Benchmarking the many-body problem

Cold Atomic Gases and Effective Interactions

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INT – March 28, 2011

Refs: C.W.J., Phys. Rev. C **82**, 031303(R) (2010).
Stetcu *et al*, PRA **76** 063613 (2007)
Alhassid, Bertsch, Fang, PRL **100** 230401 (2008)

Consider the *unitary fermi gas:*
*infinite scattering length
*zero range

If you put in a harmonic trap, then the *only* intrinsic scales (energy, length) are those of the trap!

We'll use *configuration interaction*,
or diagonalization in a shell-model basis.

The unitary fermi gas approximates the nuclear case (long scattering length, short range) but turns out to be even more challenging.

Prelude:
what goes into a shell-model calculation

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

Solve $\hat{H}\left|\Psi\right\rangle = E\left|\Psi\right\rangle$

where one expands in a Slater determinant basis:

$$\left|\Psi\right\rangle = \sum_{\alpha} c_{\alpha}\left|\alpha\right\rangle$$

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

Prelude: what goes into a shell-model calculation

The Hamiltonian is input in second quantization:

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

single-particle energies

two-body matrix elements

The single-particle energies and two-body matrix elements are integrals that implicitly depend upon the choice of single-particle wavefunctions.... but are computed externally to the CI code and are read in as **a file of numbers.** No restriction on form; can be non-local.

The BIG QUESTION:

What are these numbers? How do we get them?

Computing the Interaction

The two-body matrix element…

$$V_{ij\,kl} = \int d\vec{r} \int d\vec{r}' \cdot \phi_i^*(\vec{r}) \phi_j^*(\vec{r}') V(\vec{r} - \vec{r}') \phi_k(\vec{r}) \phi_l(\vec{r}')$$

…is a six-dimensional integral.

However, for **harmonic oscillator** single-particle states, there is an exact and **finite** transformation between the lab frame and the intrinsic frame

$$\phi_{n_1 l_1}(\vec{r}_1) \phi_{n_2 l_2}(\vec{r}_2) = \sum \langle n_1 l_1, n_2 l_2 | nl, NL \rangle \phi_{nl}(\vec{r}) \phi_{NL}(\vec{R})$$

Talmi-Moshinksy transformation bracket

Computing the Interaction

If the interaction $V = V(r)$, then one only needs to do a (finite set of) one-dimensional integrals in the relative frame:

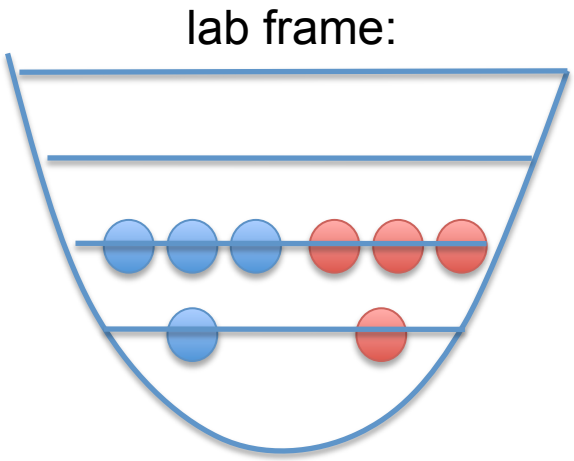
$$V_{ij\,kl} = \int d\vec{r} \int d\vec{r}' \cdot \phi_i^*(\vec{r})\phi_j^*(\vec{r}')V(\vec{r}-\vec{r}')\phi_k(\vec{r})\phi_l(\vec{r}')$$

$$V_{n'n} = \int u_{n'}(r)V(r)u_n(r)dr$$

V_{ijkl} = (finite sum over Talmi-Moshinsky brackets) × $V_{n'n}$

The trapped, two-component fermi gas at unitarity

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



V_0 tuned for infinite scattering length (cutoff-dependent)

(For example, you can find analytically for a square well the scattering length as a function of V_0 and well radius.)

Computing the Interaction

For a δ-interaction, this becomes (at first) even easier: only *s*-waves are nontrivial and the integral becomes trivial:

$V(r) = V_0\,\delta(r)$

$$V_{n'n} = \int u_{n'}(r) V(r) u_n(r) dr \quad \Rightarrow \quad V_0 \phi_{n'}(0) \phi_n(0)$$

All we have to do now is to choose V_0 to get an infinite scattering length….

Regularizing the δ-potential

In our case the cut-off is not in coordinate or momentum, but in the *harmonic oscillator quanta*.

That is, in the relative frame, we have the matrix elements $V_{n'n} = V_0 \phi_{n'}(0)\phi_n(0)$ with V_0 depending on the max value of $n = N_{max}$

But how do we determine V_0 to get a scattering length if we are now in a basis of harmonic oscillator states (all of which are bound)?

Regularizing the δ-potential

$$\frac{\hat{p}^2}{2m} + \tfrac{1}{2} m\omega^2 \hat{r}^2$$

Consider the *l* = 0 states for a 3D harmonic oscillator in the relative frame. The eigen-energies are 3/2ħω, 7/2 ħω, 11/2 ħω, 15/2 ħω ….

$$\frac{\hat{p}^2}{2m} + \tfrac{1}{2} m\omega^2 \hat{r}^2 - V_0 \delta^{(3)}(\vec{r})$$

If you have a δ-potential with an infinite scattering length + a harmonic oscillator, the eigen energies are 1/2ħω, 5/2 ħω, 9/2 ħω….

You can do this numerically by taking a finite square well with infinite scattering length and adding to it a harmonic oscillator

Regularizing the δ-potential

In the harmonic oscillator basis,

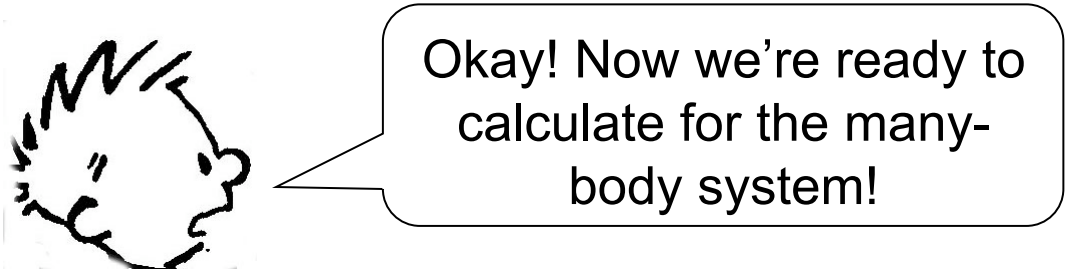
$$\hat{H}_{rel} = \frac{\hat{p}^2}{2m} + \tfrac{1}{2} m\omega^2 \hat{r}^2 - V_0 \delta^{(3)}(\vec{r})$$

$$\left\langle n' \left| \hat{H}_{rel} \right| n \right\rangle_{l=0} = \delta_{n'n}(2n + \tfrac{3}{2})\hbar\omega - V_0 \Psi_{n'}(0)\Psi_n(0)$$

One can find an analytic expression for V_0 so that the ground state has energy 1/2$\hbar\omega$ for any N_{max} (Y. Alhassid)

The rest of the spectrum, however, will be approximate due to the cut-off

The many-body calculation



Step 1: Choose a cut-off N_{max} and generate the interaction in the relative frame.

Step 2: Need to choose a many-body space – for us this is the maximal # of orbits in the lab frame, N_{orbit}

Step 3: Generate the two-body matrix elements going from the relative frame to the lab frame via Talmi-Moshinsky transformation…

….and run through a CI-shell model code!

Introduction to Effective Interactions

For nuclear physics, “hard core”
makes calculations troublesome.

Strong, short-range part of interaction means one has strong coupling to high-momentum/high energy orbits.
Bare interaction requires many orbitals to converge.

Thus, many orbits are required…too many
for most CI calculations (possible for coupled cluster)

Alternately, one creates a renormalized *effective interaction* that implicitly accounts for the sums to high-momentum states,

e.g., Brueckner G-matrices.

In more modern approaches we generally use a unitary transformation in the relative frame:

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

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.**

Effective interactions

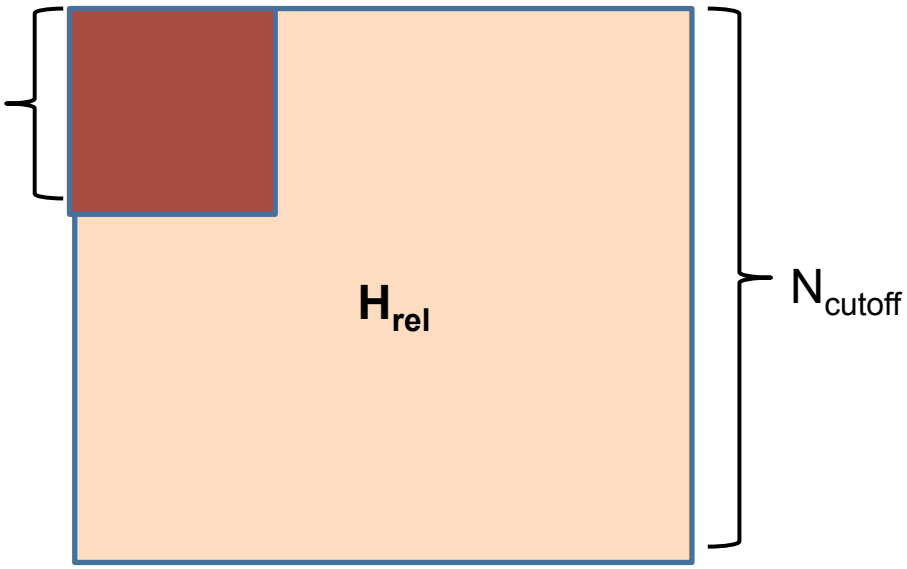
Example: Okubo-Lee-Suzuki-Okamoto (+…) methodology:

Start with some large cutoff so that the low-lying spectrum is correct (N_{cutoff} ~ 250 – 1000)

This relative space is too large to handle in a many-body calculation

We want to truncate to some smaller N_{max} ~ 2 – 10…
but want the correct spectrum in this smaller space

Relative frame:



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Effective interactions

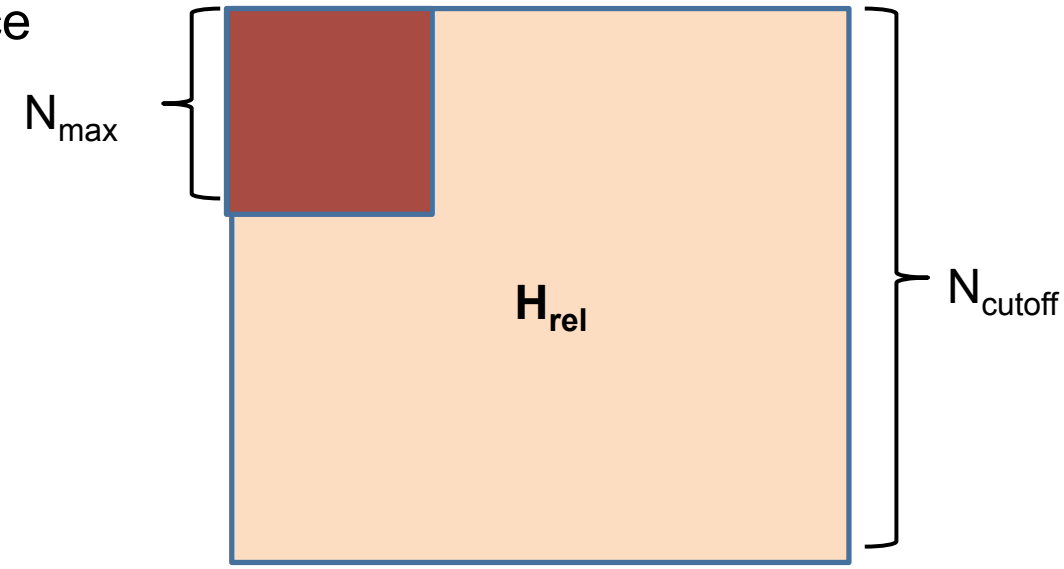
We follow the Okubo-Lee-Suzuki-Okamoto (+…) methodology:

We introduce a unitary transformation in the relative space which decouples the smaller model space (dim N_{max}) from the larger cutoff space

$$\mathbf{H_{rel}} \longrightarrow \mathbf{H'_{rel} = U^{+}H_{rel}U}$$

After this we transform to the lab frame.

Relative frame:



(NB: in the lab frame, the unitary transformation induces three-body, four-body, etc. forces)

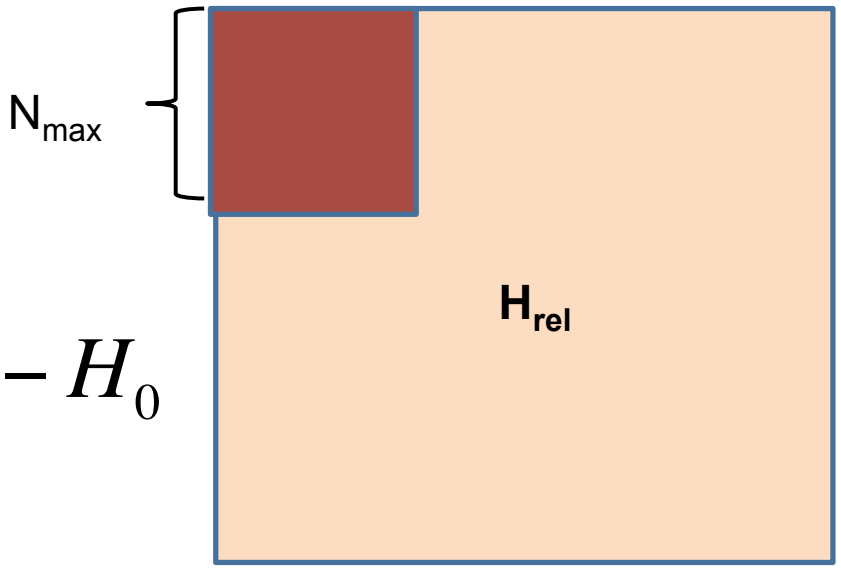
Effective interactions

An alternative one for the unitary fermi gas is the Alhassid-Bertsch-Fang, which yields (in h.o. space) a separable interaction.

Here the unitary transformation is only implied, not explicit. The result depends only on N_{max} , not N_{cutoff}.

$$V_{eff} = U^{+}(H_0 + V)U - H_0$$

Relative frame:



Alhassid et al *PRL* 100 230401 (2008)

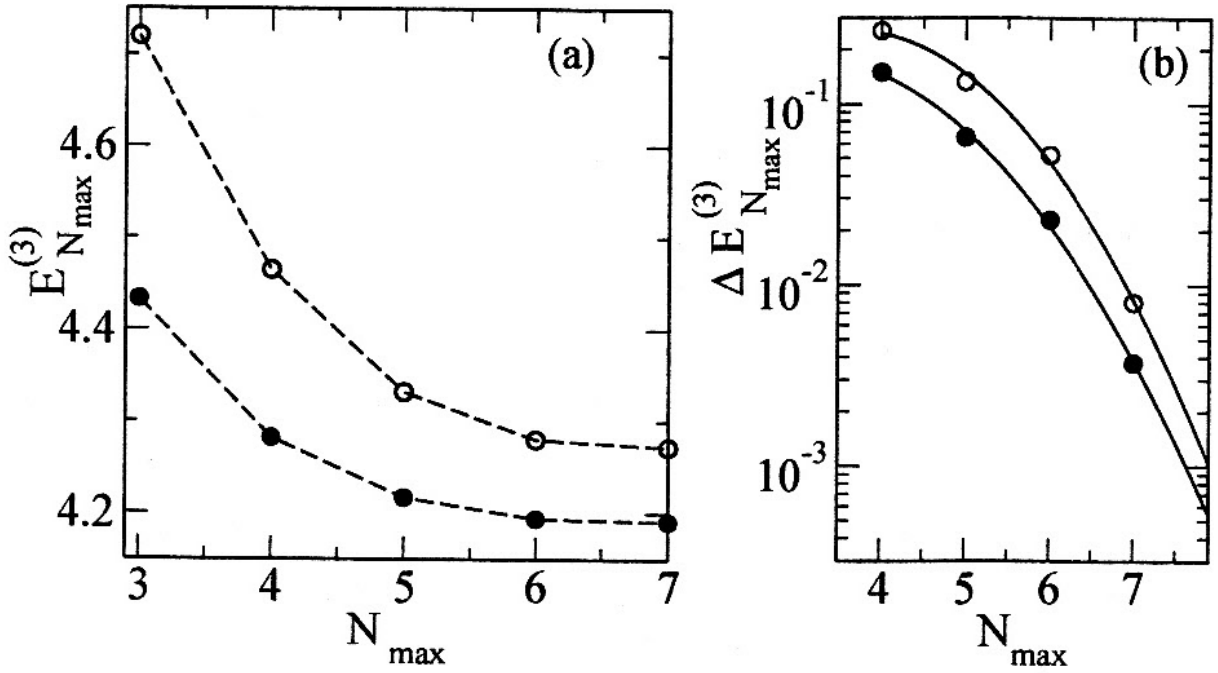


FIG. 1: Convergence in $N_{\max}$ for the $A = 3$ ground-state energy. (a) $E^{(q)}_{N_{\max}}$ versus $N_{\max}$ for $q = 3$. Open circles correspond to the renormalized contact interaction and solid circles to the interaction defined by (8) and (10). (b) $\Delta E^{(3)}_{N_{\max}}$ versus $N_{\max}$ in a logarithmic scale. All energies are in units of $\hbar\omega$.

q+1 = dimension in relative space (max relative excitement is 2q hw) = cutoff in relative harmonic oscillator
= "V-low-N_{max}"

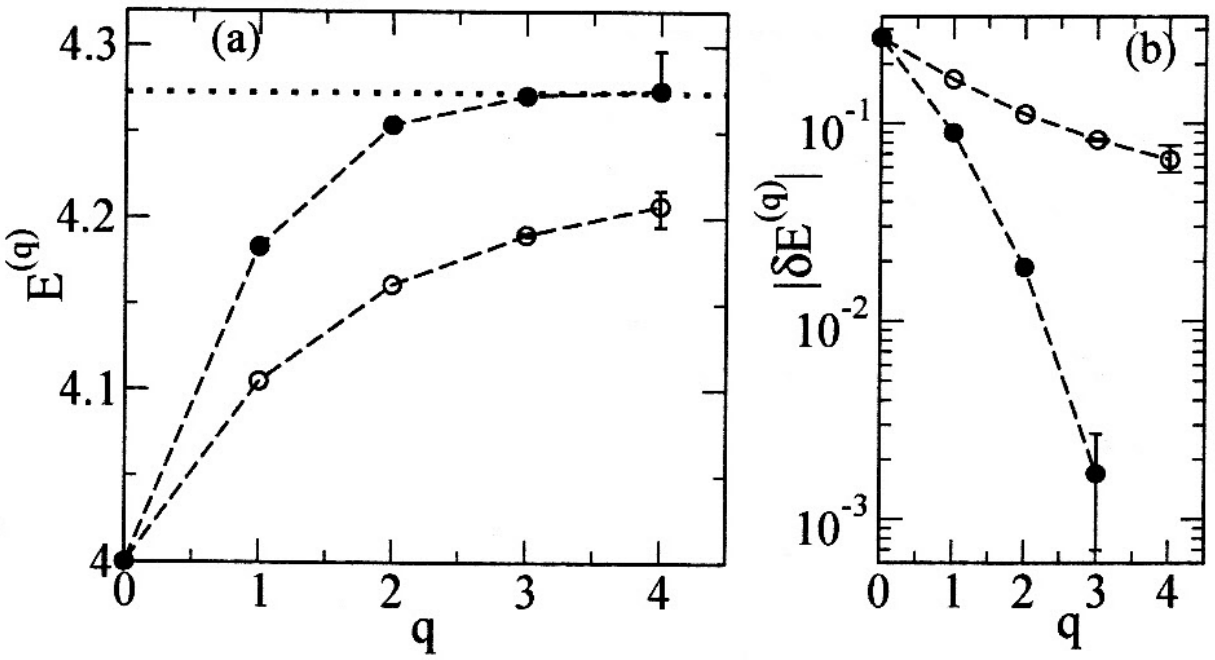
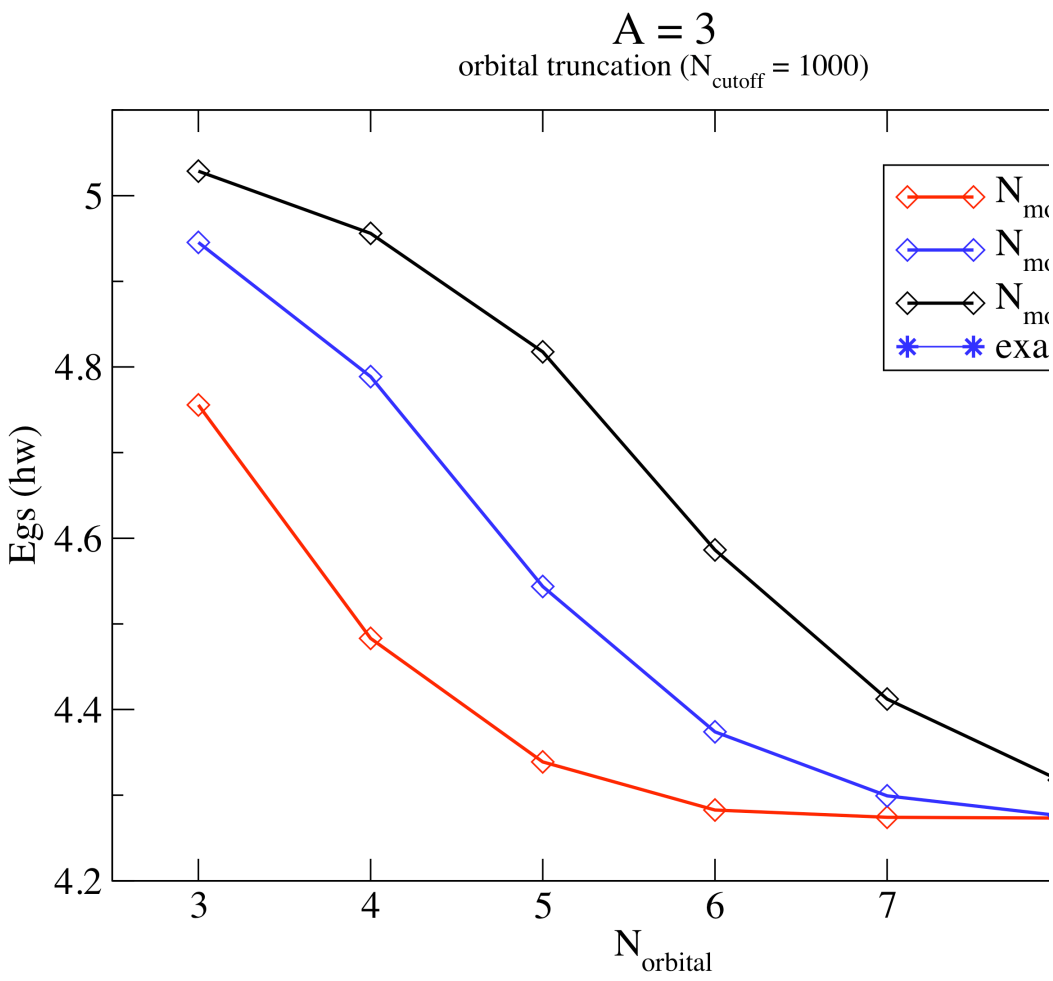
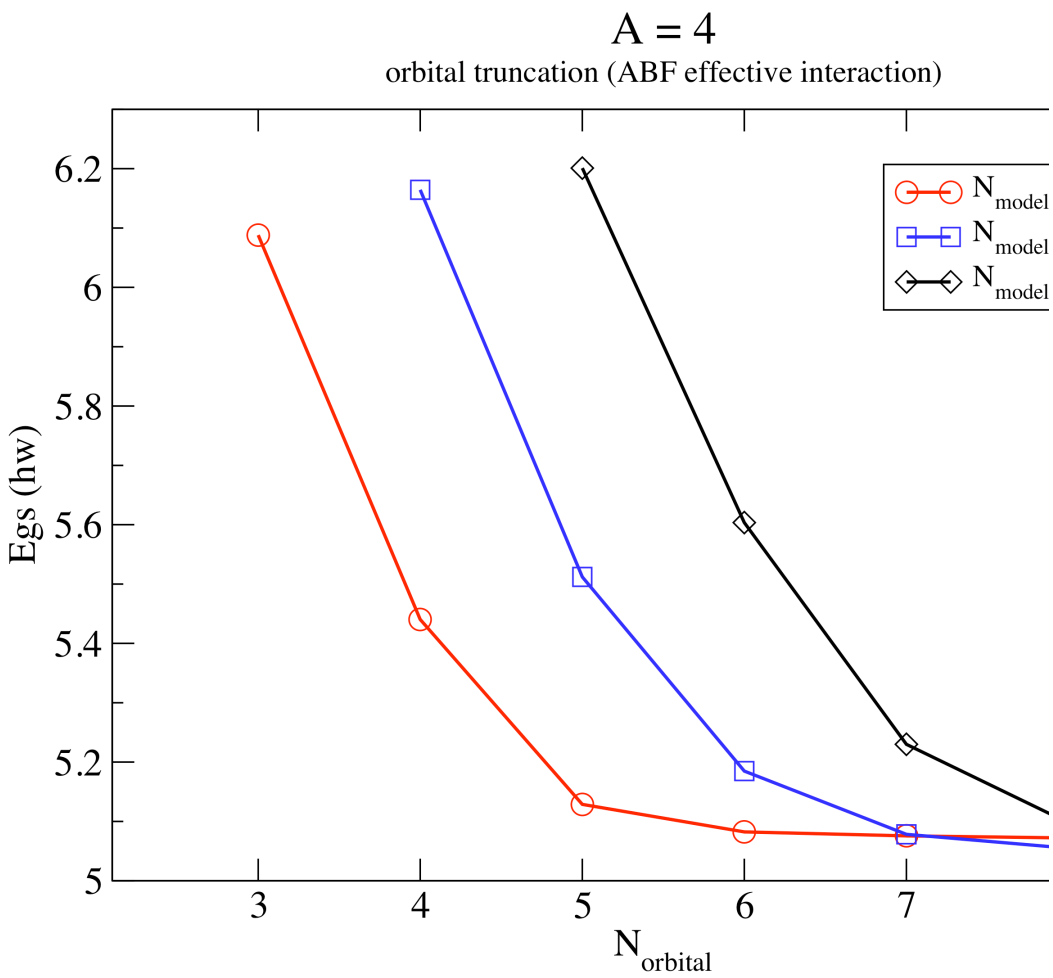


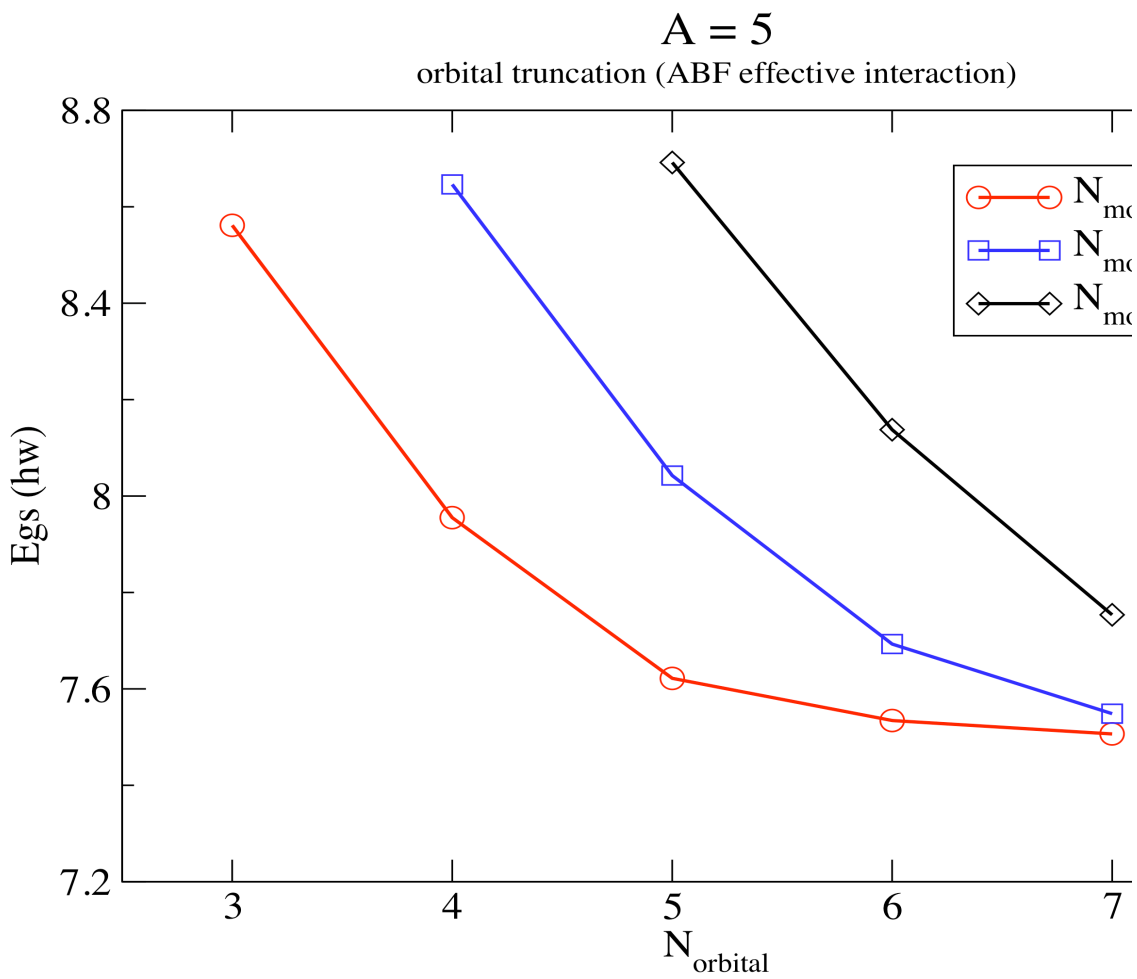
FIG. 2: Convergence of the q-regulated energies for the $A = 3$ ground state. (a) $E^{(q)}$ versus q for both interactions (symbols and units as in Fig. 1). The dotted line is the exact ground-state energy. (b) The error $|\delta E^{(q)}|$ in a logarithmic scale.

After extrapolating to large N_{orbit} for fixed q (cut-off), must extrapolate to large q.

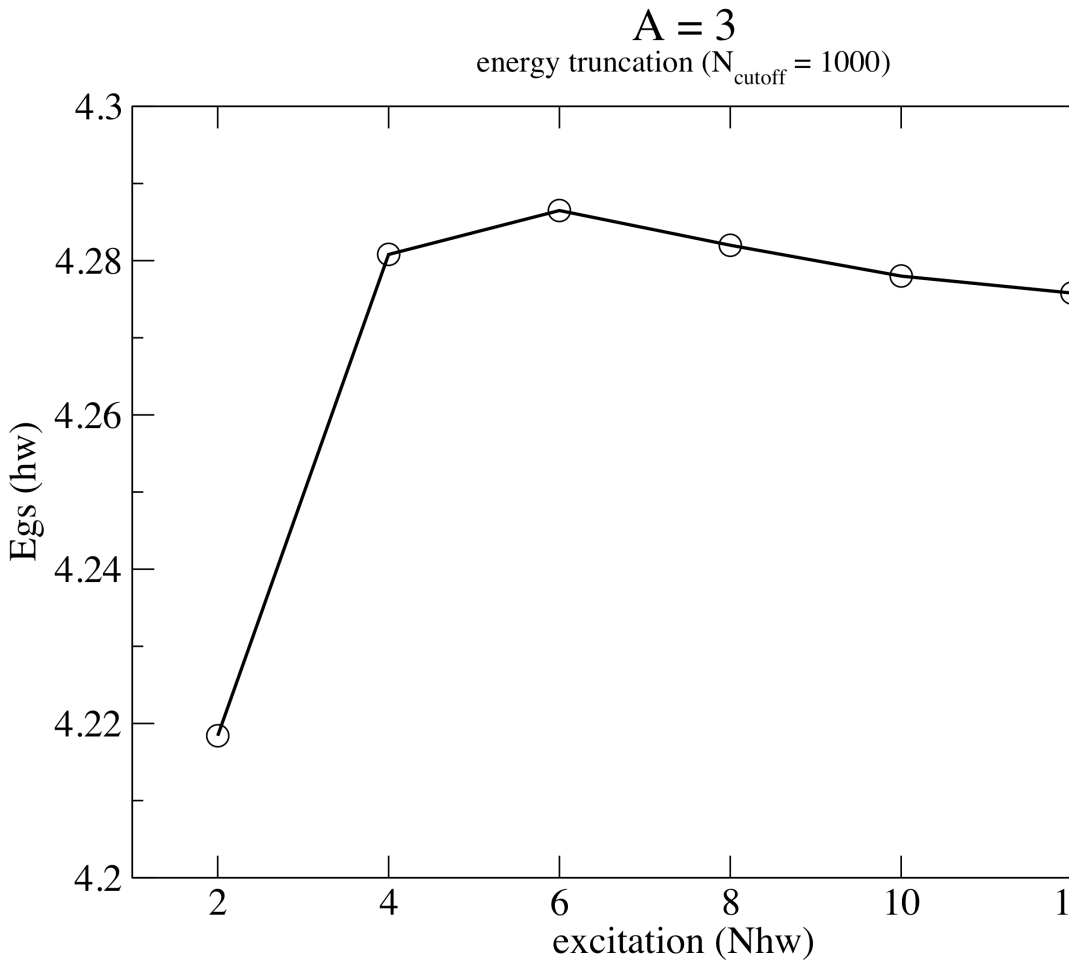
Using Okubo-Lee-Suzuki; requires large initial cutoff



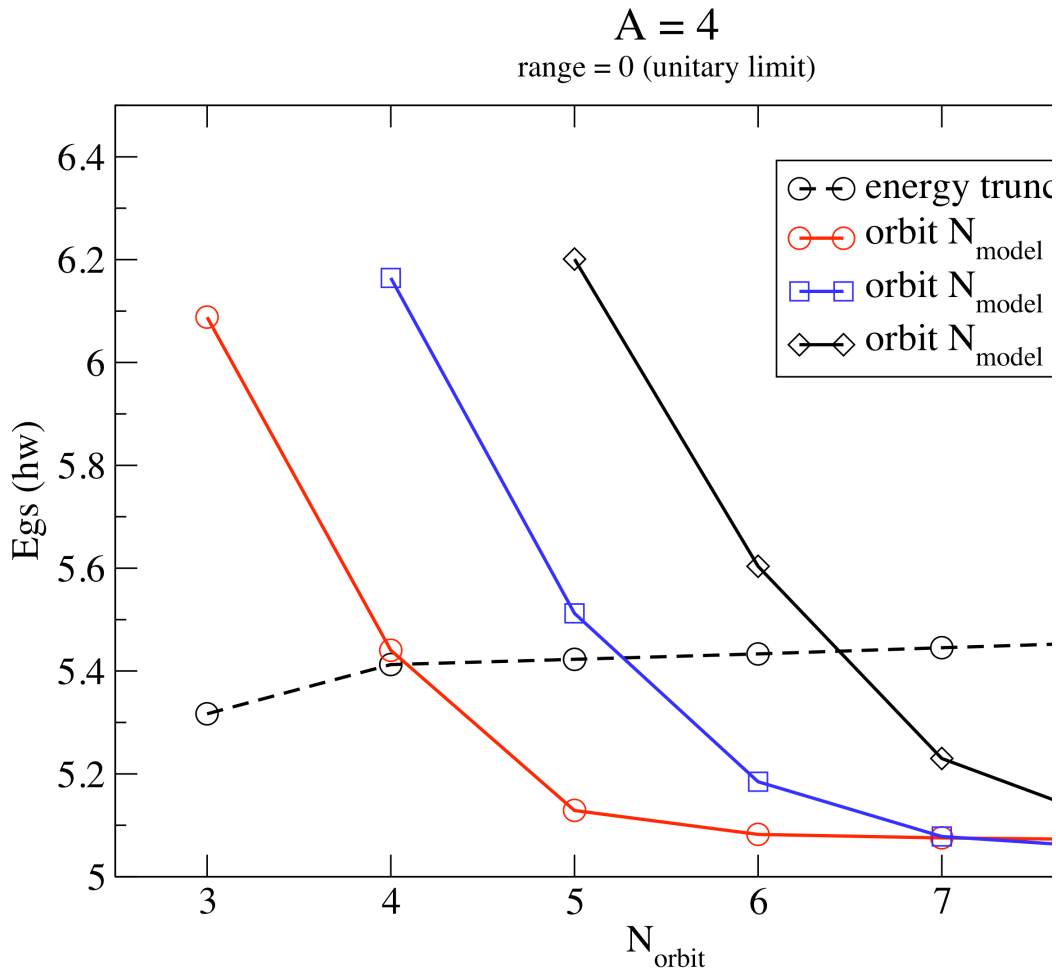

A = 4
orbital truncation (ABF effective interaction)
Egs (hw)
6.2
6
5.8
5.6
5.4
5.2
5
3
4
5
6
7
N orbital
N model
N model
N model


A = 5
orbital truncation (ABF effective interaction)
8.8
8.4
8
7.6
7.2
Egs (hw)
3
4
5
6
7
N orbital
N mc
N mc
N mc

The same “energy” or Nhw truncation as used in the “no-core shell model” in nuclear physics



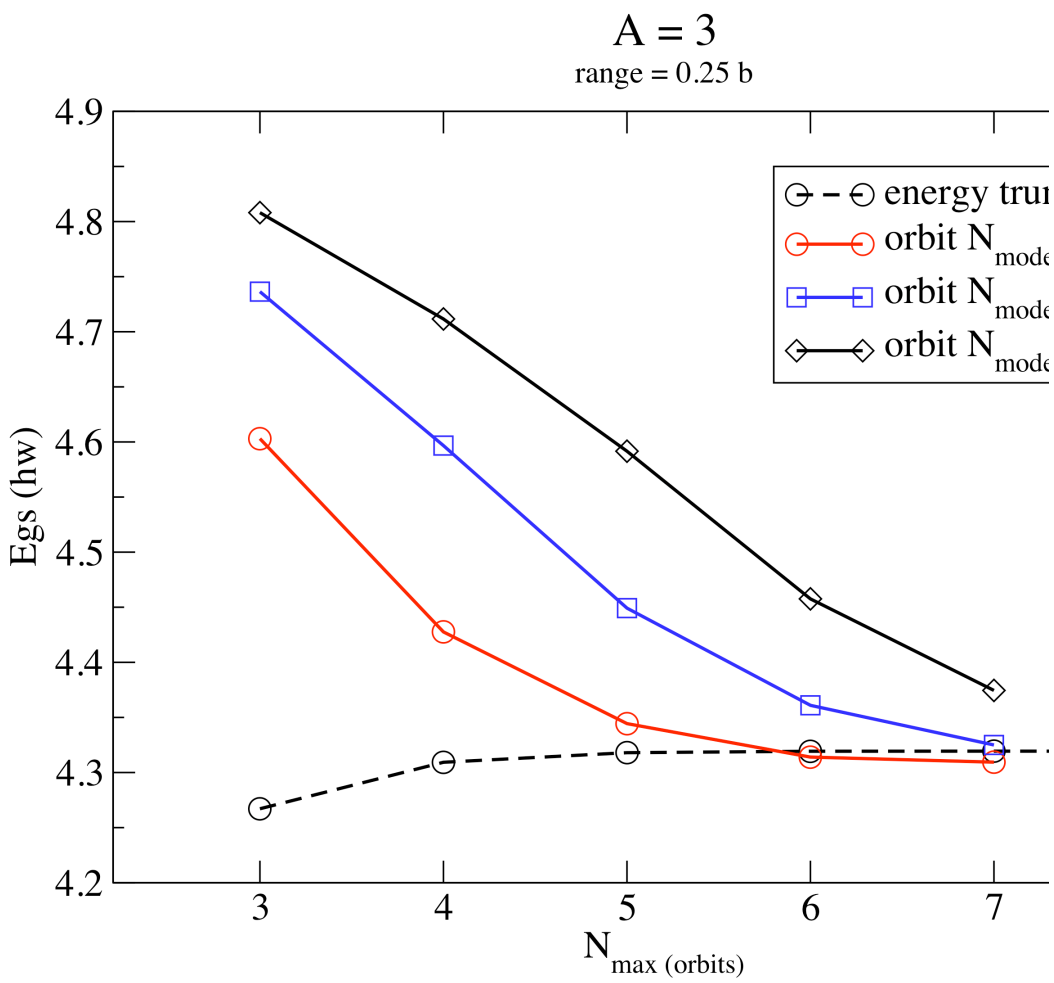
The same "energy" or Nhw truncation as used in the "no-core shell model" in nuclear physics – slow convergence (see also Stetcu *et al*, PRA **76** 063613 (2007))

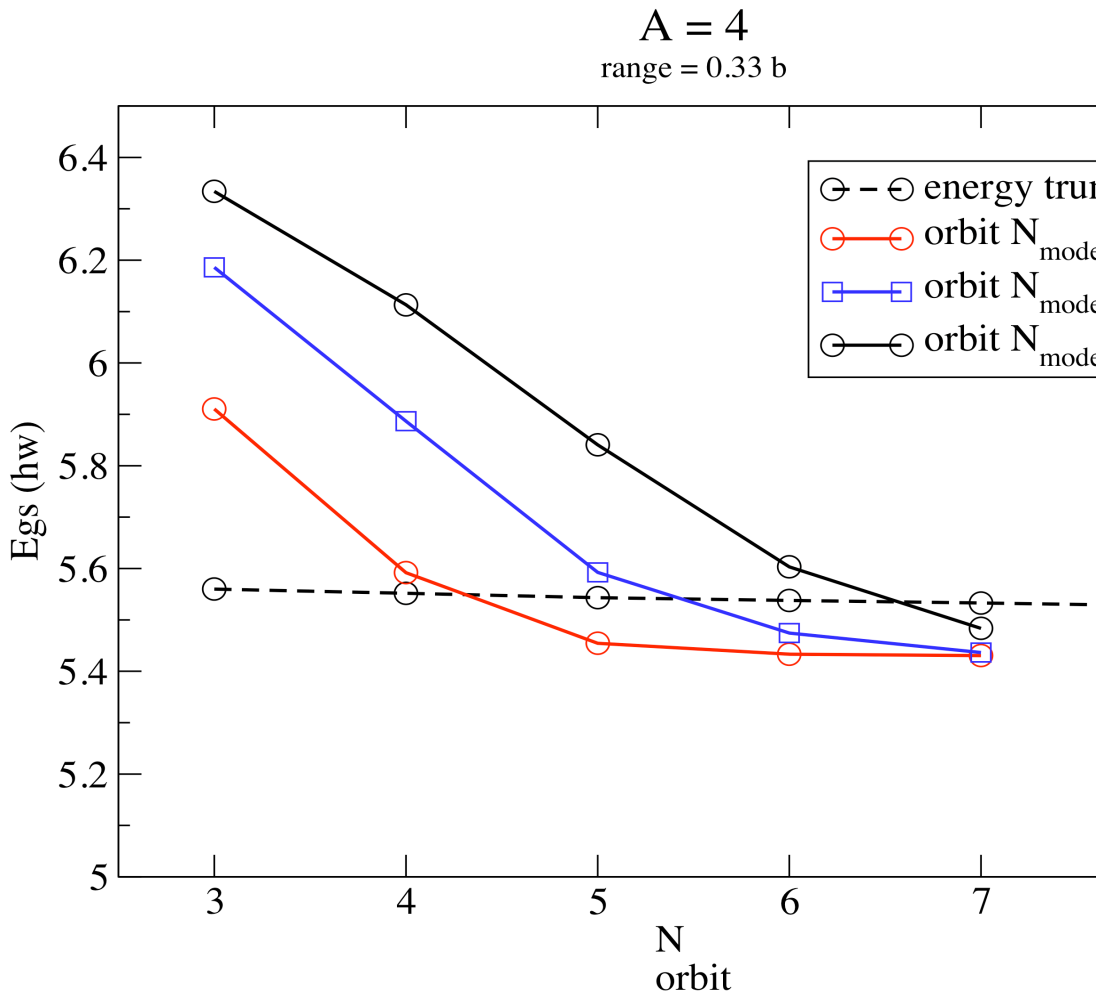


What's behind the slow convergence?

The culprit seems to be the zero range.

We can test this by using a finite square well but with infinite scattering length.


A = 3
range = 0.25 b
4.9
4.8
4.7
4.6
4.5
4.4
4.3
4.2
Egs (hw)
3
4
5
6
7
N max (orbits)
energy trui
orbit N mode
orbit N mode
orbit N mode


A = 4
range = 0.33 b
Egs (hw)
6.4
6.2
6
5.8
5.6
5.4
5.2
5
3
4
5
6
7
N
orbit
energy trui
orbit N
mode
orbit N
mode
orbit N
mode

Making effective interactions more effective

"Hard core" or short range makes calculations troublesome.

Hence, one creates a renormalized *effective interaction*
that implicitly accounts for the sums to high-momentum states,
today via unitary transformations

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

This is often traced back to the need for 3-body forces.
Effective interactions also induce 3- (and *A*-) body forces.

Making effective interactions more effective

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...

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 $E_\alpha{}^0$ be the experimental (target) energies.

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

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

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

Hellmann-Feynman theorem:

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

Here we're working in the *lab frame* and adjusting the two-body matrix elements V_{ijkl}

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

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

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

$$\cong \sum_\alpha \left(E_\alpha^0 - E_\alpha - \sum_i \partial E_\alpha / \partial c_i \cdot \delta c_i \right)^2$$

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

$$\cong \sum_\alpha \left(E_\alpha^0 - E_\alpha - \sum_i \partial E_\alpha / \partial c_i \cdot \delta c_i \right)^2$$

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

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

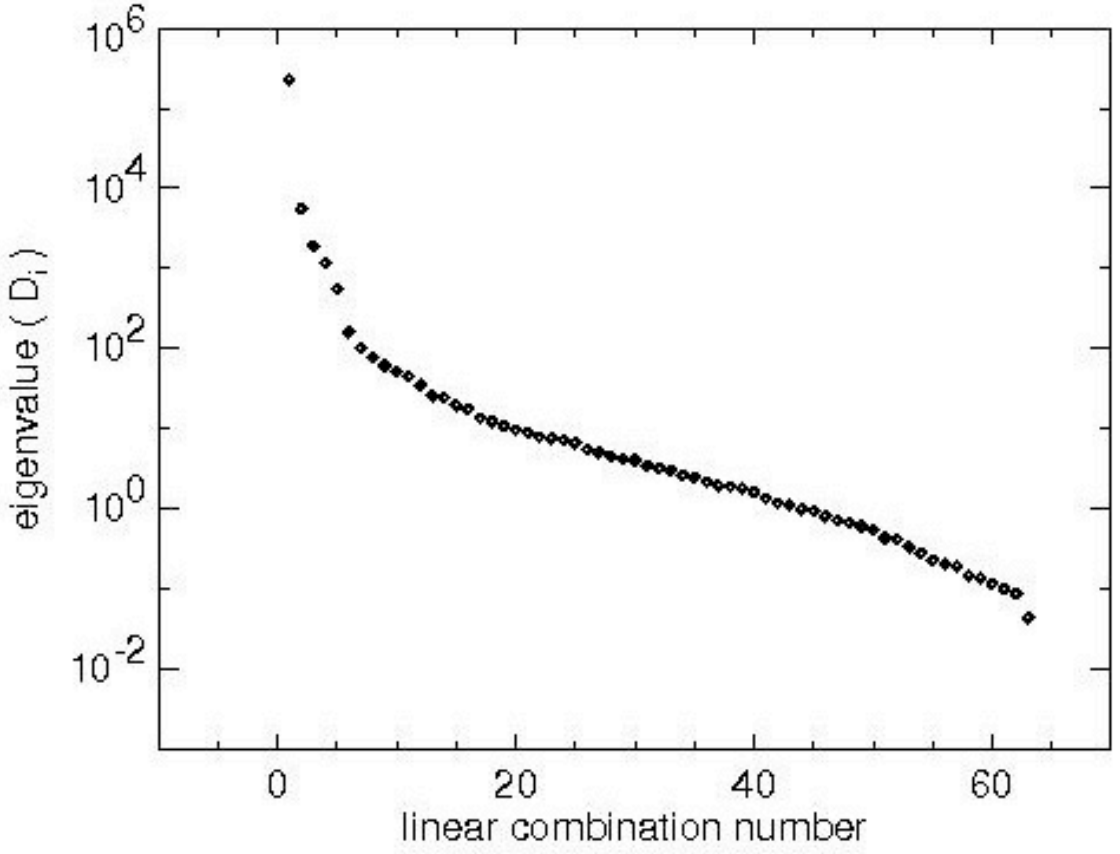
Formally the solution to $\mathbf{B}^T\mathbf{B}\vec{c} = \mathbf{B}^T\delta\vec{E}$

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

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

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

SVD eigenvalues
for USDB in *sd*-shell

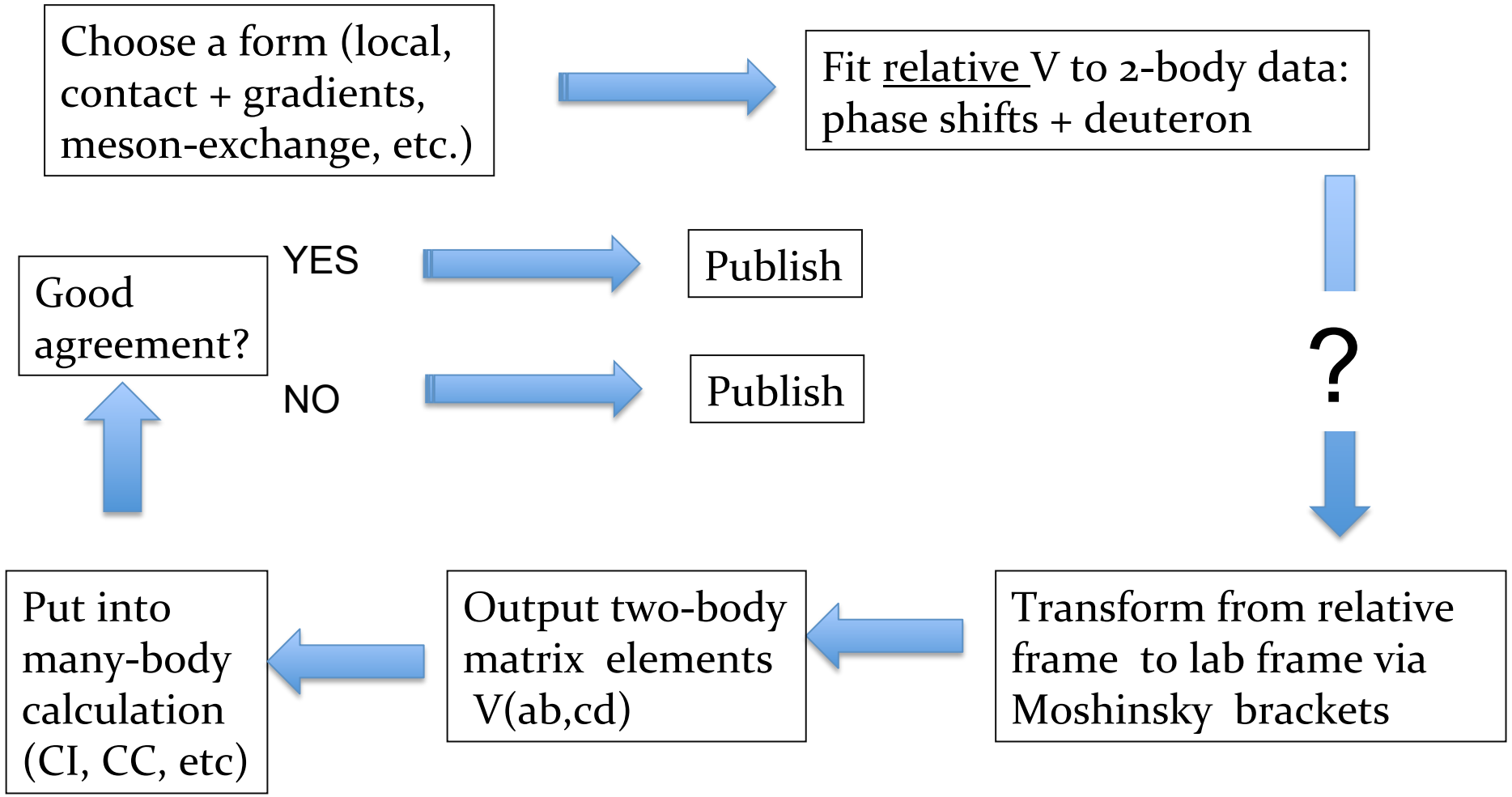


What about "realistic" effective nuclear interactions?

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

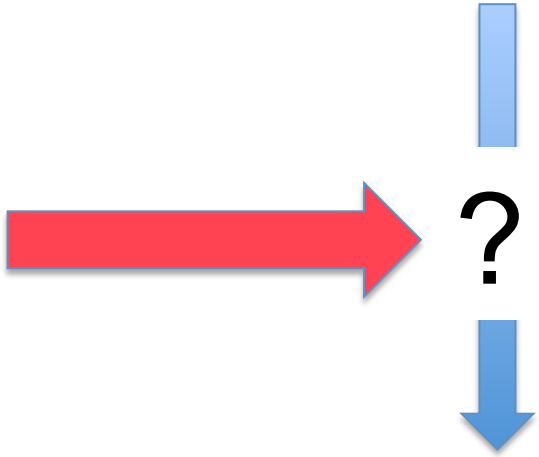
A: Match experimental data!

Life cycle of a realistic interaction:



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

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

Transform from relative frame to lab frame via Moshinsky brackets

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., the INOY and JISP16 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?

Never waste a crisis, *or*, Cracking the off-shell degrees of freedom in in "realistic" 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

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

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

USDB etc: work in lab frame, perturb Hamiltonian

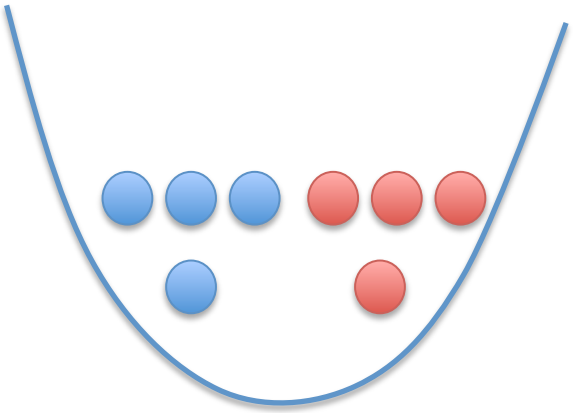
New: we perturb the generators of the unitary transformation in the relative frame

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

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

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

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



V_0 tuned for infinite scattering length (cutoff-dependent)

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

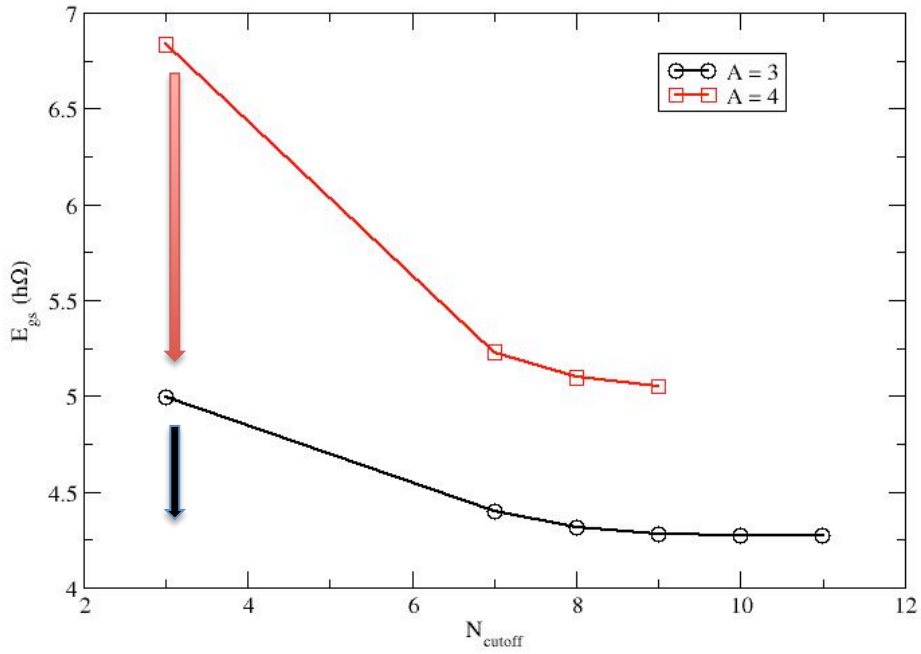
Sample application: cold atomic gases at unitarity in a harmonic trap

Only *s*-wave channel in relative coordinates

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

Slow convergence in CI calculations.

Use ABF regularization
Alhassid, Bertsch, Fang, PRL**100**, 230401(2008)
with cutoff of 10ħΩ
(in relative *s*-channel)



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

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

Use ABF regularization
with cutoff of 10ħΩ
(in relative *s*-channel).

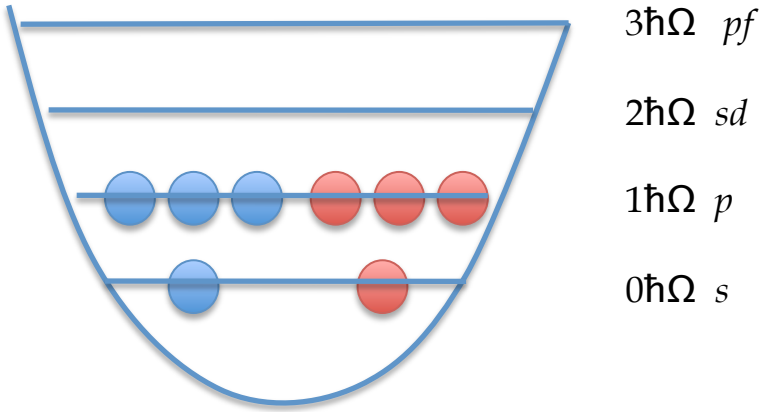
In lab frame, cutoff of 3ħΩ

For preliminary study:

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

A = 4, 0^+,1^+, 2^+

or to A = 3-10 g.s.



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

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

Fit to 5 states in A = 3,4;
"prediction" is comparison against g.s. of all A = 3-10
(all energies in units of trap hw)

starting H_{rel}	initial rms	fit rms	rms of prediction
bare	0.62	0.10	0.32
ABF	1.06	0.06	0.37

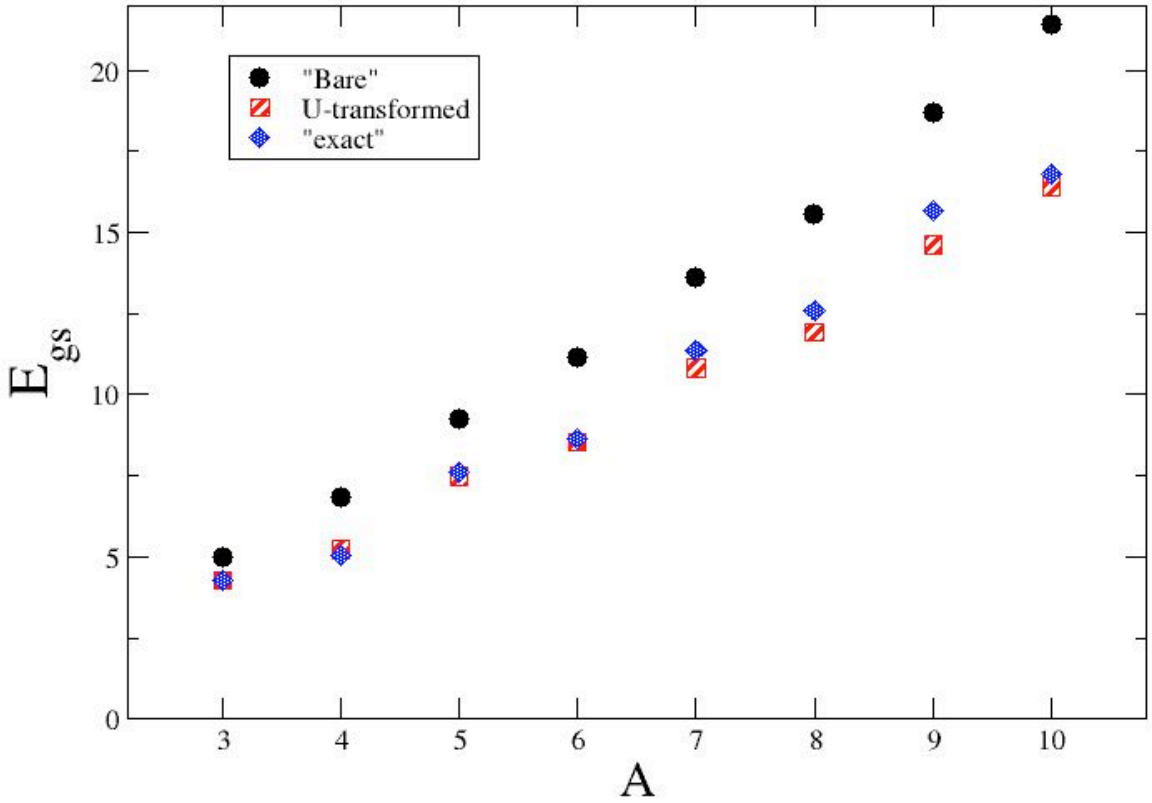
Fit to g.s. energies of A = 3-10
(all energies in units of trap hw)

starting H_{rel}	initial rms	fit rms
bare	1.16	0.28
ABF	2.32	0.25

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 only 1 generator (d/dr)



Conclusions and summary

I have discussed two powerful tool for analyzing and "improving" effective interactions:

-- Singular value decomposition, to find most important degrees of freedom when fitting to data

-- similar behavior both with empirical and random interactions

-- Unitary transformations, to adjust off-shell matrix elements

Conclusions and summary

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)