac{\partial \chi^2}{\partial \delta c_i} = 0 \quad \Rightarrow \quad \sum_j \left(\sum_\alpha \frac{\partial E_\alpha}{\partial c_i} \frac{\partial E_\alpha}{\partial c_j} \right) \delta c_j = \sum_\alpha \frac{\partial E_\alpha}{\partial c_i} \left(E_\alpha^0 - E_\alpha \right)$$

This has the form $\mathbf{B}^T \mathbf{B} \vec{c} = \mathbf{B}^T \delta \vec{E}$

Formally the solution is $\vec{c} = \left(\mathbf{B}^T \mathbf{B} \right)^{-1} \mathbf{B}^T \delta \vec{E}$ but

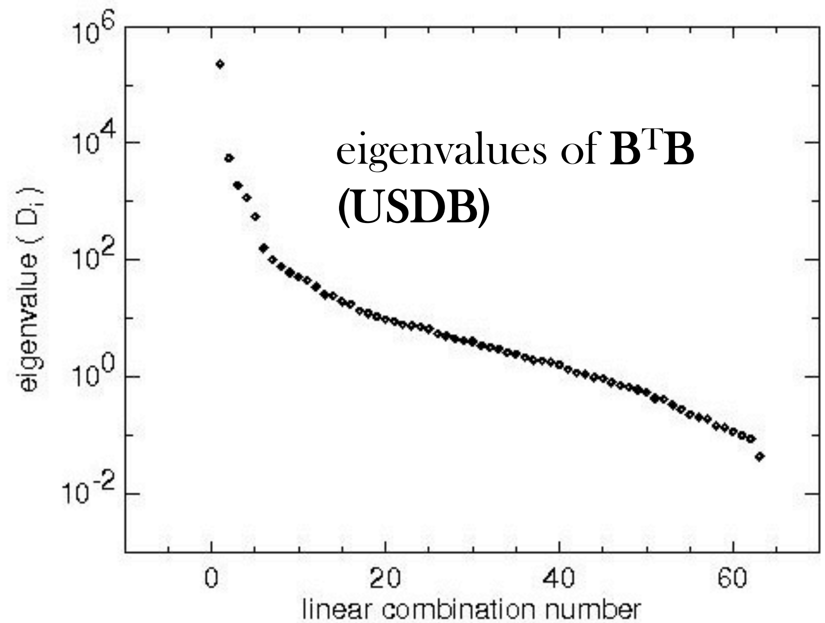
$B_{\alpha i} = \frac{\partial E_\alpha}{\partial c_i}$ may be singular or nearly so

Thus one does a singular value decomposition—find the eigenvalues of $\mathbf{B}^{\mathrm{T}}\mathbf{B}$ and truncate.

Part 2: SVD analysis of random and non-random interactions

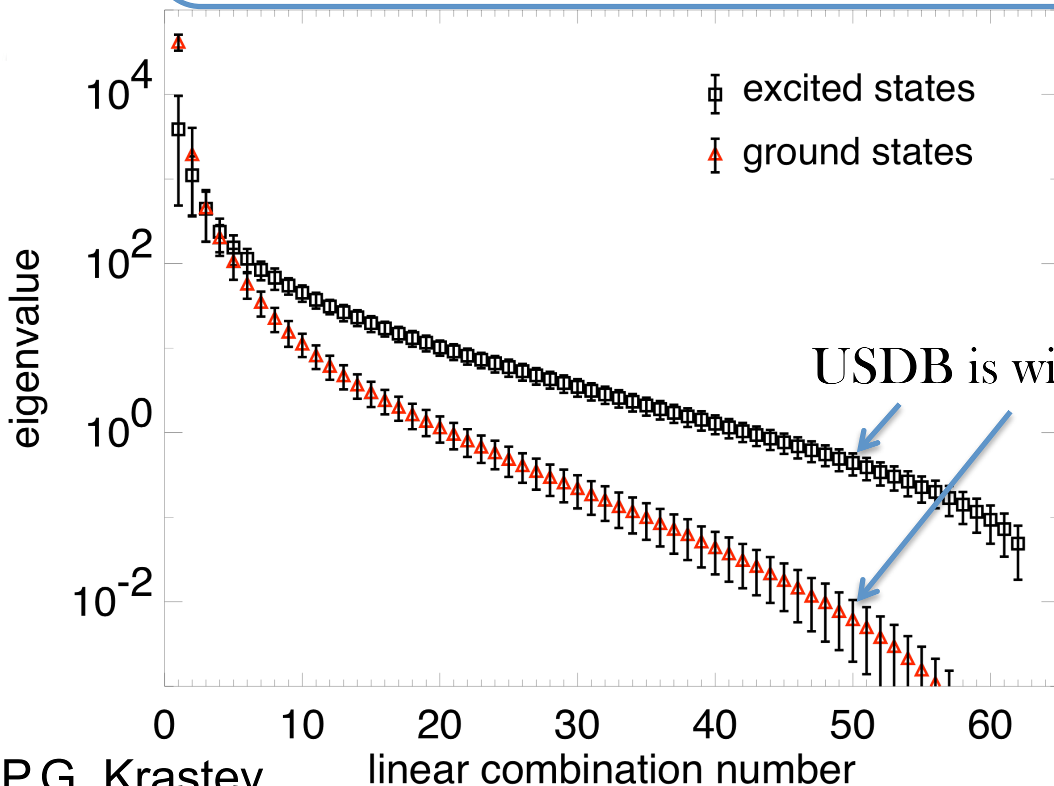
Let's review: Given an interaction and a set of states $\{|\alpha>\}$, one can use the Hellmann-Feynman theory to compute the sensitivity of the spectrum to perturbations in the Hamiltonian

$$B_{\alpha i} = \frac{\partial E_\alpha}{\partial c_i} = \langle \alpha | \hat{H}_i | \alpha \rangle$$



Part 2: SVD analysis of random and non-random interactions

Is there something *special* about the nuclear interaction? What about other interactions? Suppose we take a ***random*** interaction?



USDB is within the error bars

Johnson and P.G. Krastev, PRC **81**, 054303 (2010).

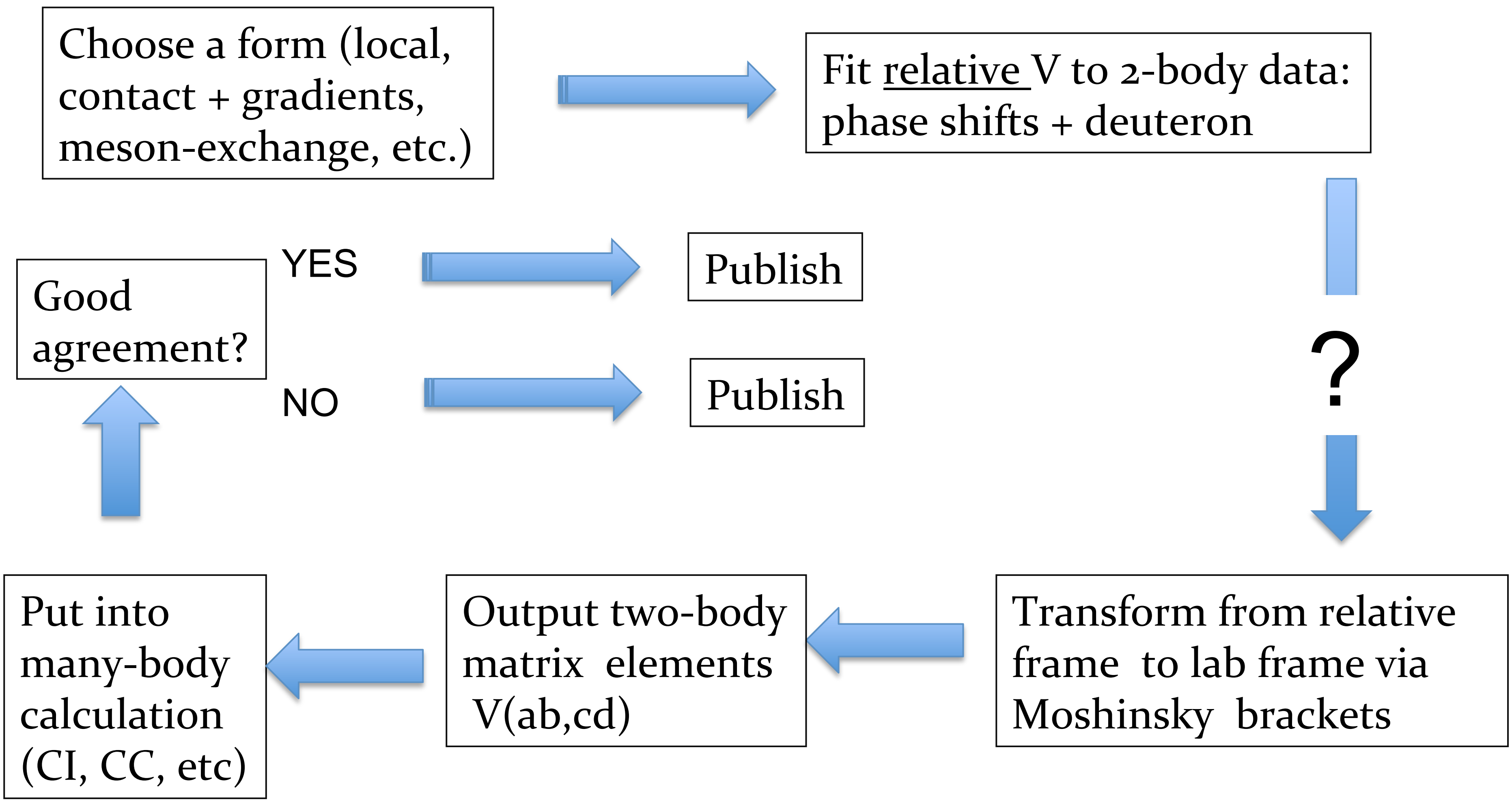
Interlude:
What about "realistic" effective nuclear interactions?

Q: What does it mean to be "realistic"?

A: Match experimental data!

Interlude: What about "realistic" effective nuclear interactions?

Life cycle of a realistic interaction:



Interlude: What about "realistic" effective nuclear interactions?

Life cycle of a realistic interaction:

Fit relative V to 2-body data:
phase shifts + deuteron

Here is where one needs to "renormalize" the short-range/ high momentum part of the interaction

?

Transform from relative frame to lab frame via Moshinsky brackets

Today this renormalization is accomplished via unitary transformations that preserve two-body data (phase shifts, bound states)

Interlude: What about "realistic" effective nuclear interactions?

Some common unitary transformations are Okubo-Lee-Suzuki, $V_{low\text{-}k}$, and the similarity renormalization group (SRG).

They all have the same goal: soften the short-range/high-*p* behavior while preserving two-body (on-shell) data. **In other words, they modify the off-shell behavior, which can only be seen in many-body (A = 3 and higher) systems.**

There have been some other attempts to choose different off-shell behavior, e.g., UCOM, INOY and JISP16 interactions.

Interlude: What about "realistic" effective nuclear interactions?

They all have the same goal: soften the short-range/high-p behavior while preserving two-body (on-shell) data. **In other words, they modify the off-shell behavior, which can only be seen in many-body (A = 3 and higher) systems.**

$$\hat{H}_{eff} = \hat{U}^{-1}\hat{H}\hat{U} = e^{-\hat{A}}\hat{H}e^{\hat{A}}$$

Can we choose the **best** generator **A** of the unitary transformation...
the same way we fitted semi-empirical interactions?

Part 3: Cracking the off-shell degrees of freedom in in "realistic" interactions

A Modest Proposal: $\hat{H}_{eff} = \hat{U}^{-1}\hat{H}\hat{U} = e^{-\hat{A}}\hat{H}e^{\hat{A}}$

We can expand the antisymmetric operator **A** in a series of "base" operators: $\hat{A} = \sum_i c_i \hat{A}_i$

Then we can find perturbations of the unitary transformation $\hat{H}_{eff} \approx \hat{H} + \sum_i c_i [\hat{H}, \hat{A}_i]$

Then we compute

$$B_{\alpha i} = \frac{\partial E_\alpha}{\partial c_i} = \left\langle \alpha \left| \left[\hat{H}, \hat{A}_i \right] \right| \alpha \right\rangle$$

and do SVD as before...

Part 3: Cracking the off-shell degrees of freedom in in "realistic" interactions

$$\hat{H}_{eff} = \hat{U}^{-1}\hat{H}\hat{U} = e^{-\hat{A}}\hat{H}e^{\hat{A}}$$

This is *just like* the SVD fits to semi-empirical interactions such as USDB, GXPF1, etc, except

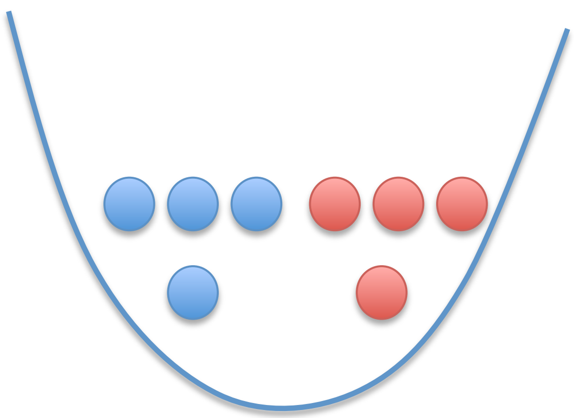
<u>USDB etc</u>: work in lab frame, perturb Hamiltonian

<u>New: </u> we perturb the generators of the unitary transformation in the relative frame

$$B_{\alpha i} = \frac{\partial E_\alpha}{\partial c_i} = \langle \alpha \| [\hat{H}, \hat{A}_i] \| \alpha \rangle$$

Sample application: cold atomic gases at unitarity in a harmonic trap

$$\hat{H} = \sum_i -\frac{\hbar^2}{2m}\nabla_i^2 + \tfrac{1}{2} m\Omega^2 r_i^2 - V_0 \sum_{i<j} \delta(\vec{r}_i - \vec{r}_i)$$



V_0 tuned for infinite scattering length (cutoff-dependent)

Sample application: cold atomic gases at unitarity in a harmonic trap

Only *s*-wave channel in relative coordinates

$$\hat{H} = \sum_i -\frac{\hbar^2}{2m}\nabla_i^2 + \tfrac{1}{2} m\Omega^2 r_i^2 - V_0 \sum_{i<j} \delta(\vec{r}_i - \vec{r}_i)$$

Use ABF regularization
Alhassid, Bertsch, Fang, PRL**100**, 230401(2008)
in relative frame with harmonic oscillator basis up to NħΩ

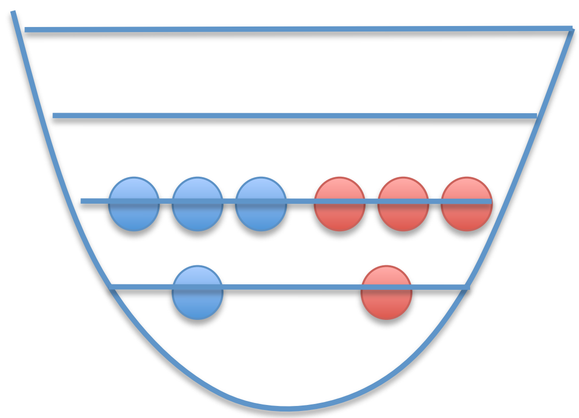
$$\langle n'l | \hat{H}_{rel} | nl \rangle$$

If cutoff at 10ħΩ (q=5) then a 6x6 symmetric matrix

Sample application: cold atomic gases at unitarity in a harmonic trap

Then need to transform from the relative frame to the lab frame (also in harmonic oscillator basis) using Talmi-Brody-Moshinsky brackets

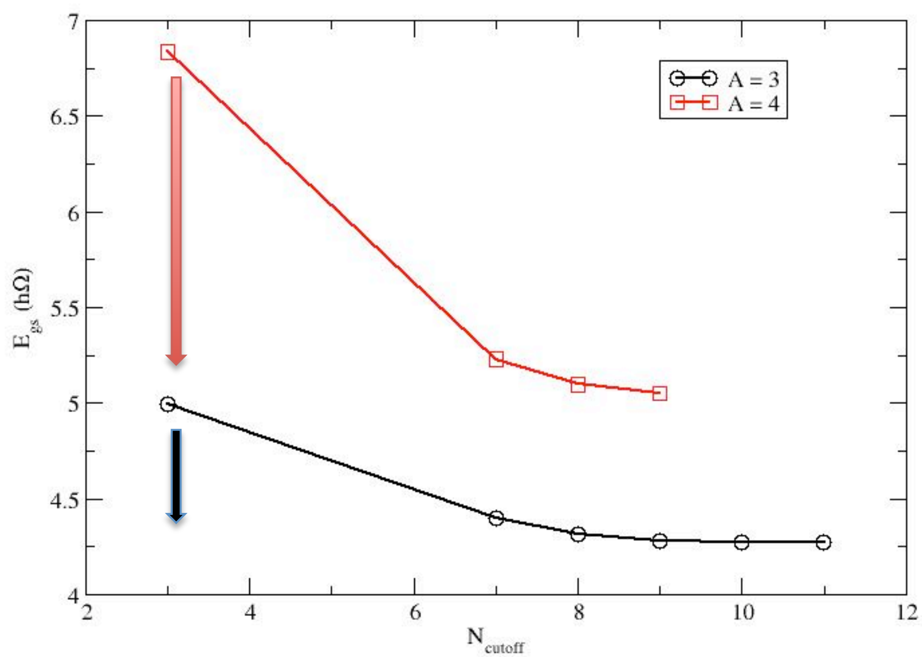
So there are *two* parameters for the system: the cutoff in the relative frame and the number of h.o. shells in the lab frame.



Sample application: cold atomic gases at unitarity in a harmonic trap

Use ABF regularization with cutoff of $10\hbar\Omega$ (in relative *s*-channel).

Slow convergence in CI calculations.



Part 3: Cracking the off-shell degrees of freedom in in "realistic" interactions

Sample application: cold atomic gases at unitarity in a harmonic trap

$$\hat{H}_{eff} = \hat{U}^{-1}\hat{H}\hat{U} = e^{-\hat{A}}\hat{H}e^{\hat{A}}$$

In the relative frame, with a 8hΩ , then **H**, **A**, and **U** are all 5 x 5 matrices. (Then go from relative to lab via Moshinsky).

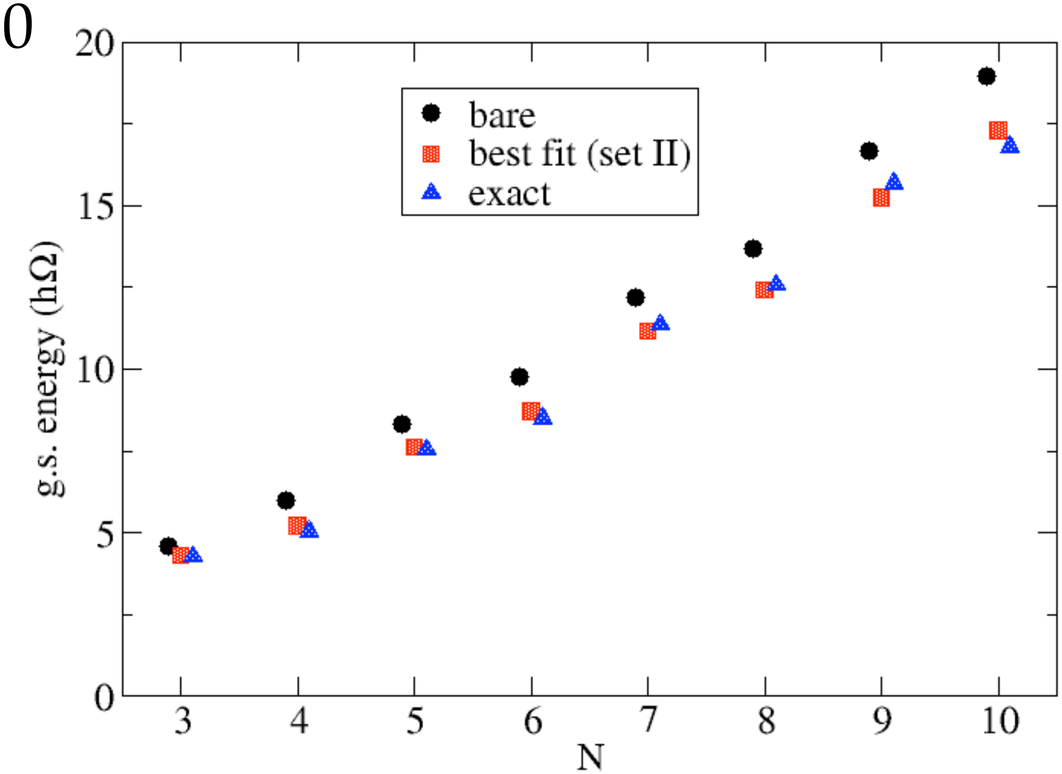
There are thus 10 generators of **A.**

Part 3: Cracking the off-shell degrees of freedom in in "realistic" interactions

Sample application: cold atomic gases at unitarity in a harmonic trap

Using all generators, fit to g.s. energies for N = 3-10

starting rms = 2.32
final rms = 0.25

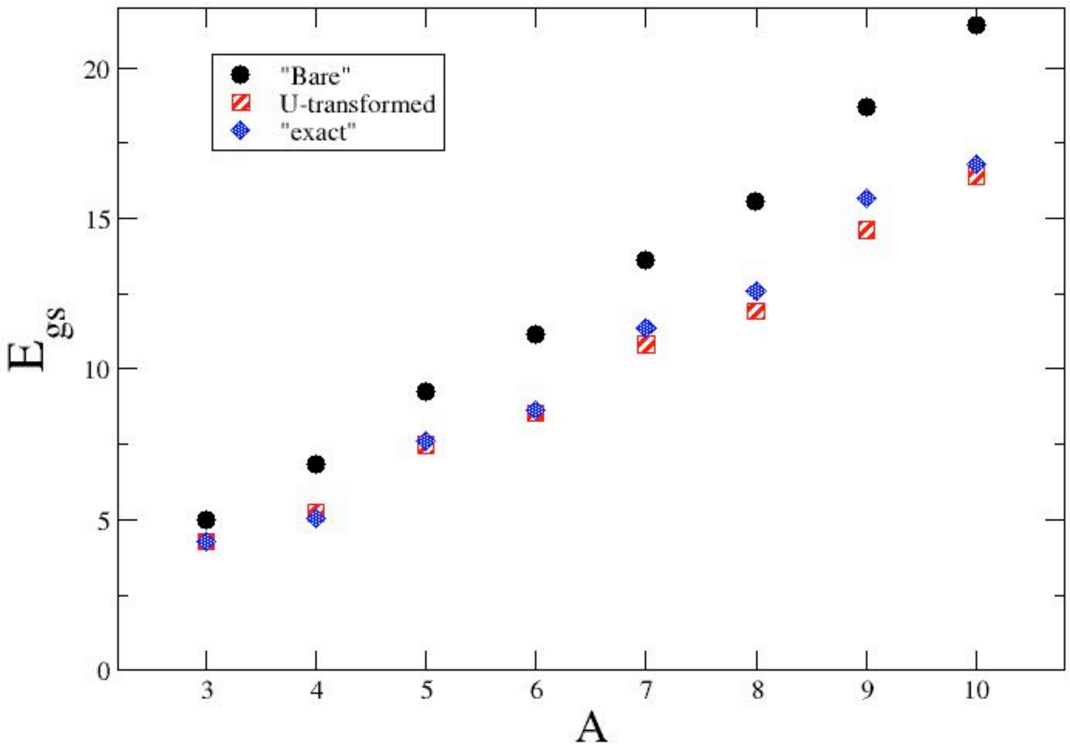


Sample application: cold atomic gases at unitarity in a harmonic trap

Using only 1 generator (d/dr) (very much like UCOM)

Fit to A =3, 1^-, 0^+
A = 4, 0^+, 1^+, 2^+

starting rms = 2.32
final rms = 0.58



I have developed a general formalism using unitary transformations that (a) preserve desired properties (on-shell matrix elements, eigenvalues) and (b) can be fitted to data.

Preliminary application to a cold atomic gas at unitarity is promising.

Next step: apply to nuclear systems
(more complicated, multi-channel;
not only binding energies, but also spin-orbit splitting usually attributed to 3-body forces)

Center of mass without exact factorization

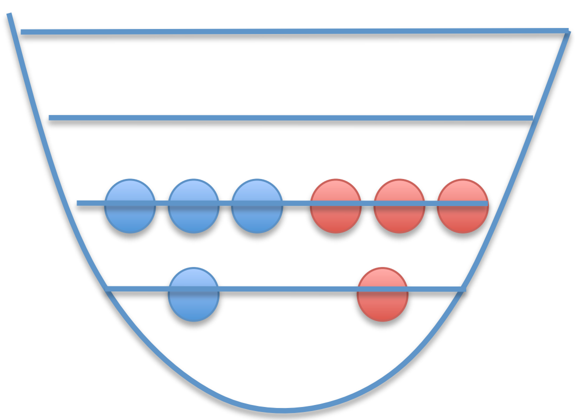
Center-of-mass is an important contamination in nuclear structure calculations.

A theorem (Palumbo, later Lawson) showed that in a h.o. basis, a specific truncation (the NhΩ truncation) guarantees a system with a translationally invariant interaction can decouple relative from c.m. motion.

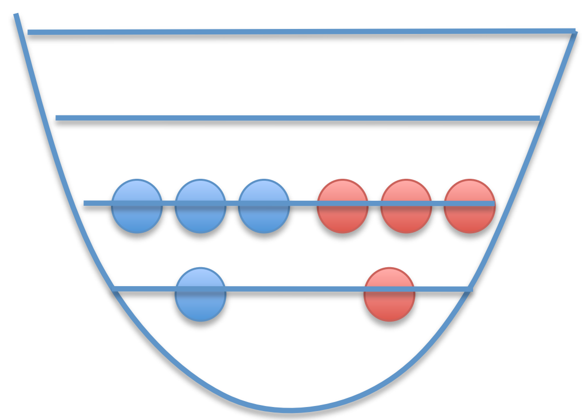
However a more "natural" truncation is by maximal orbits: this is natural in Hartree-Fock, coupled-cluster, etc.

A tale of two truncations

orbit truncation: all excitations



NħΩ (or energy) truncation: only those excitations in noninteracting h.o. with energy ≤NħΩ

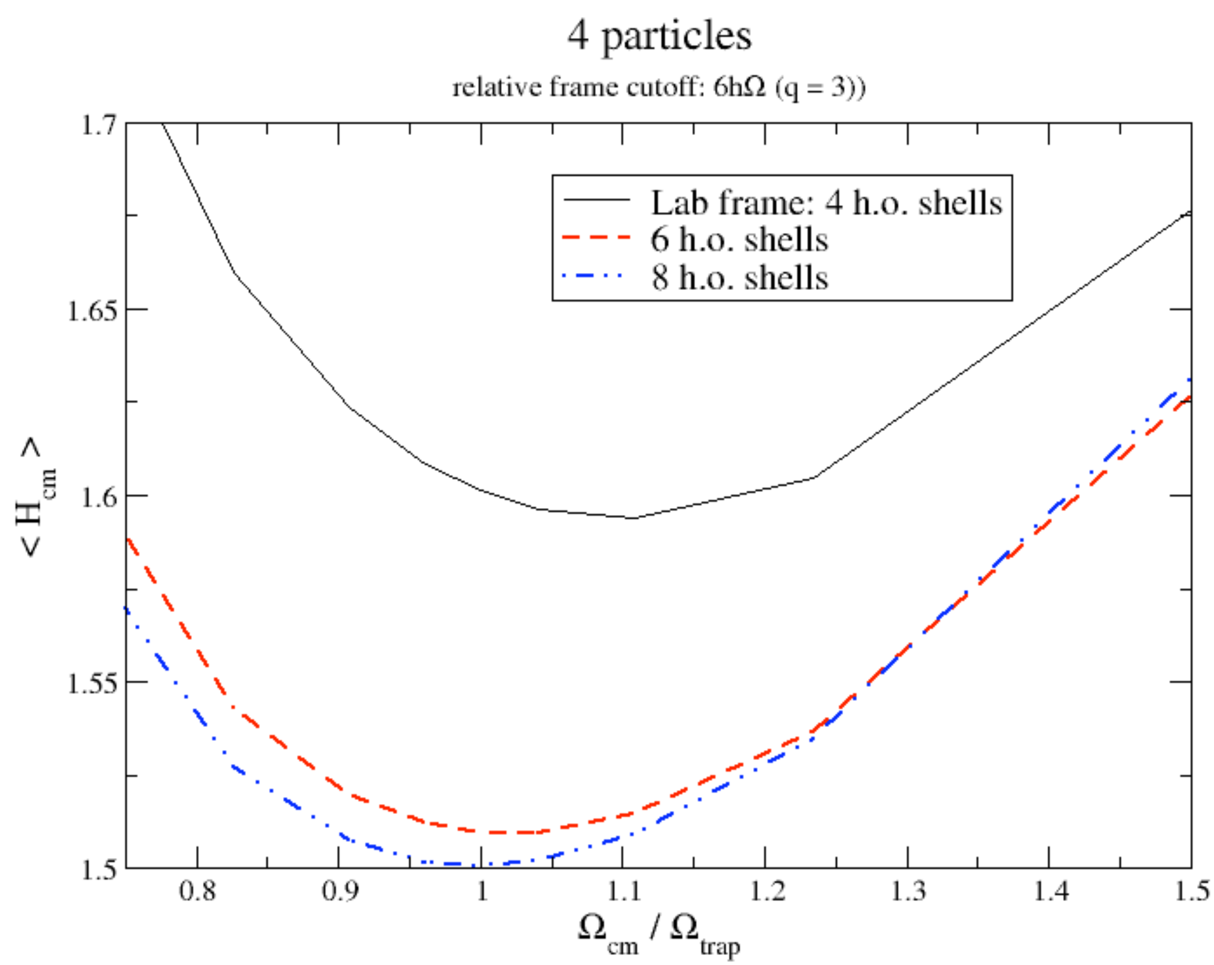


But is the orbit truncation bad?

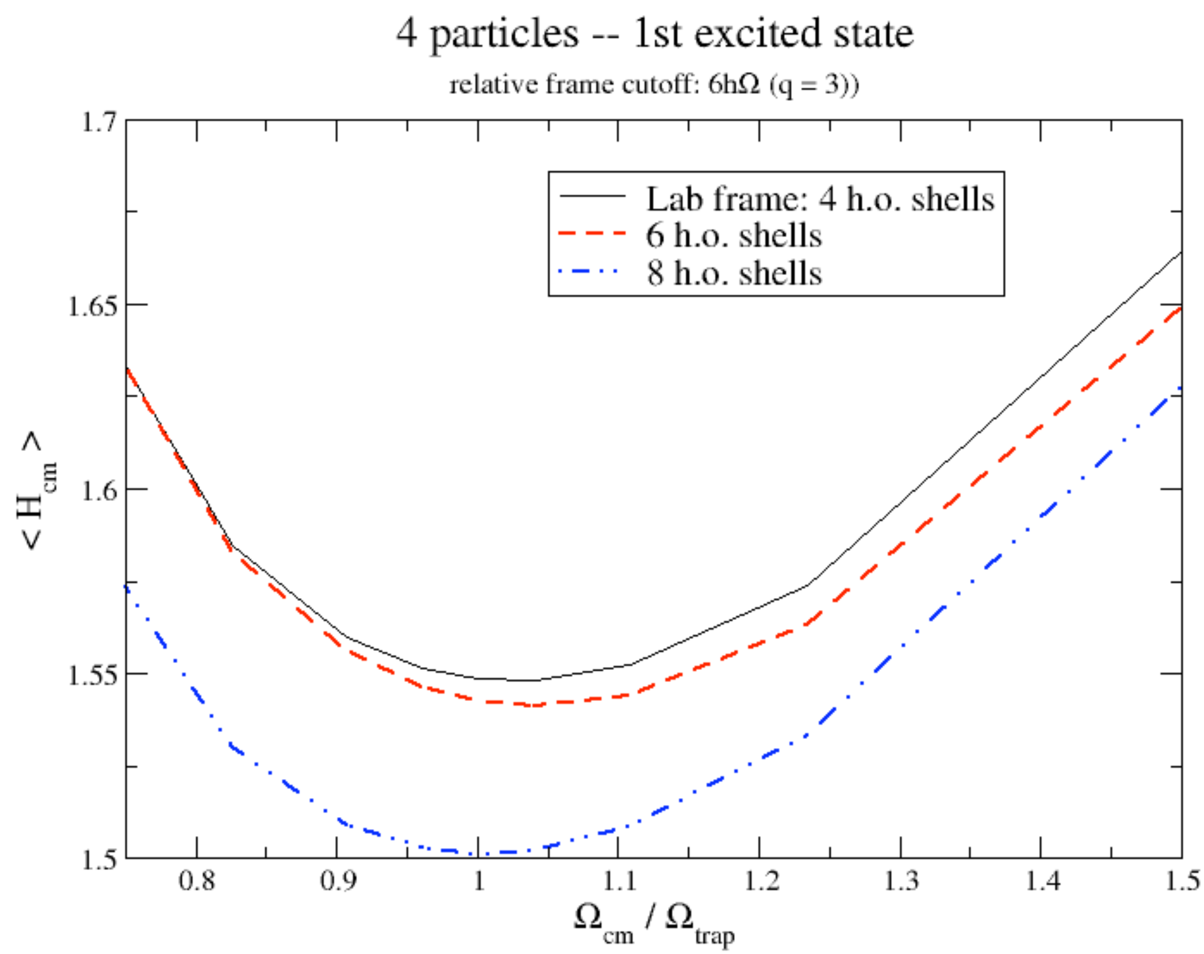
Hagen, Papenbrock, and Dean: in CC, look at $< H_{cm} >$

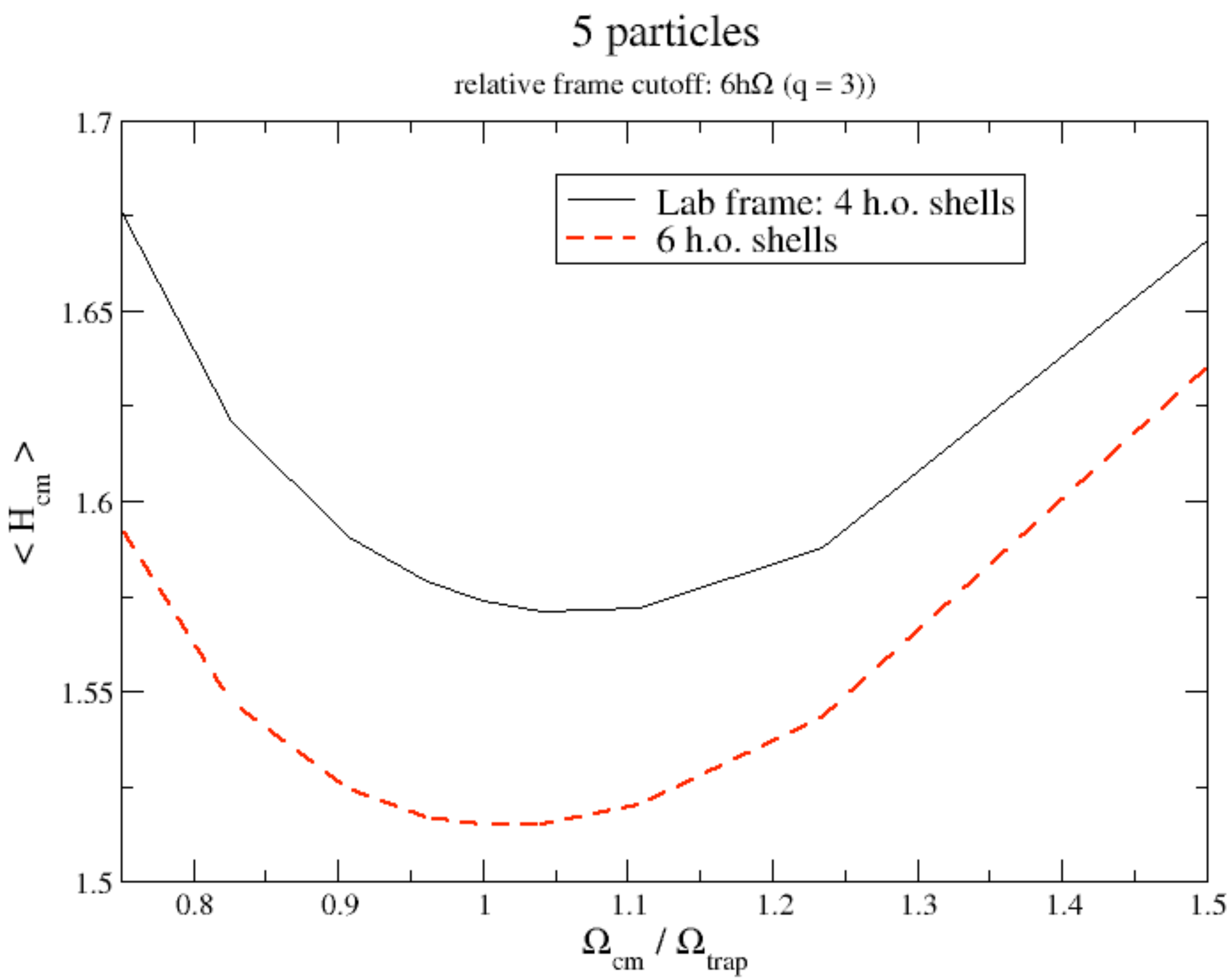
H_{cm} is minimized, only with h.o. frequency different from the basis

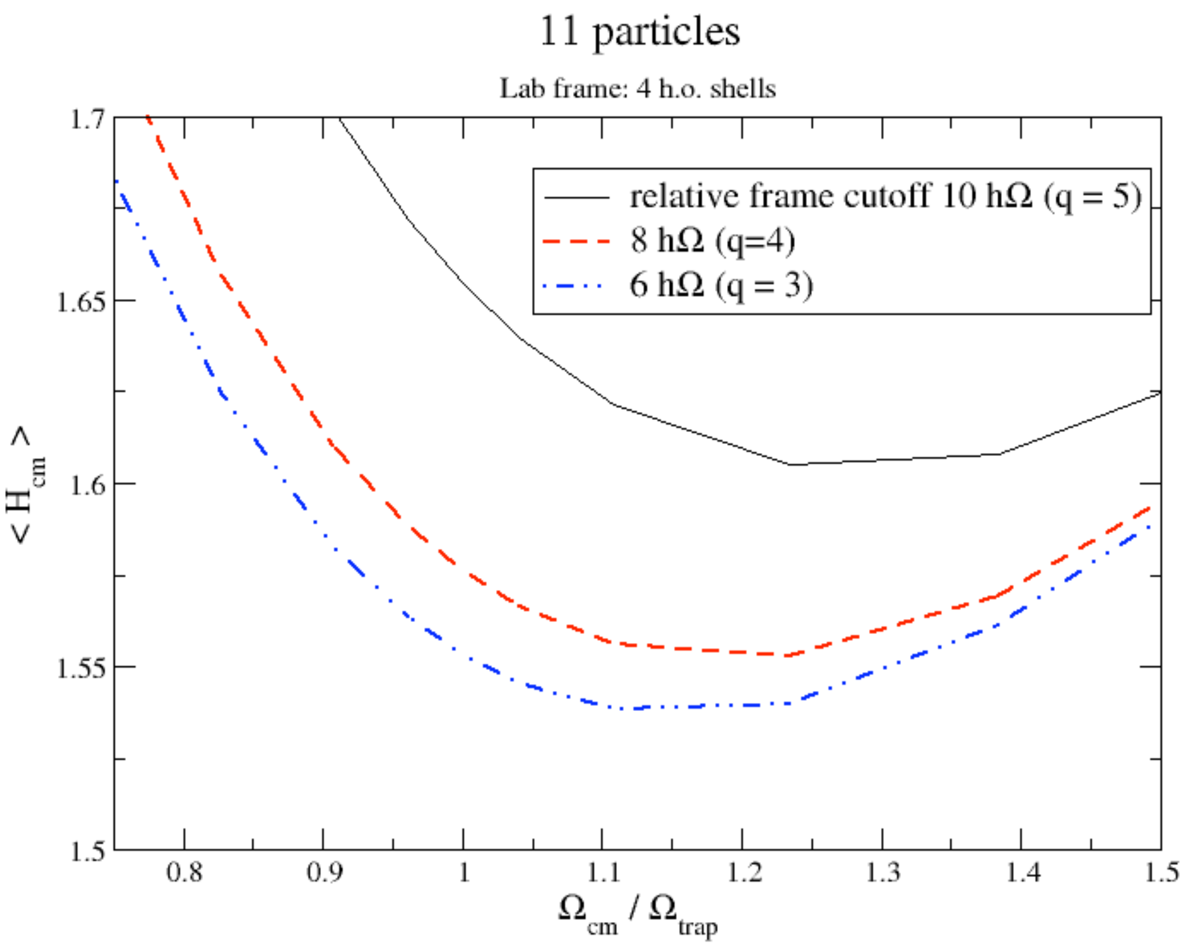
Roth, Gour, and Piecuch: in importance-truncated CI, look also at perturbations by adding βH_{cm}; considerable contamination in orbital truncation


4 particles
relative frame cutoff: 6hΩ (q = 3))
Lab frame: 4 h.o. shells
6 h.o. shells
8 h.o. shells
1.7
1.65
1.6
1.55
1.5
0.8
0.9
1
1.1
1.2
1.3
1.4
1.5
< H_cm >
Ω_cm / Ω_trap

Making Effective Interactions More Effective




5 particles
relative frame cutoff: 6hΩ (q = 3))
Lab frame: 4 h.o. shells
6 h.o. shells
< H_cm >
Ω_cm / Ω_trap
1.7
1.65
1.6
1.55
1.5
0.8
0.9
1
1.1
1.2
1.3
1.4
1.5



Need to look at sensitivity to adding $\beta H_{cm;}$

Work is under way for nuclei