Spectral distribution theory
and
the evolution of forces
under
the similarity renormalization group

Calvin W. Johnson
San Diego State University
"Insert Motto Here"

"This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics, under Award Number DE-FG02-96ER40985"

Spectral distribution theory
and
the evolution of forces
under
the similarity renormalization group
applied to nuclear many-body systems
for the purpose of illustrating prinicples of physics

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"Insert Motto Here"

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Motivation:

Modern high-performance computing is both a blessing and a curse

We can calculate to higher precision and with less tuning

But we nearly drown in numbers:
for example

- No-core shell model dimension > 10^{10} basis states
- Number of 3-body matrix elements ~ $10^7 – 10^{10}$

(cf. K. Hebeler's talk)

- …

Richard Hamming: "The purpose of computing is insight, not numbers"

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Motivation:

Can we find more succinct ways to characterize *ab initio* nuclear physics?

(Example: describe wavefunctions in terms of group irreps
--SU(3), SU(4), L and S subgroups of SU(2) --

One finds very similar L-S decomposition between *ab initio* chiral forces and phenomenological Cohen-Kurath force CWJ, Phys. Rev. C **91**, 034313 (2015))

Spectral distribution theory and SRG……

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Motivation:

Can we find more succinct ways to characterize *ab initio* nuclear physics?

Today: "Spectral distribution theory" a.k.a. "Statistical spectroscopy"

What's that mean?

Spectral distribution theory =
Averages, traces, and number operators

Spectral distribution theory and SRG……

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My talk in a nutshell:

1. **A case study: No-core shell model (NCSM) (= matrix diagonalization) of ^{12}C under evolution of the similarity renormalization group (SRG)**

2. **Under SRG:**
   Some things change a lot,
   some things change a little → illuminated by SDT

3. **"Yes, but what can you do for me?"**

   Compare and contrast interactions
   A path to better truncation/single particle orbits?

Work in progress!!

Spectral distribution theory and SRG……

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Configuration interaction a.k.a. interacting shell model (including the *no-core shell model*)

Diagonalize the nuclear Hamiltonian in a basis (typically Slater determinants with fixed quantum numbers such as total J_z = "M-scheme" or total J "J-scheme" or other quantum numbers e.g. SU(3) or symplectic or….)

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$$\mathbf{H}\vec{v} = E\vec{v}$$

Spectral distribution theory and SRG……

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$$\mathbf{H}\vec{v} = E\vec{v}$$

Dimensions up to ~ 10^{10}
can choose a smaller basis with richer physics (J-scheme, SU(3)-scheme, symplectic scheme) but more complicated to calculate
or
simpler basis easy to calculate with but large dimensions (M-scheme)

Configuration interaction a.k.a. interacting shell model
(including the *no-core shell model*)

Diagonalize the nuclear Hamiltonian in a basis

$$\left(\quad \infty \times \infty \quad \right) \left(\quad \right) = E \left(\quad \right)$$

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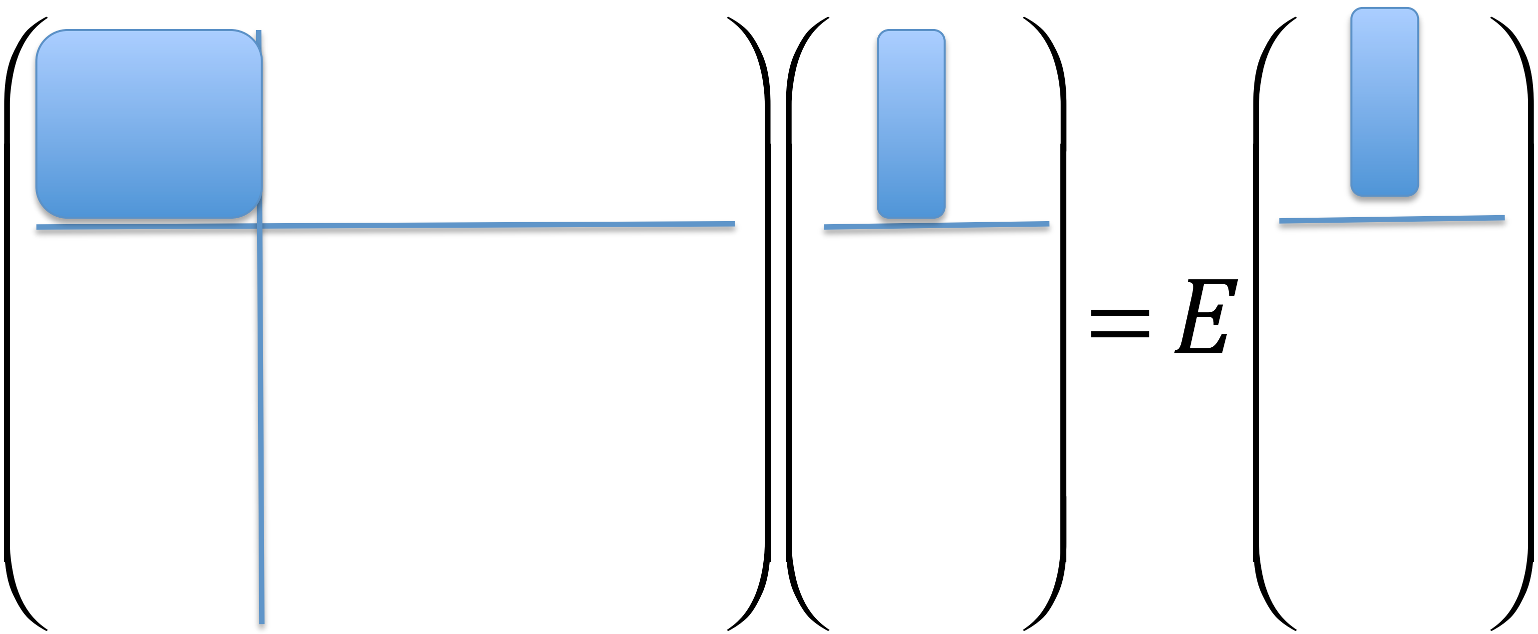
Configuration interaction a.k.a. interacting shell model (including the *no-core shell model*)

Diagonalize the nuclear Hamiltonian in a basis

Truncate to "smaller" space



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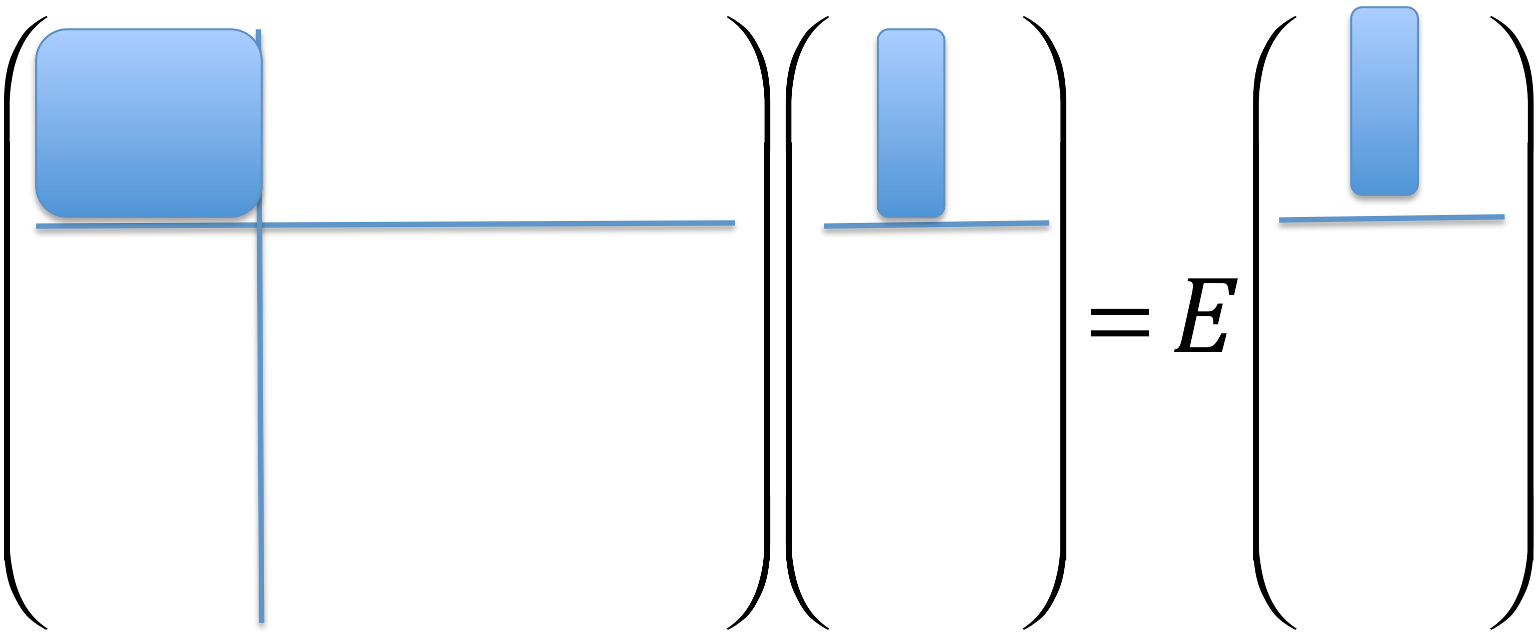
Truncate to “smaller” space



Strategies for successful truncation:

- Choose truncated space with lowest diagonals (guided by importance truncation/perturbation theory)
- Transform via unitary transformation -> decoupled or diagonal-dominated

Spectral distribution theory and SRG……

Truncate to "smaller" space

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Strategies for successful truncation:

E.g., Hartree-Fock changes the single-particle basis so that
(a) energy of starting state is lowest, and
(b) 1p-1h states decoupled from 0p-0h

Spectral distribution theory and SRG……

Truncate to "smaller" space

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The *similarity renormalization group* (SRG) and related unitary transformations drives the Hamiltonian towards the "diagonal" in the *a*-body space ($a = 2,3,4\ldots$) and applies it in the *A*-body space.

Spectral distribution theory and SRG……

Truncate to "smaller" space

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$$\frac{d\hat{H}(s)}{ds} = \left[\hat{\eta}, \hat{H}(s)\right]$$ typically $$\hat{\eta} = \left[\hat{T}, \hat{H}(s)\right]$$

Spectral distribution theory and SRG……

Truncate to "smaller" space

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Strategies for successful truncation:

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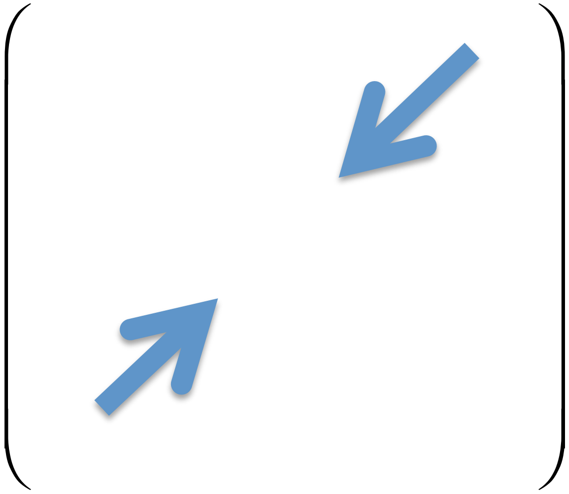

Spectral distribution theory and SRG……

Truncate to "smaller" space

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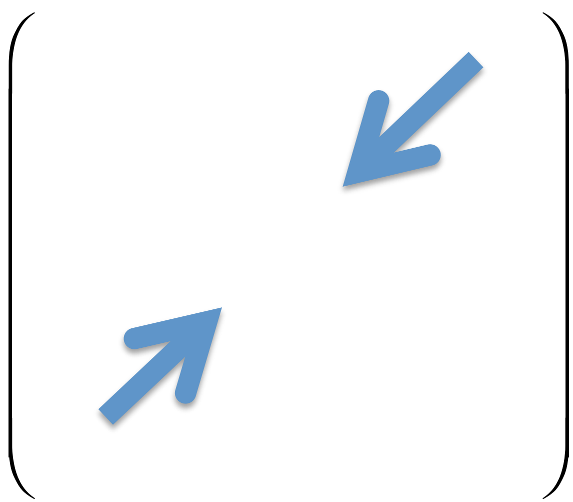
Strategies for successful truncation:

The *similarity renormalization group* (SRG) and related unitary transformations drives the Hamiltonian towards the "diagonal" in the *a*-body space (*a* = 2,3,4…) and applies it in the *A*-body space.

In "original recipe" SRG evolution is done in (relative) momentum space for 2 or 3 or particles



$\lambda = s^{-1/4}$ measures the effective momentum (wave number) cutoff from SRG

then transformed to lab frame (single-particle coordinates) for A particles

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So let's do an example calculation:

- **carry out SRG** on Entem-Machleidt N3LO chiral force (code from P. Navratil) **in relative frame and transform to lab frame (2-body only)**

***Apply to "typical" nucleus, ^{12}C**
at N_{max} = 6 (M-scheme dimension = 30 M)

Calculations done using BIGSTICK code:

C. W. Johnson, W. E. Ormand, and P. G. Krastev, Comp. Phys. Comm. **184**, 2761-2774 (2013).

Spectral distribution theory and SRG……

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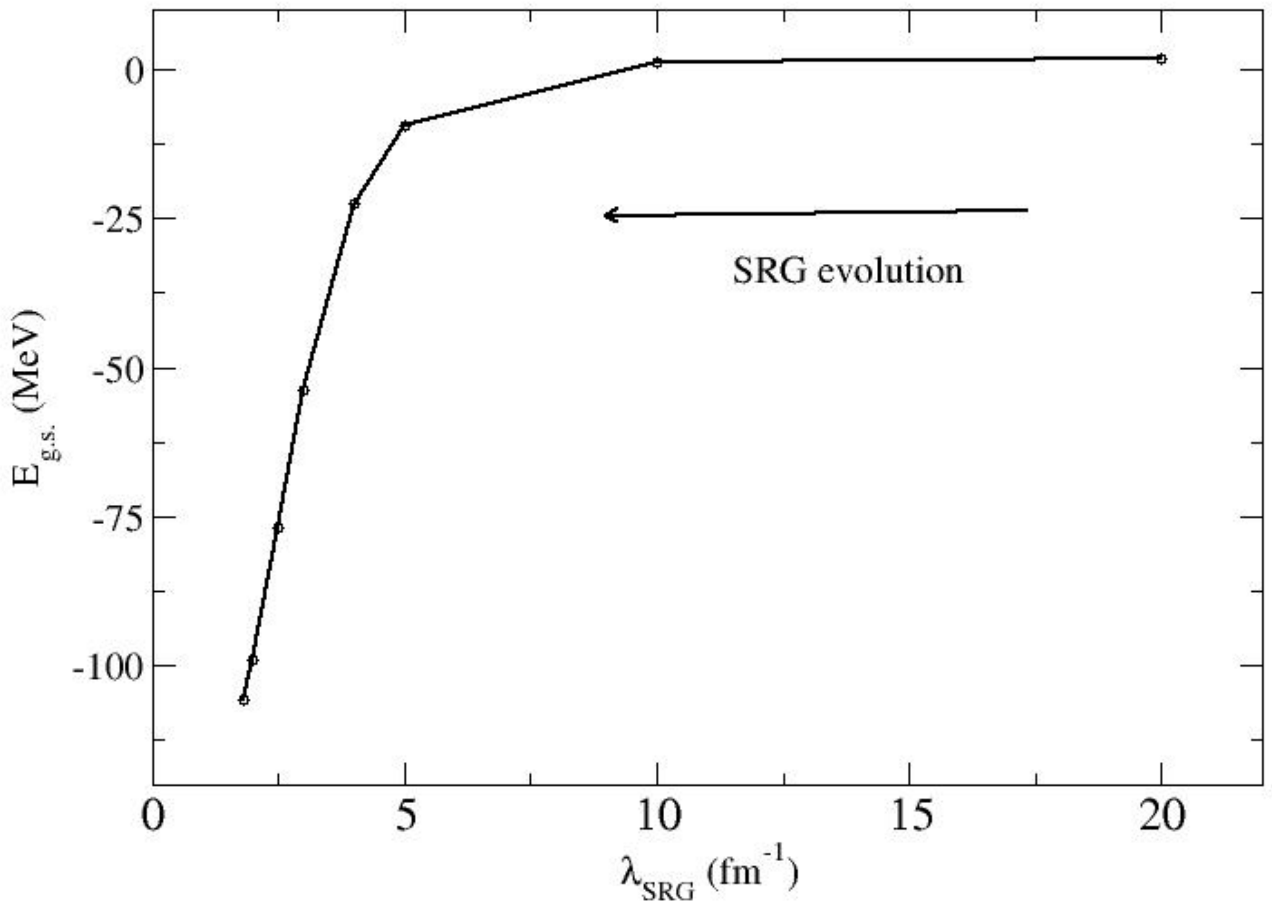
Example: ^{12}C at N_{max} =6, basis $\hbar\omega$ = 20 MeV

(chiral Entem & Machleidt N3LO via P. Navratil)



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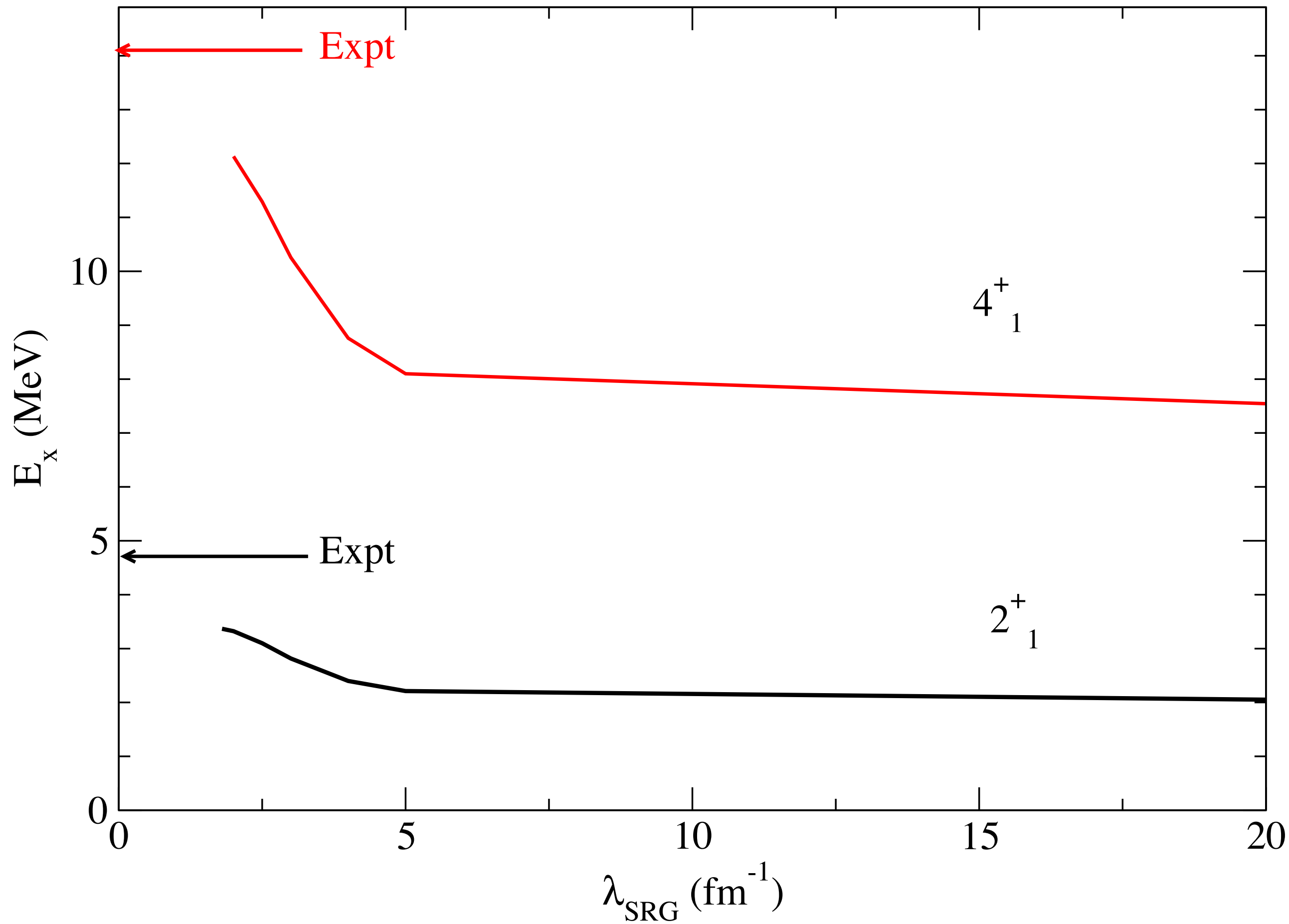

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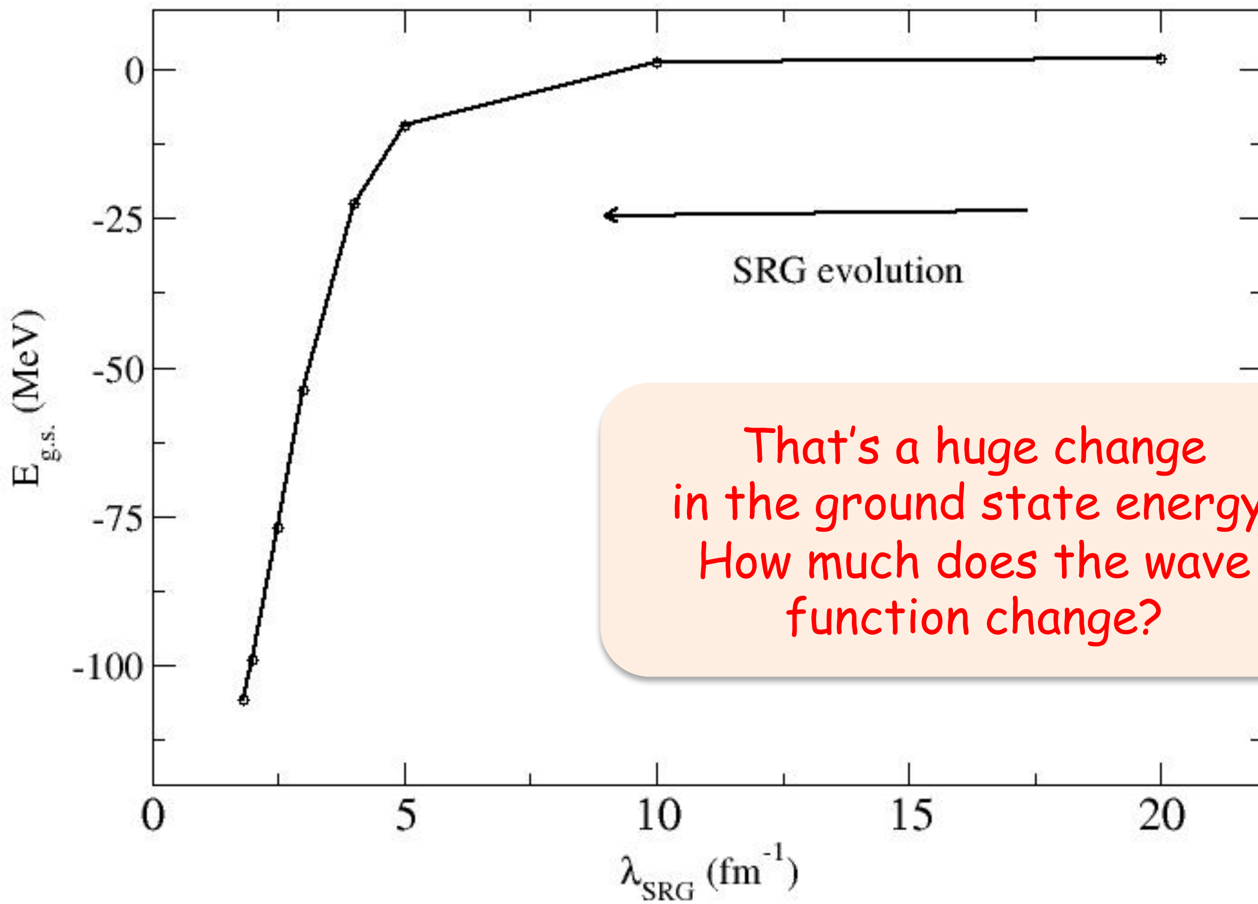

That’s a huge change
in the ground state energy!
How much does the wave
function change?

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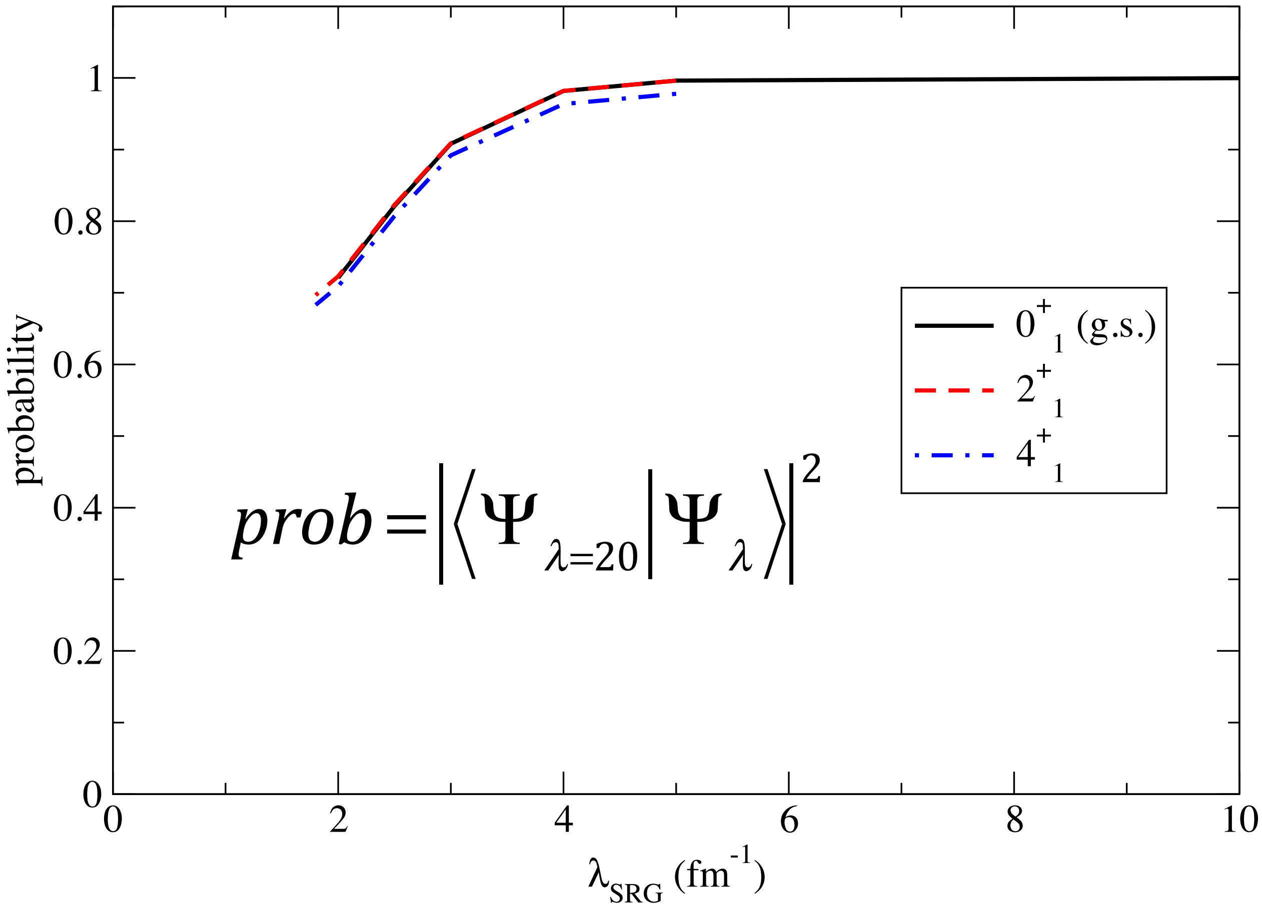

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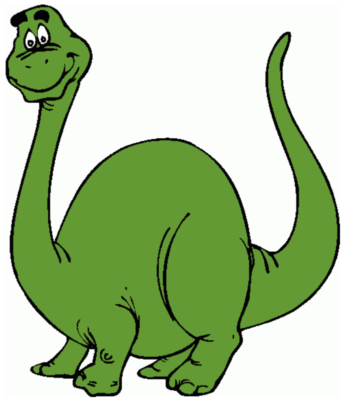

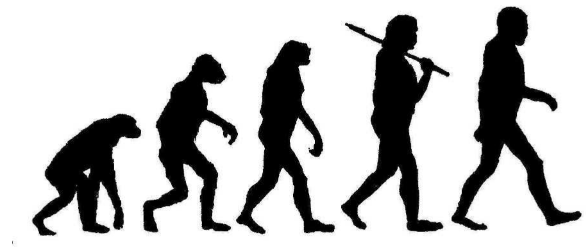

$$\mathbf{H}_{\lambda=20}\vec{v} = E\vec{v}$$

"Unevolved"

$$\mathbf{H}_{\lambda=2}\vec{v} = E\vec{v}$$

"Evolved"

The **eigenvalue** changes a **huge** amount but the **eigenvector** only changes a little!

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Introducing…

SPECTRAL DISTRIBUTION THEORY

SPECTRAL DISTRIBUTION THEORY

Introduced by J. Bruce French and collaborators,
spectral distribution theory or *statistical spectroscopy*
is at heart very simple:

averages over the spectrum

SPECTRAL DISTRIBUTION THEORY

Introduced by J. Bruce French and collaborators, *spectral distribution theory* or *statistical spectroscopy* is at heart very simple:

averages over the spectrum

This is accomplished through traces of many-body matrices

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SPECTRAL DISTRIBUTION THEORY

Let **H** be a Hamiltonian for *A* particles.

Let D be the dimension of the A-particle system.

The *centroid* is the average energy of the spectrum, given by a trace:

$$\bar{E} = \frac{1}{D} tr\mathbf{H}$$

SPECTRAL DISTRIBUTION THEORY

$$\bar{E} = \frac{1}{D} tr\mathbf{H}$$

It turns out the centroid is easy to calculate directly from the one+two-body matrix elements

Spectral distribution theory and SRG……

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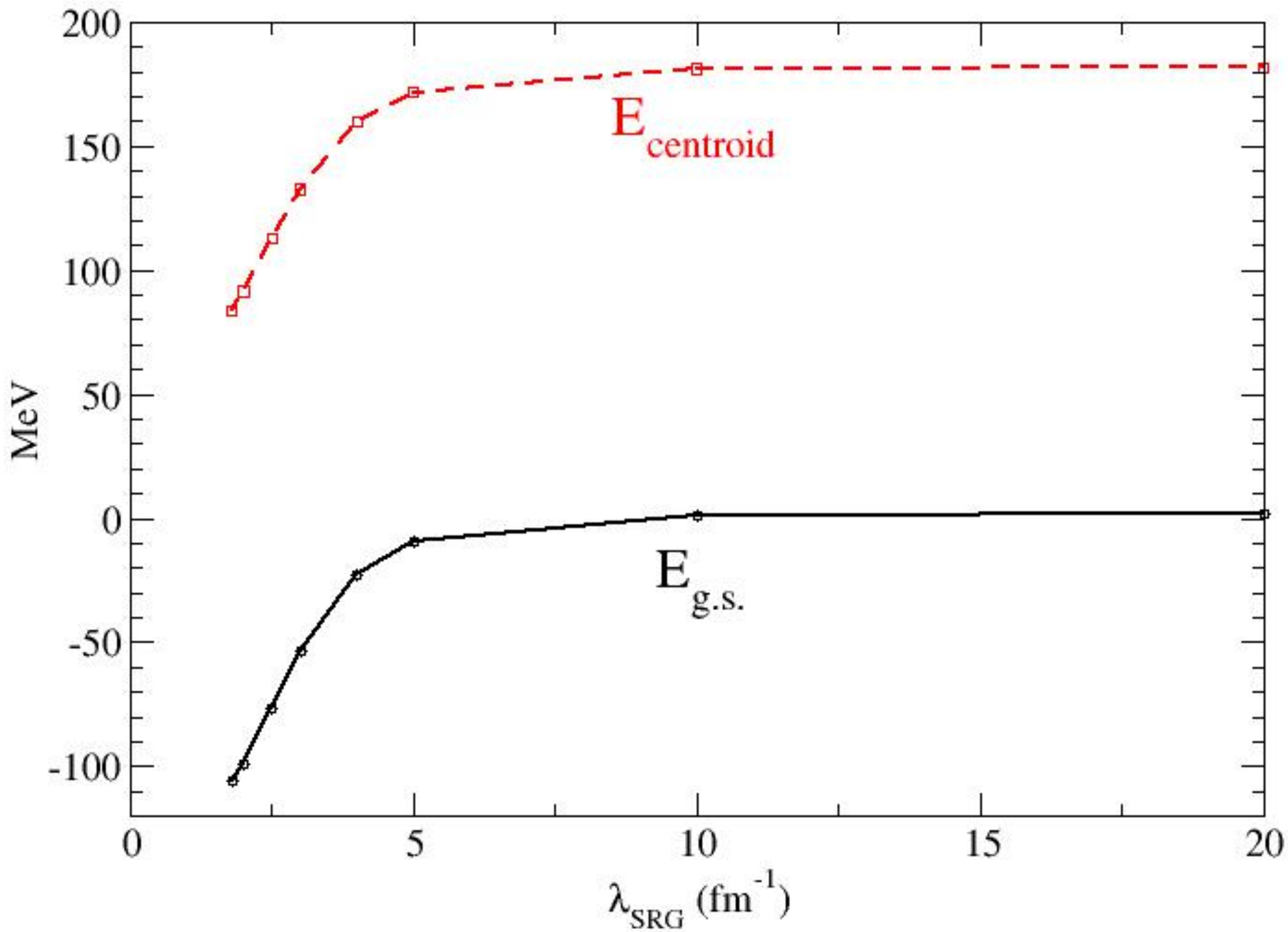

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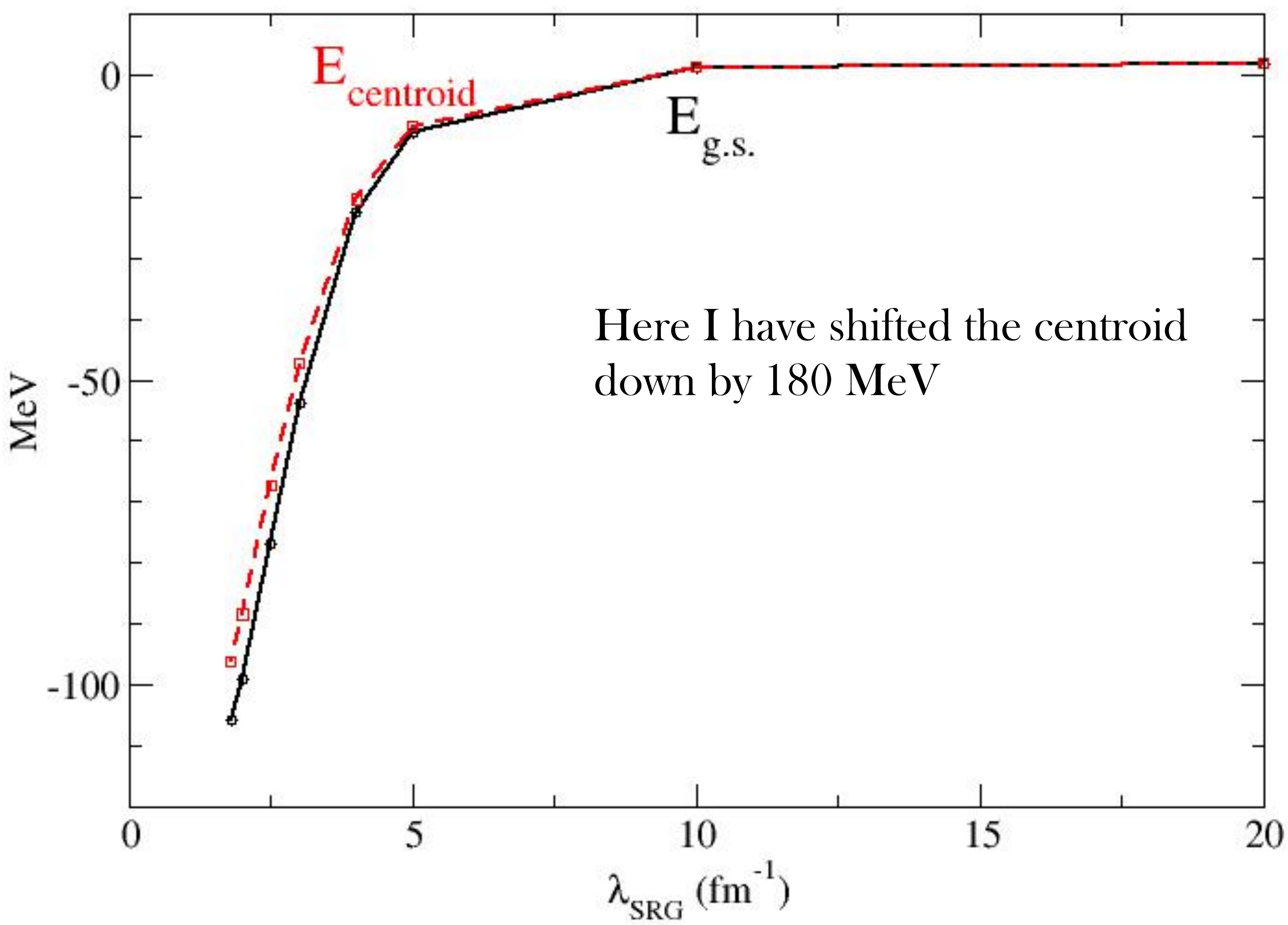

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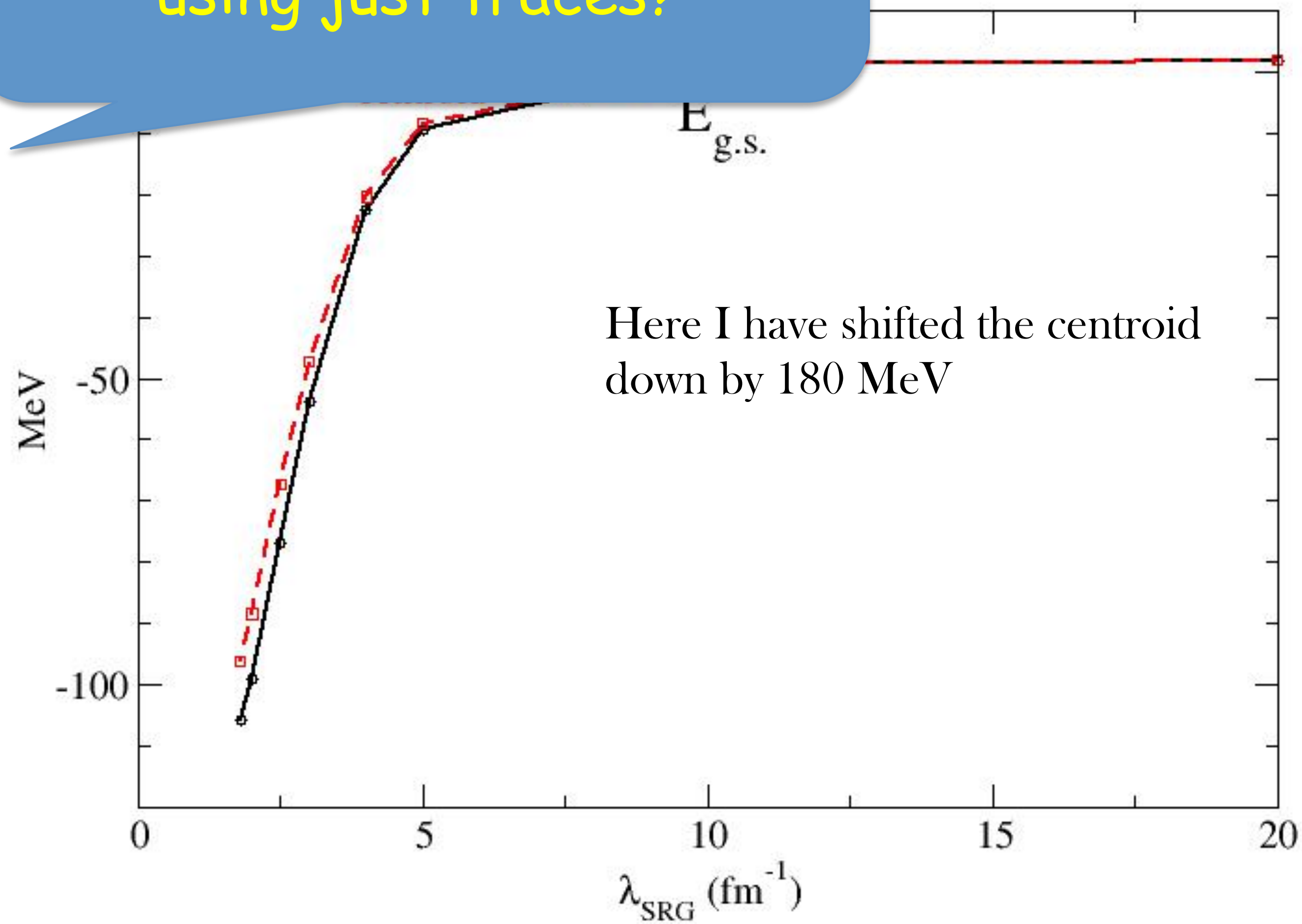
Example
(chiral En

That's amazing!
What else can one calculate using just traces?



Spectral distribution theory and SRG……

That's amazing!
What else can one calculate using just traces?

One can define an inner product!

And thus define the *distance* between Hamiltonians!

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Spectral distribution theory and SRG……

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That's amazing!
What else can one calculate using just traces?

One can define an inner product!
And thus define the *distance* between Hamiltonians!

$$\left(\hat{H}_1, \hat{H}_2\right) \equiv \frac{1}{D} tr\left\{\left(\hat{H}_1 - \bar{E}_1\right)\left(\hat{H}_2 - \bar{E}_2\right)\right\}$$

This is also straightforward to calculate directly: Launey, Sarbadhicary, Dytrych, and Draayer, *Computer Physics Communications* 185, (2014): 254.

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magnitude $\left|\hat{H}\right| = \sqrt{\left(\hat{H},\hat{H}\right)}$ = width of spectrum

cosine of angle between two Hamiltonians $= \dfrac{\left(\hat{H}_1,\hat{H}_2\right)}{\left|\hat{H}_1\right|\left|\hat{H}_2\right|}$

Spectral distribution theory and SRG……

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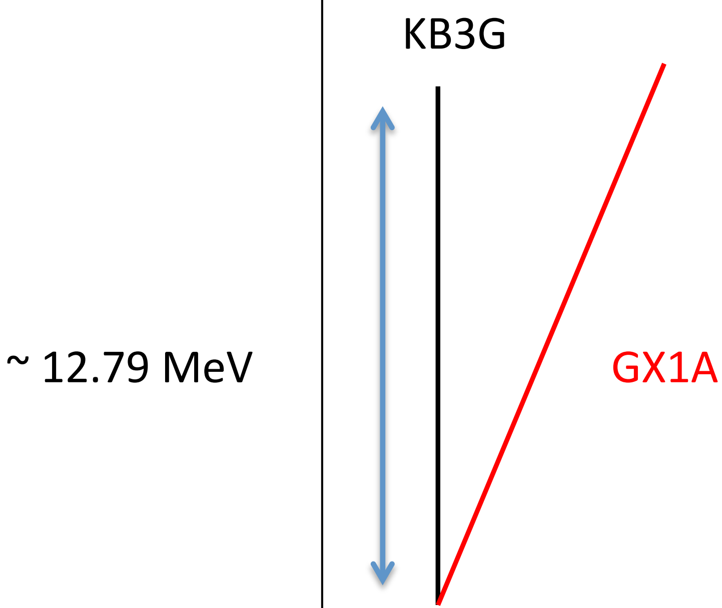

Example: in *pf* shell, for ^{57}Fe, KB3G interactions vs. GX1A

Spectral distribution theory and SRG……

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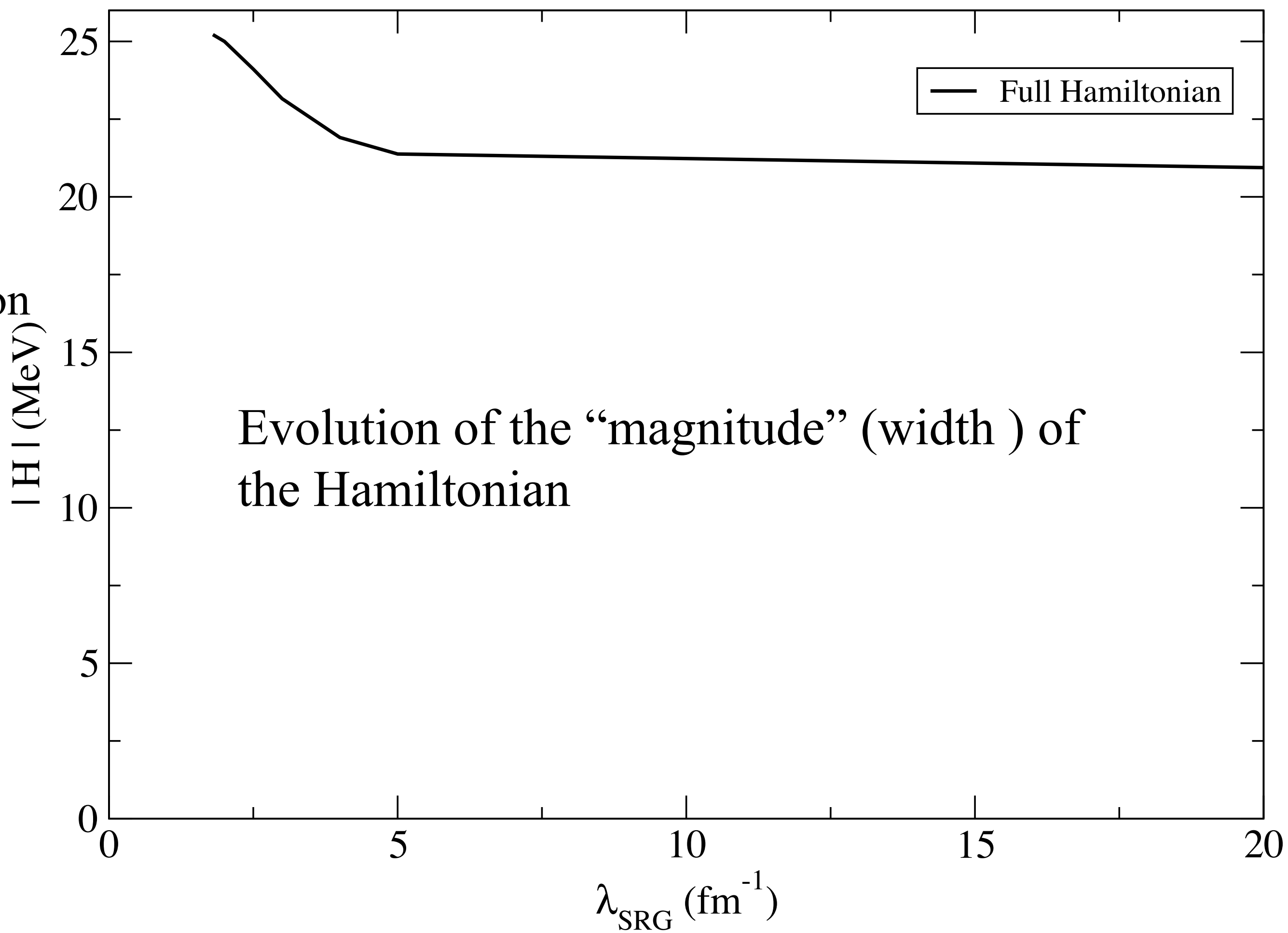
Example: ^{12}C "Full configuration" basis ħω = 20 MeV
(chiral Entem & Machleidt N3LO via P. Navratil)

These traces computed in full configuration in 3 major h.o. shells (0s-0p-1s0d)



Spectral distribution theory and SRG……

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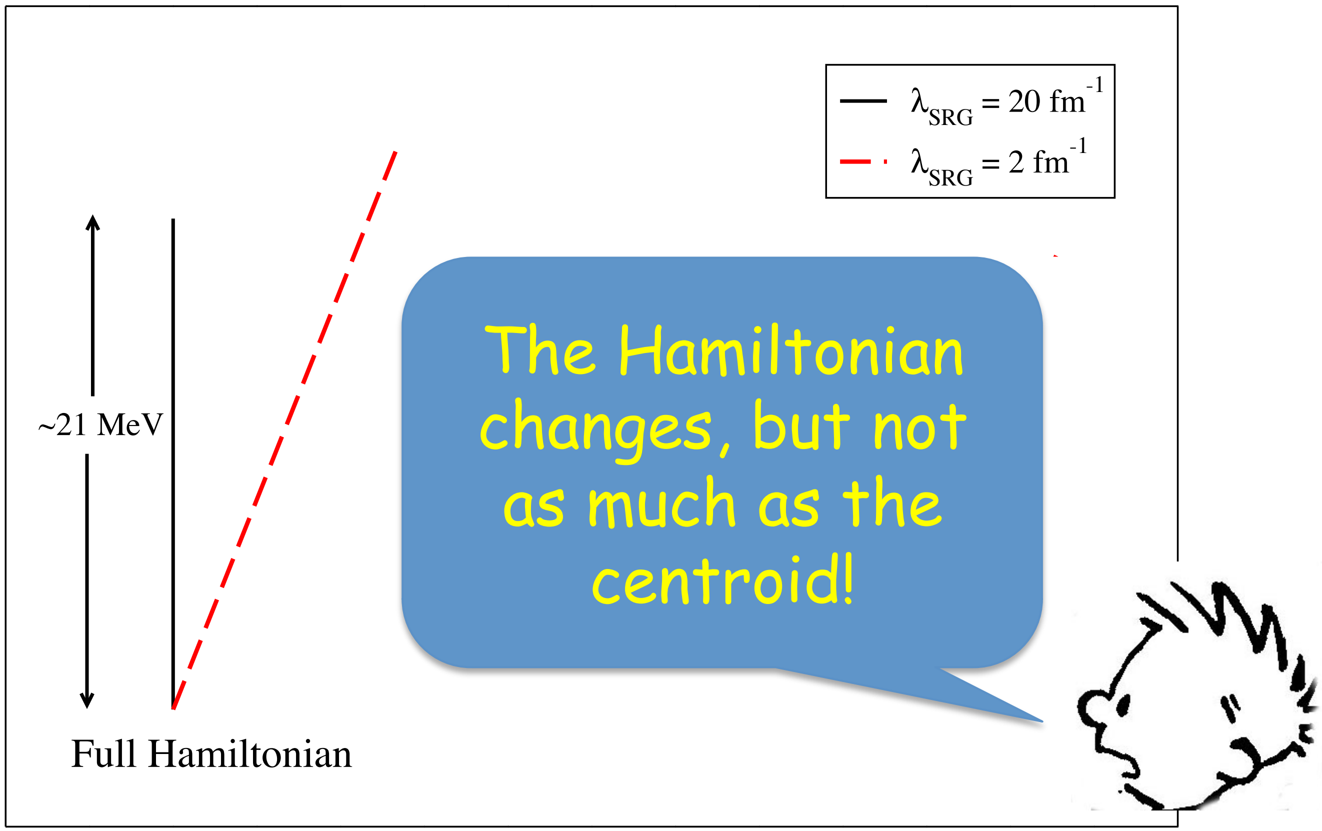

Spectral distribution theory and SRG……

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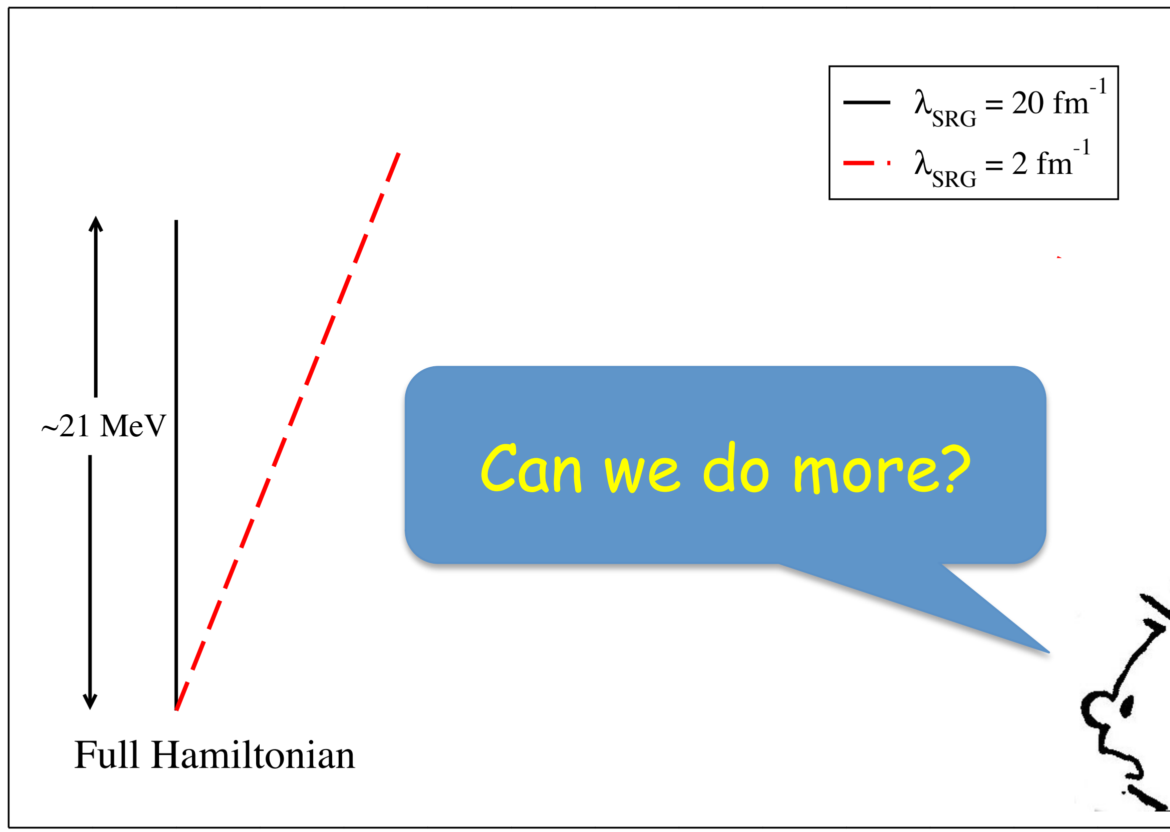

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SPECTRAL DISTRIBUTION THEORY

Yes we can!

The centroid is computed from the *monopole* terms in the Hamiltonian, that is, all terms that look like number operators:

$$\hat{H}_{mono} = \sum_a \varepsilon_a \hat{n}_a + \sum_{ab} V_{ab} \hat{n}_a \left(\hat{n}_b - \delta_{ab} \right)$$

n_a is the number of particles in orbit a

Spectral distribution theory and SRG……

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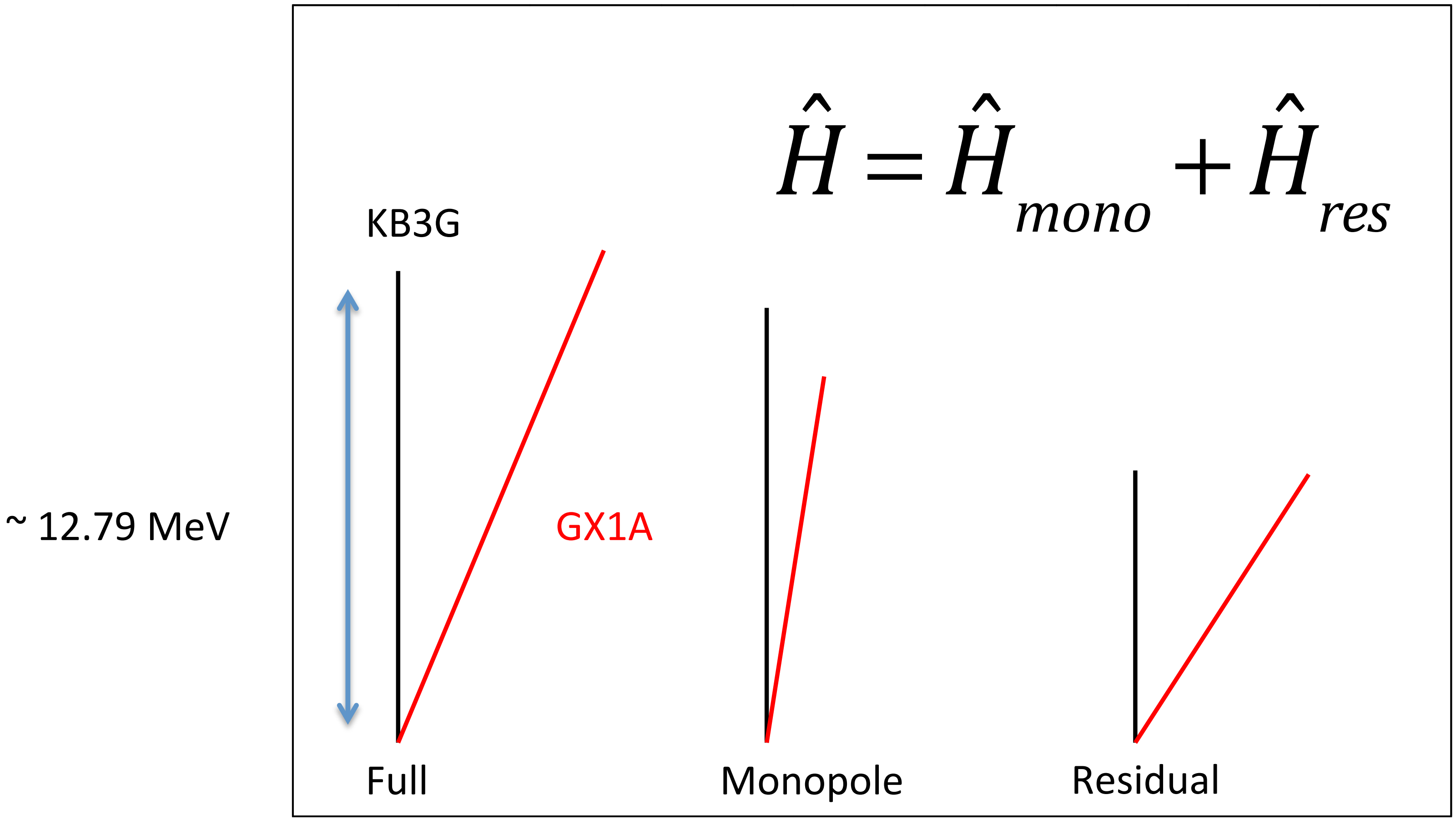
Example: in *pf* shell, for ^{57}Fe,
KB3G interactions vs. GX1A



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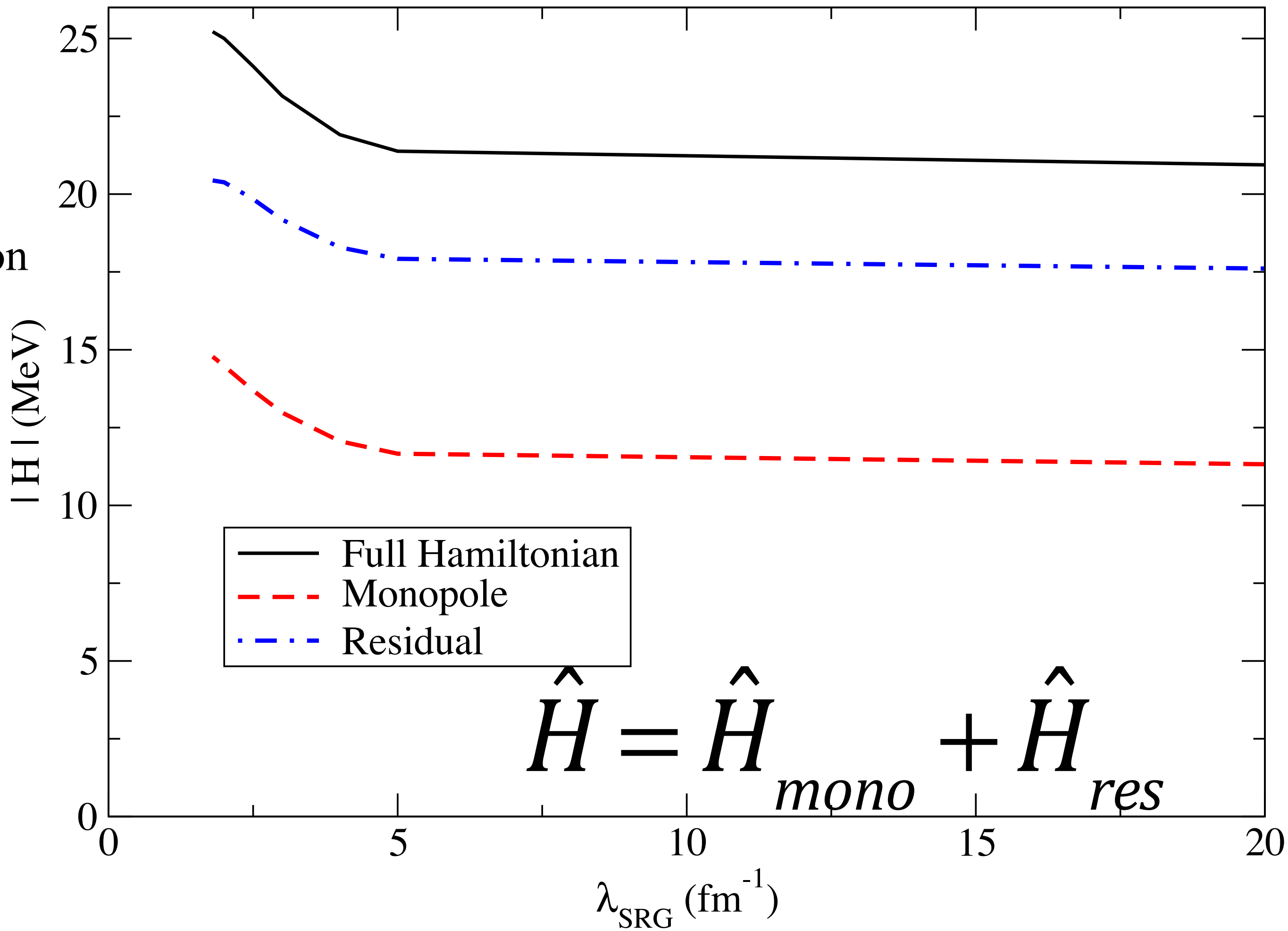

$$\hat{H} = \hat{H}_{mono} + \hat{H}_{res}$$

Spectral distribution theory and SRG……

Example: ^{12}C "Full configuration" basis ħω = 20 MeV
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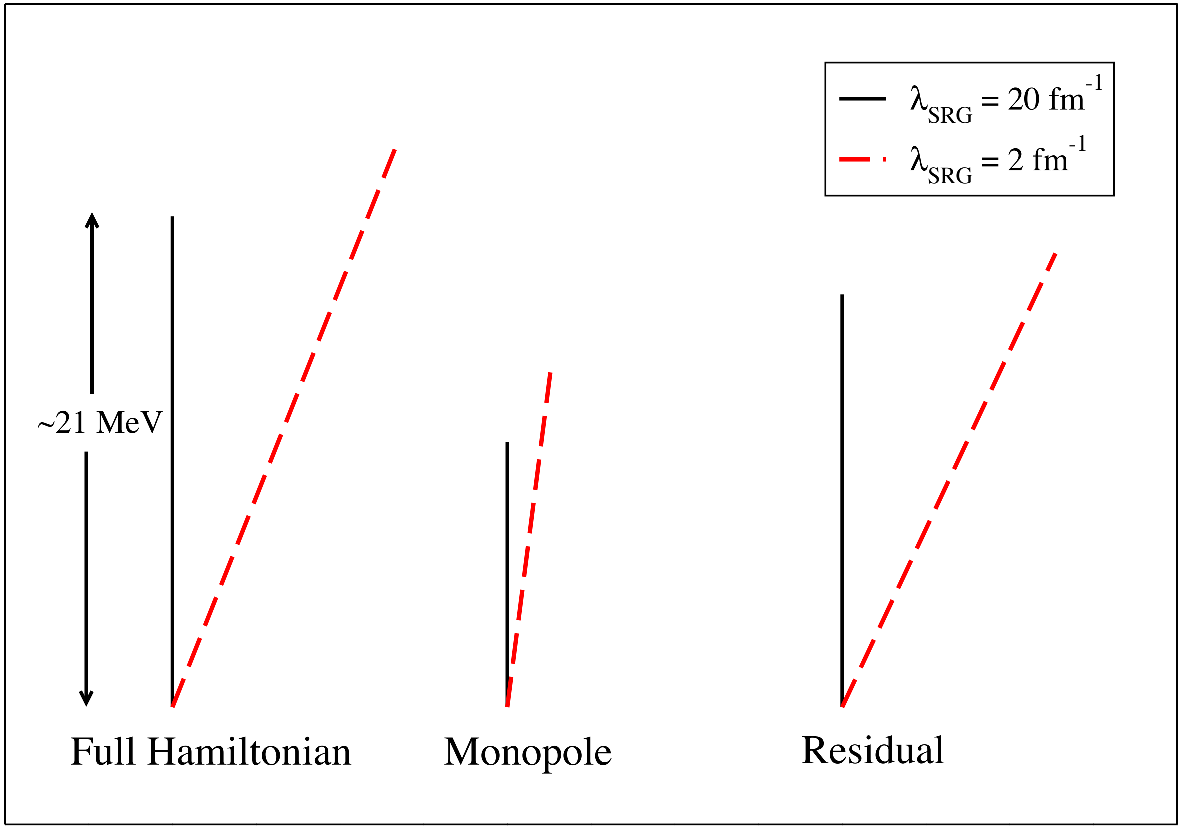

Because the trace is calculated using number operators, we can introduce *configuration averages*

A *configuration* is the subspace of all states (Slater determinants) with fixed occupation, i.e.,

$(0d_{5/2})^4(1s_{1/2})^1(1p_{3/2})^2$ **etc**

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A *configuration* is the subspace of all states (Slater determinants) with fixed occupation, i.e.,

$(0d_{5/2})^4(1s_{1/2})^1(1p_{3/2})^2$ **etc**

One can introduce a projection operator $\mathbf{P}_\alpha$ for the subspace defined by a configuration and use it for the traces, e.g., the *configuration centroid*

$$\bar{E}_\alpha = \frac{1}{D_\alpha} tr \mathbf{P}_\alpha \hat{H}$$

Spectral distribution theory and SRG……

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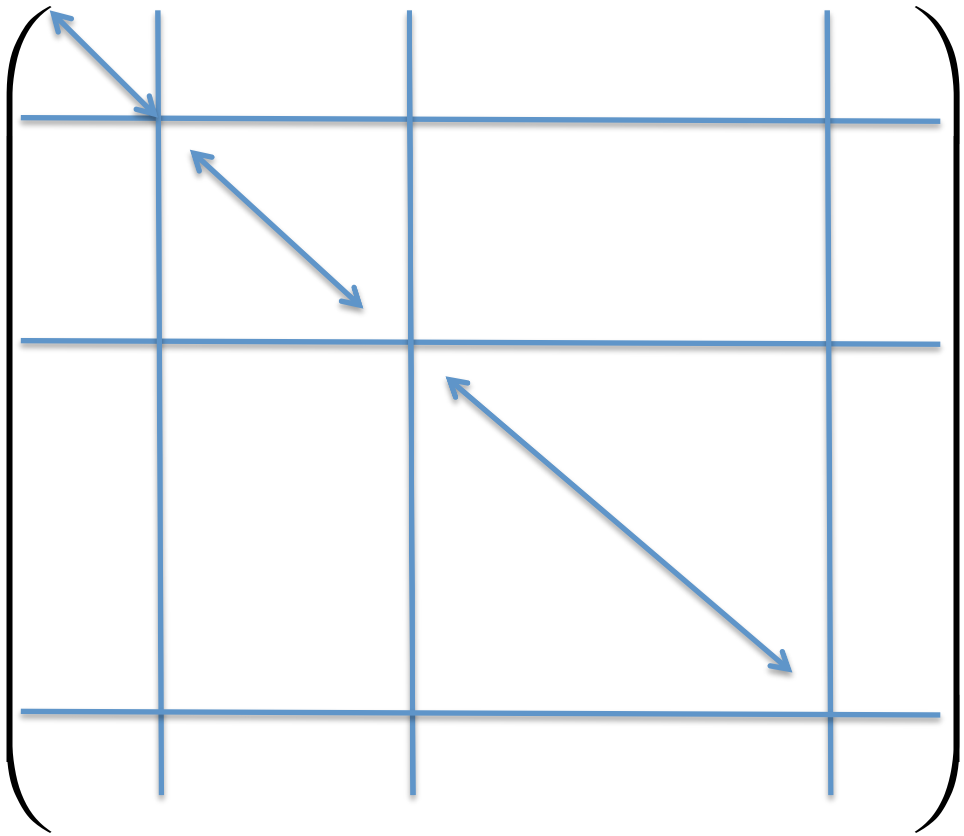
$$\bar{E}_\alpha = \frac{1}{D_\alpha} tr \mathbf{P}_\alpha \hat{H}$$

Configuration subspaces

$$H =$$



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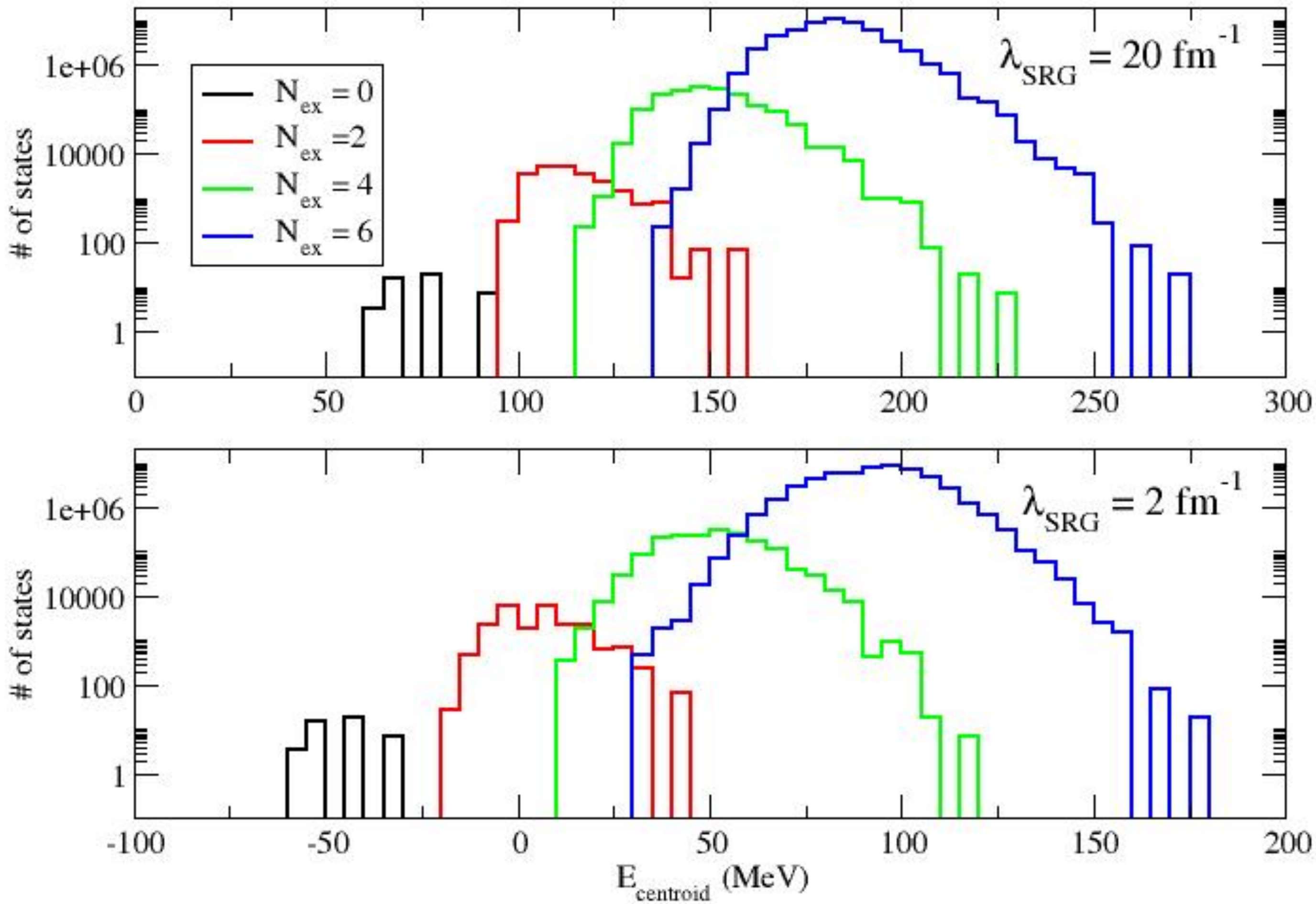
Example: ^{12}C at N_{max} =6, basis ħω = 20 MeV
(chiral Entem & Machleidt N3LO via P. Navratil)

Distribution of configuration centroids (vs binned dimensions of configurations)



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Example: ^{12}C at N_{max} =6, basis ħω = 20 MeV
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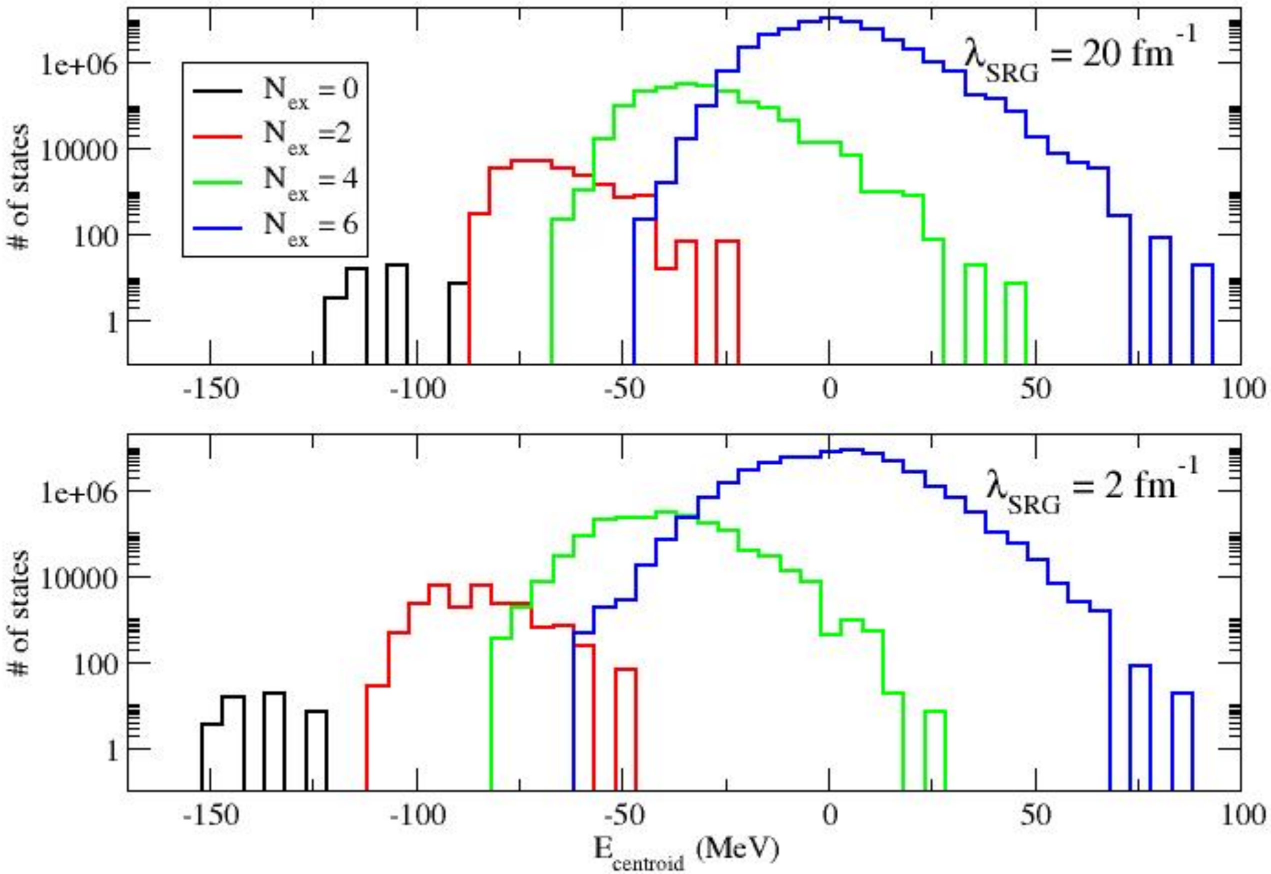
Here I have shifted so overall centroid is at E = 0



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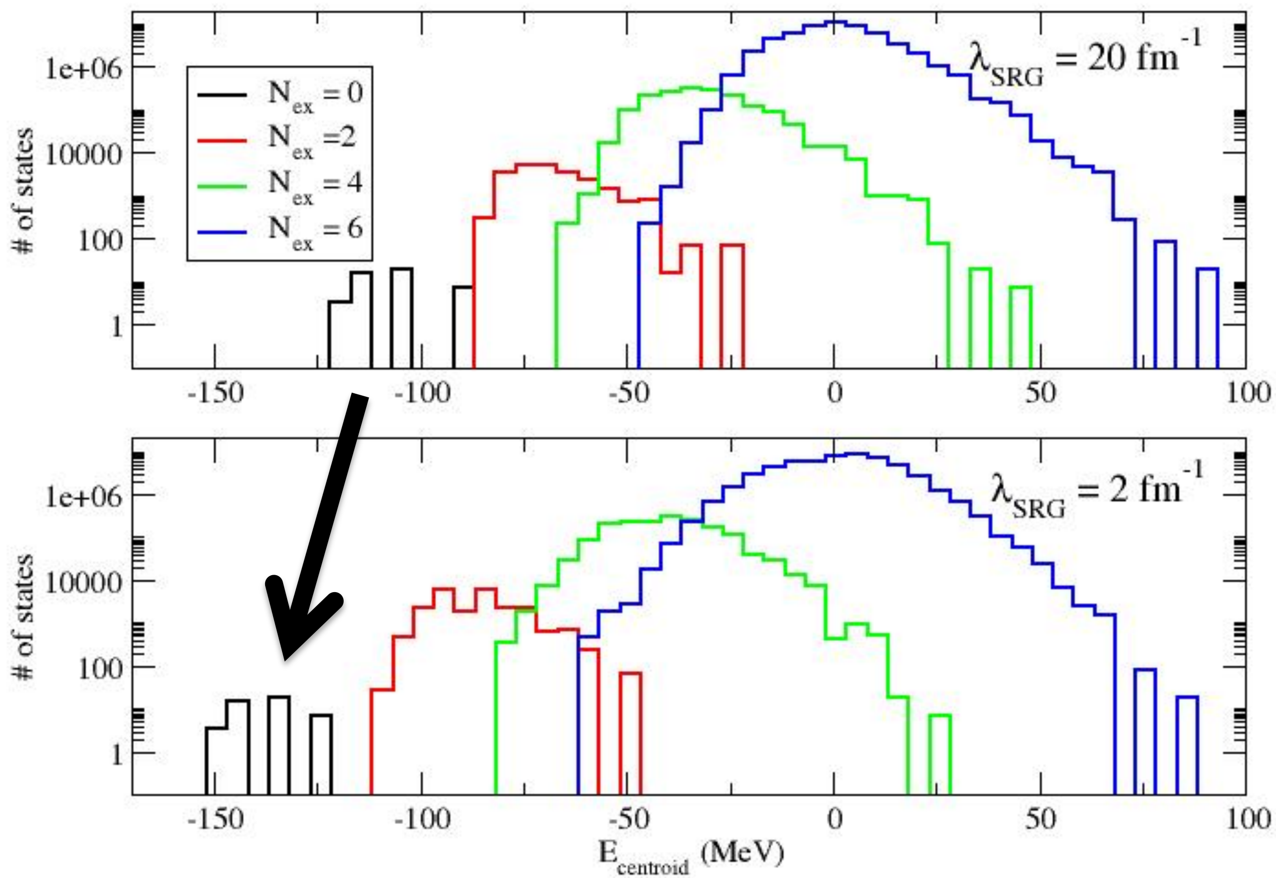
Example: ^{12}C at N_{max} =6, basis ħω = 20 MeV
(chiral Entem & Machleidt N3LO via P. Navratil)

The y-axis is log scale

all averages (traces) are over the *entire* spectrum and thus dominated by the middle of the spectrum



Spectral distribution theory and SRG……

Example: ^{12}C at N_{max} =6, basis ħω = 20 MeV
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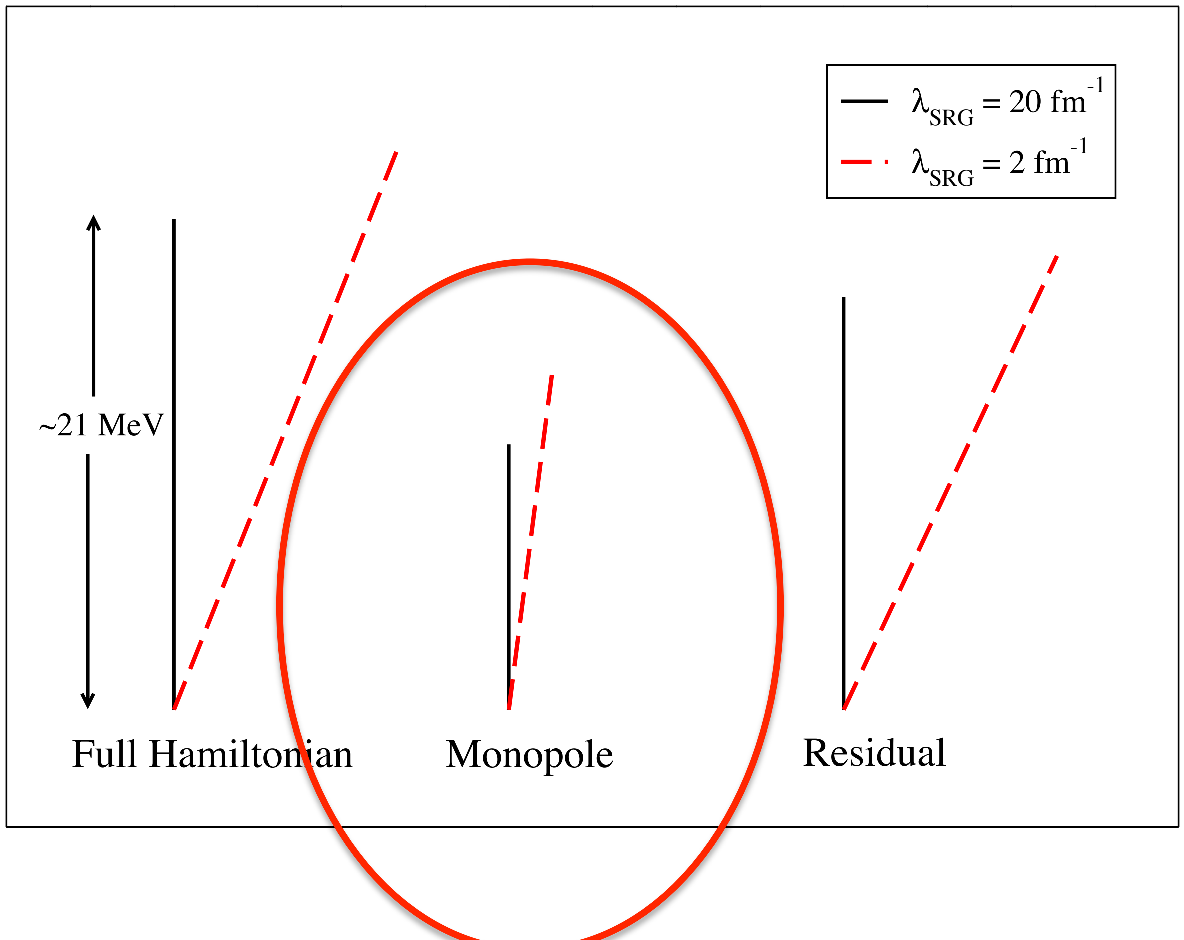
The downside of spectral averaging is it has less weighting at extremes (g.s.) where we care the most.



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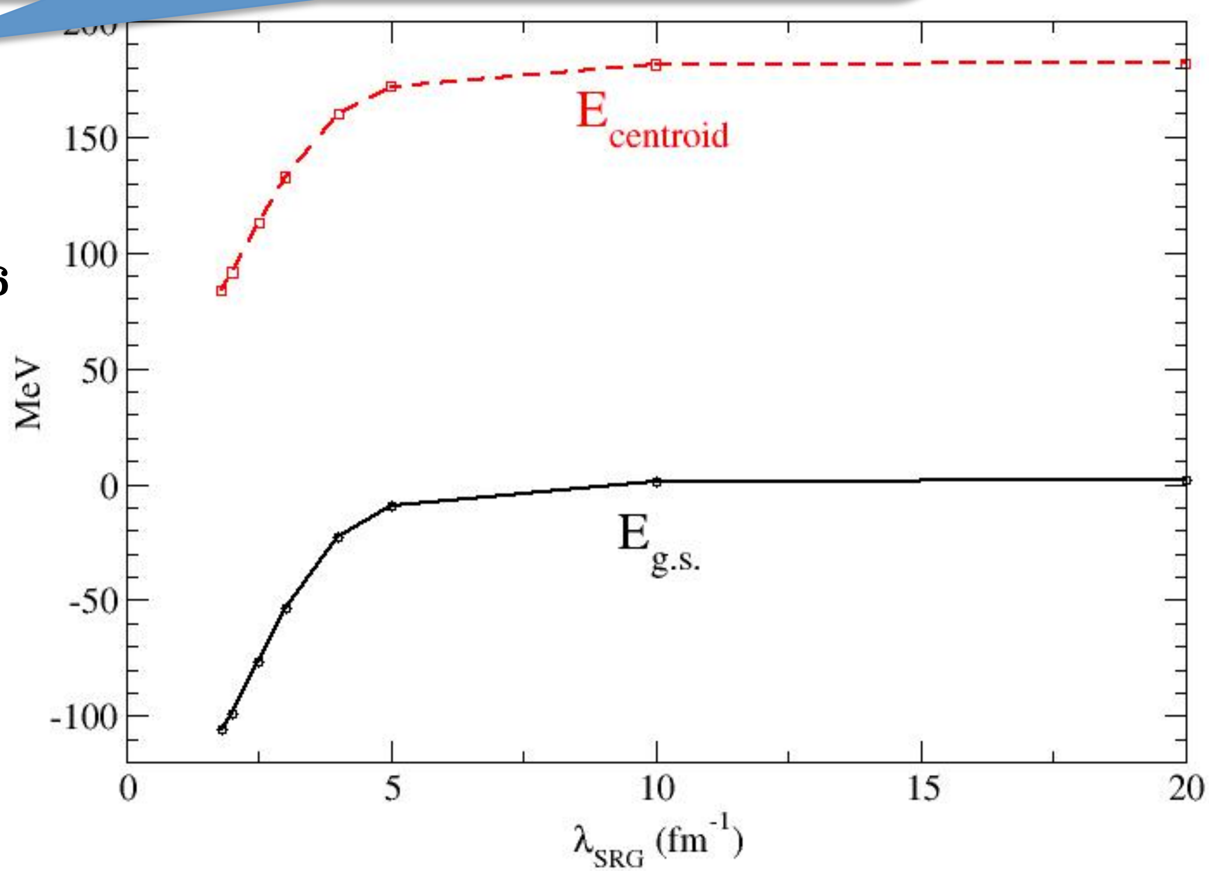
Despite the spectral averaging, we saw the g.s. energy track the centroid

^{12}C at N_{max} =6



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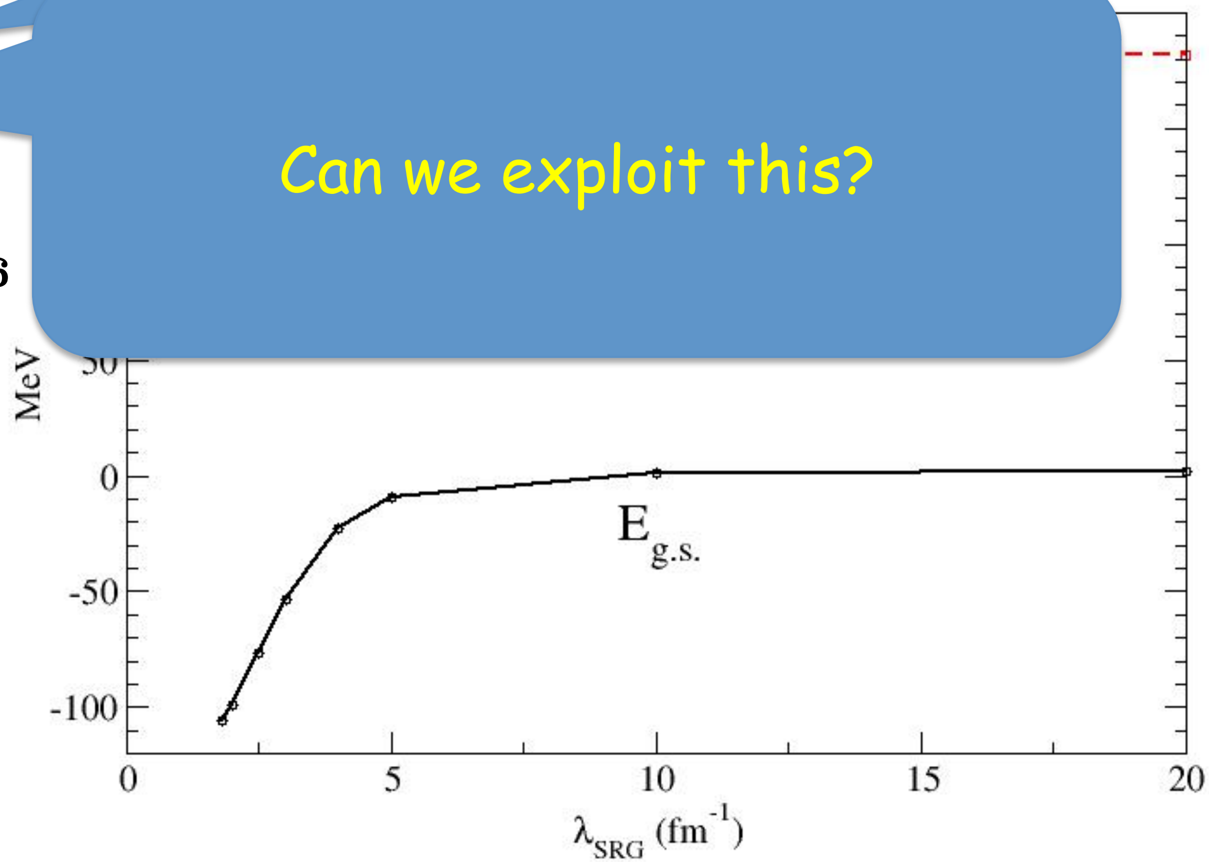
Despite the spectral averaging, we saw the g.s. energy track the centroid

Can we exploit this?

^{12}C at N_{max} =6



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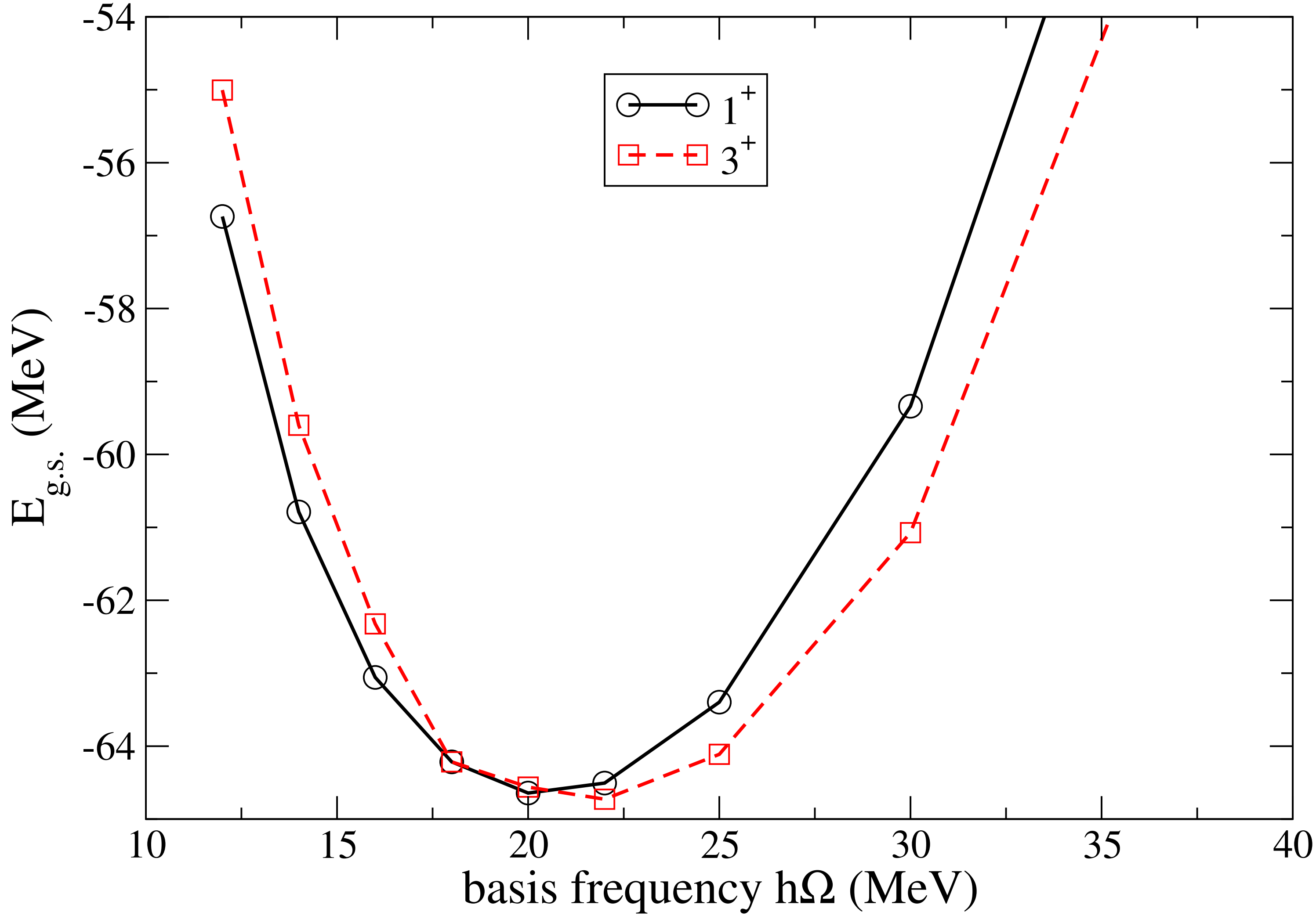
Example: ^{10}B at N_{max} =6
(chiral Entem & Machleidt N3LO via P. Navratil)



Spectral distribution theory and SRG……

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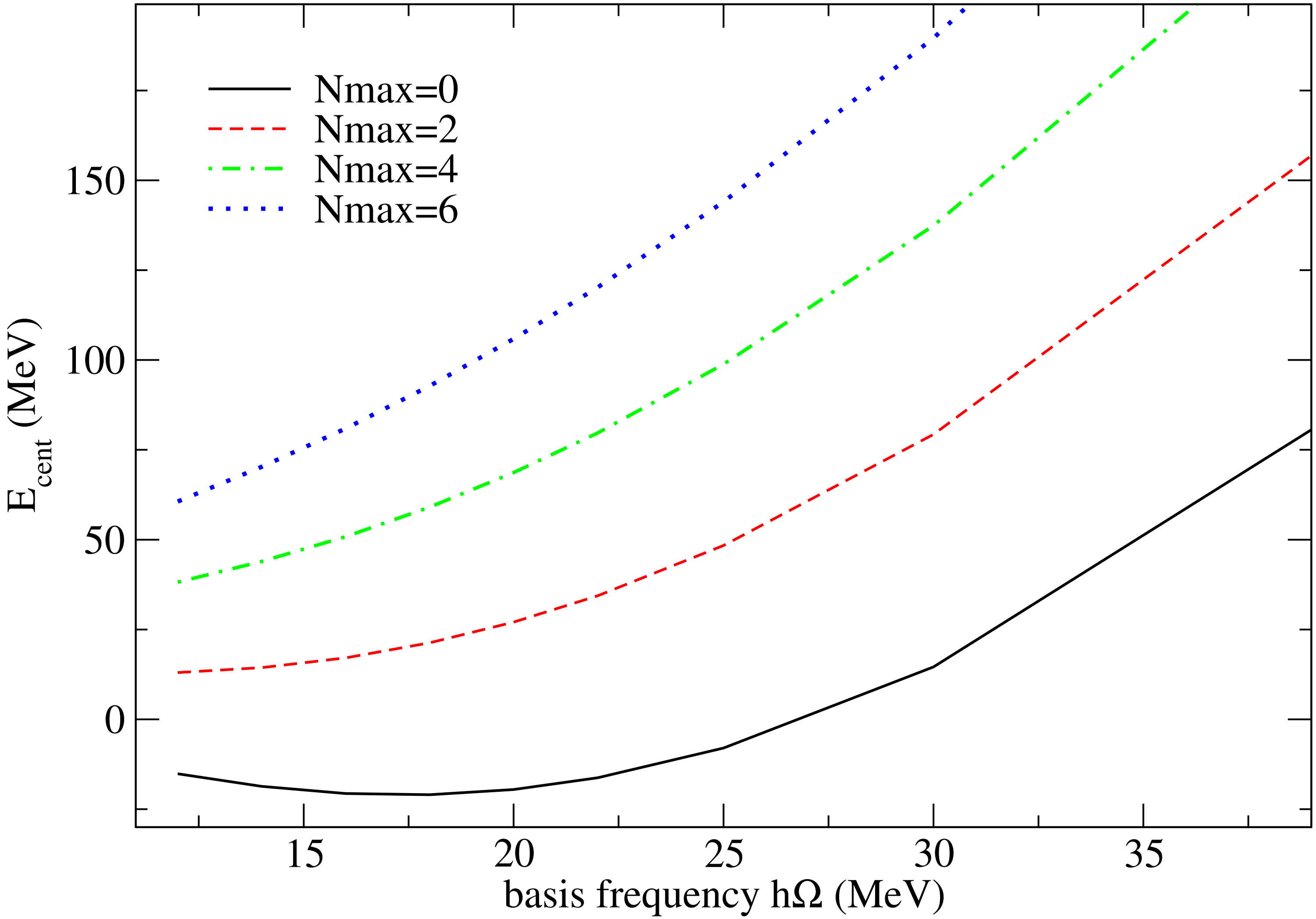

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Spectral distribution theory and SRG......

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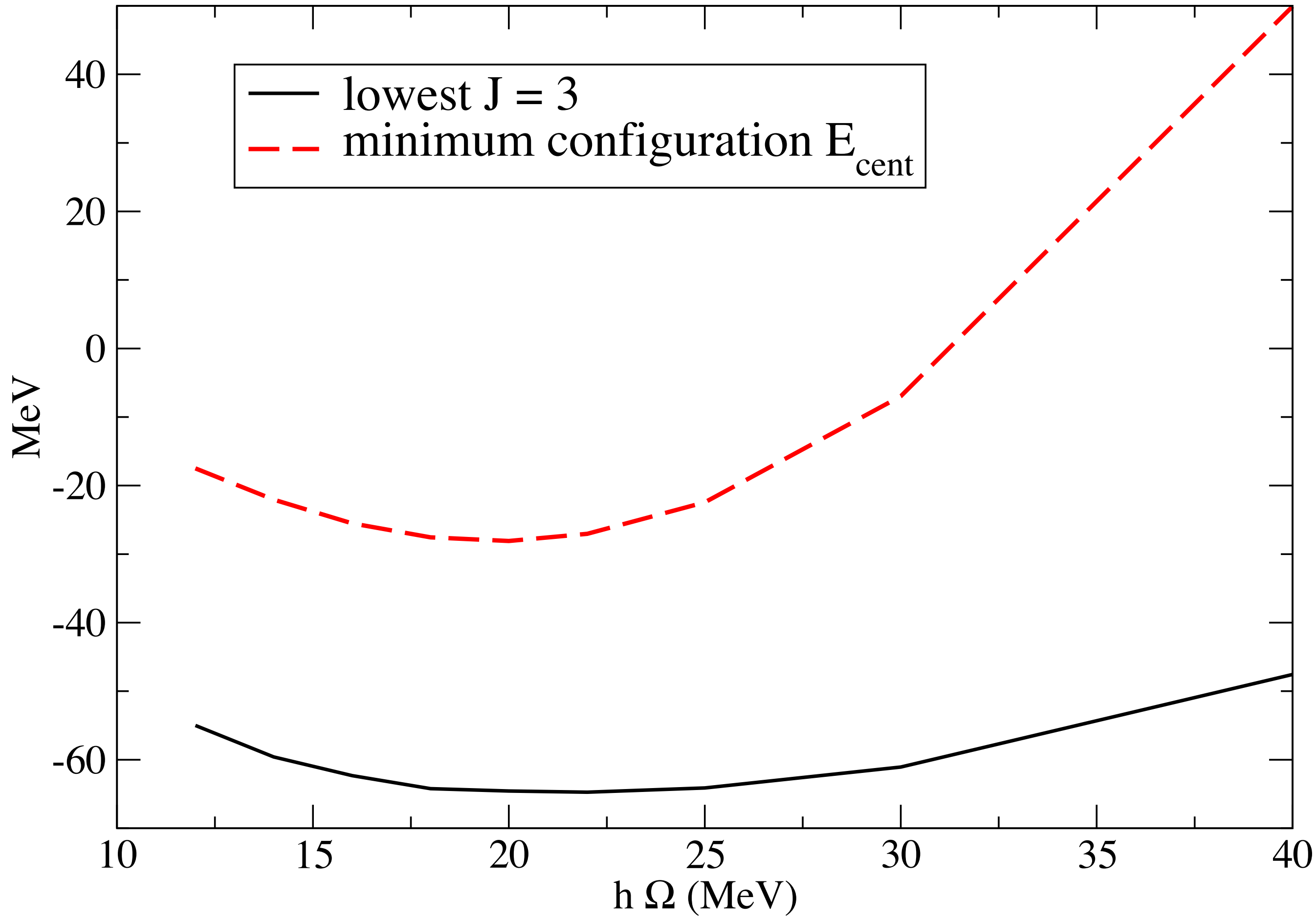

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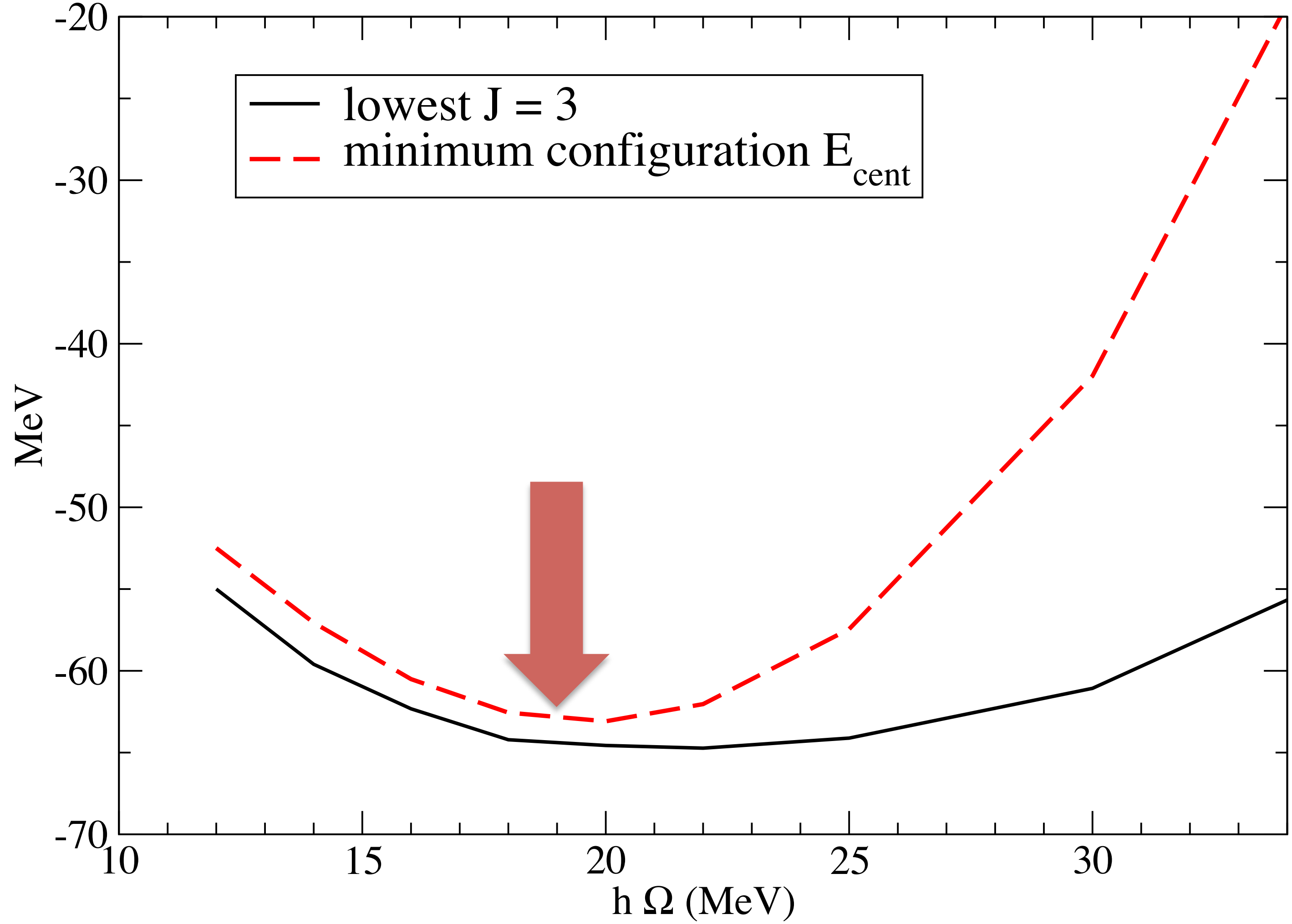

Spectral distribution theory and SRG……

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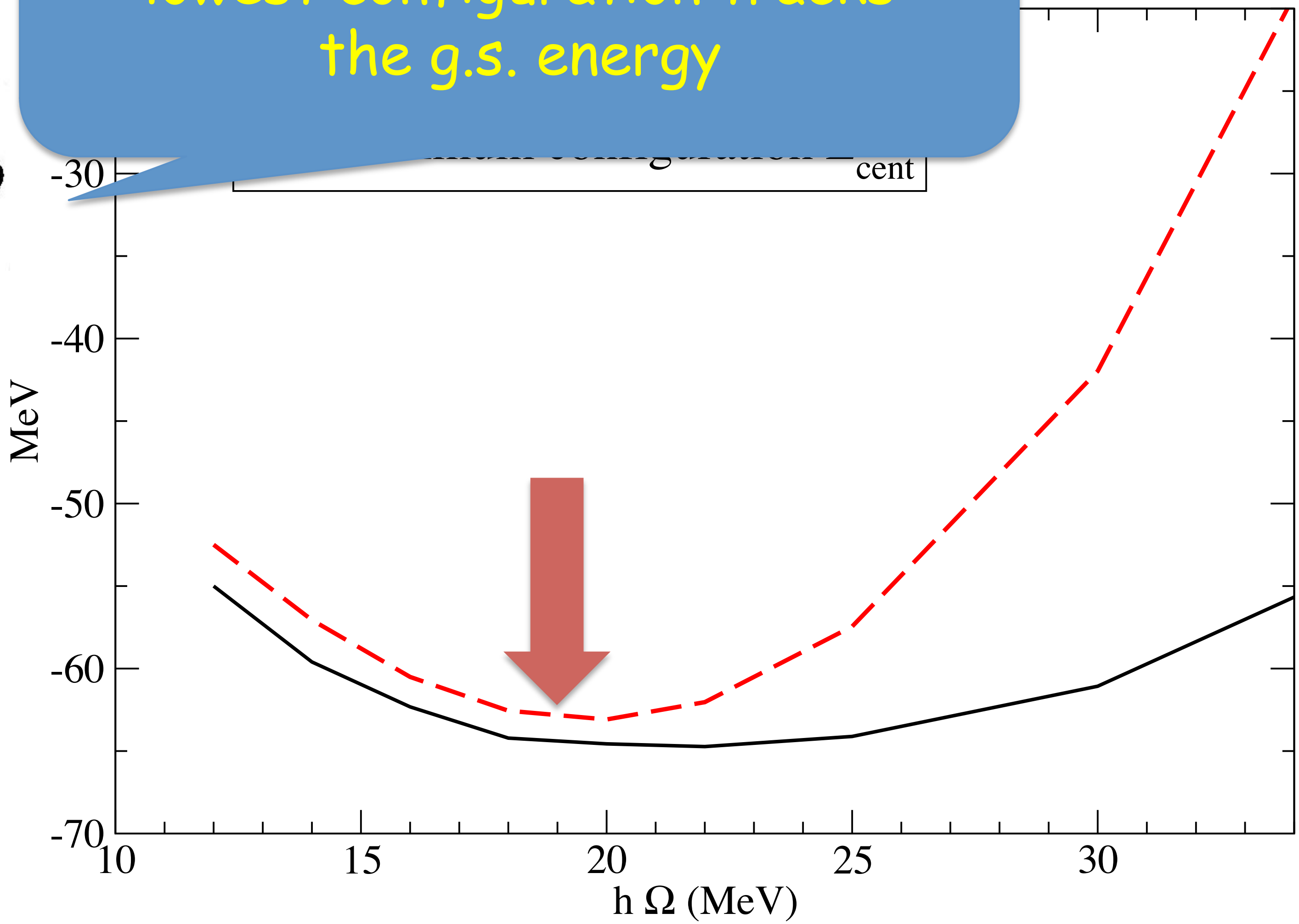
For this example, the lowest configuration tracks the g.s. energy



Spectral distribution theory and SRG……

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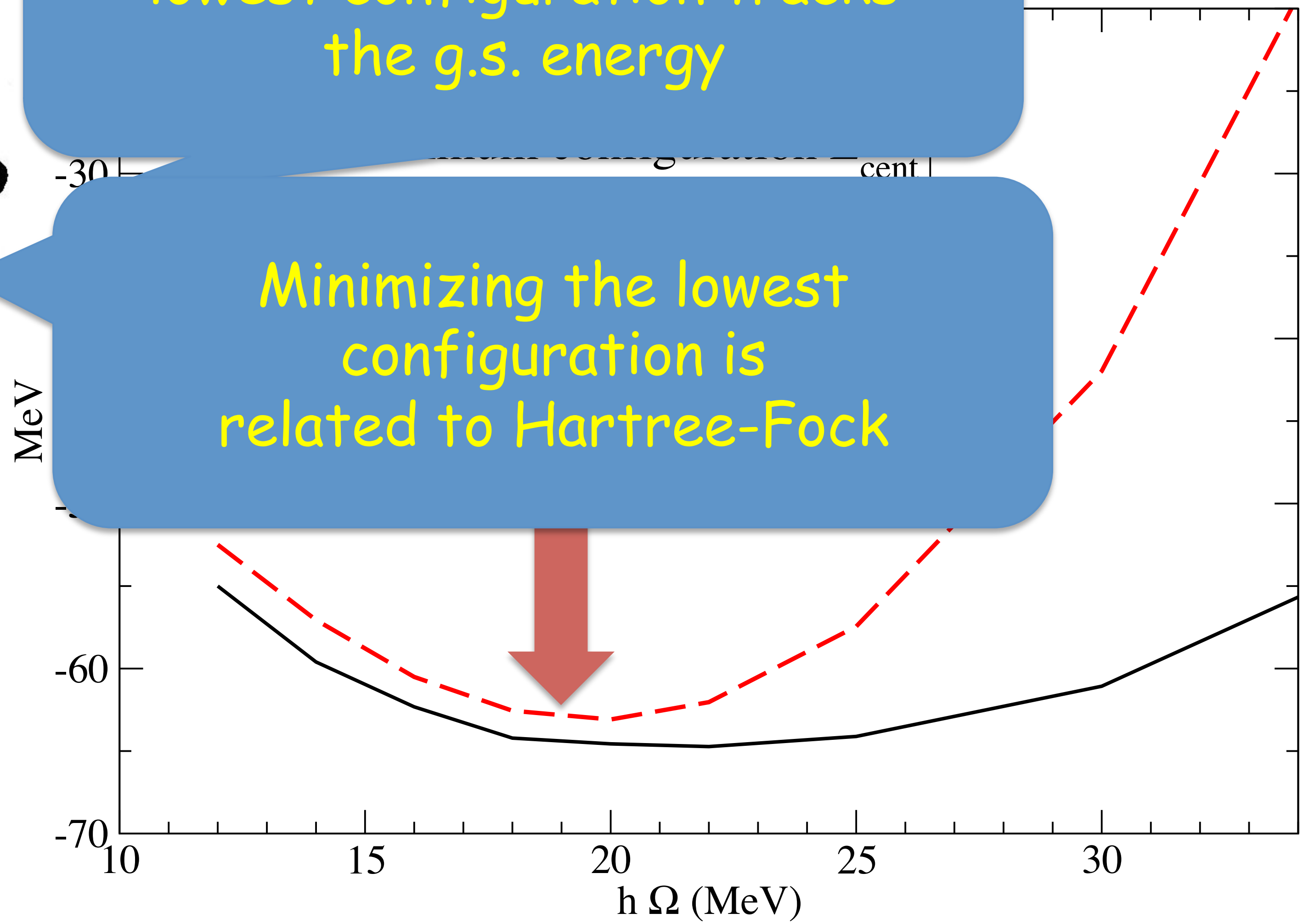
For this example, the lowest configuration tracks the g.s. energy

Minimizing the lowest configuration is related to Hartree-Fock



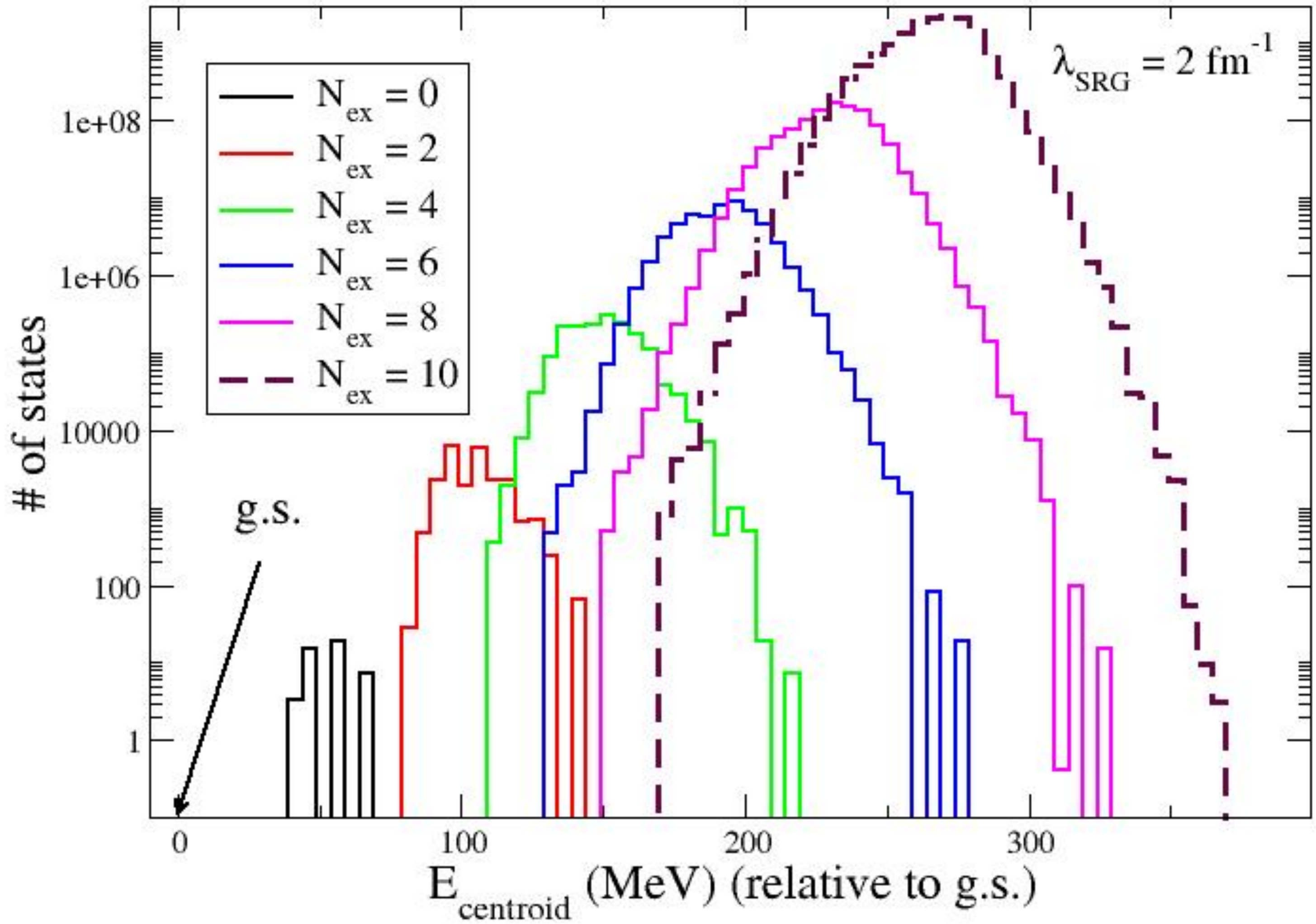
Spectral distribution theory and SRG……

What about the many-body truncations?

Typically we use a N_{max} cutoff for NCSM, but is that best?

Spectral distribution theory and SRG……

Example: ^{12}C basis ħω = 20 MeV
(chiral Entem & Machleidt N3LO via P. Navratil)

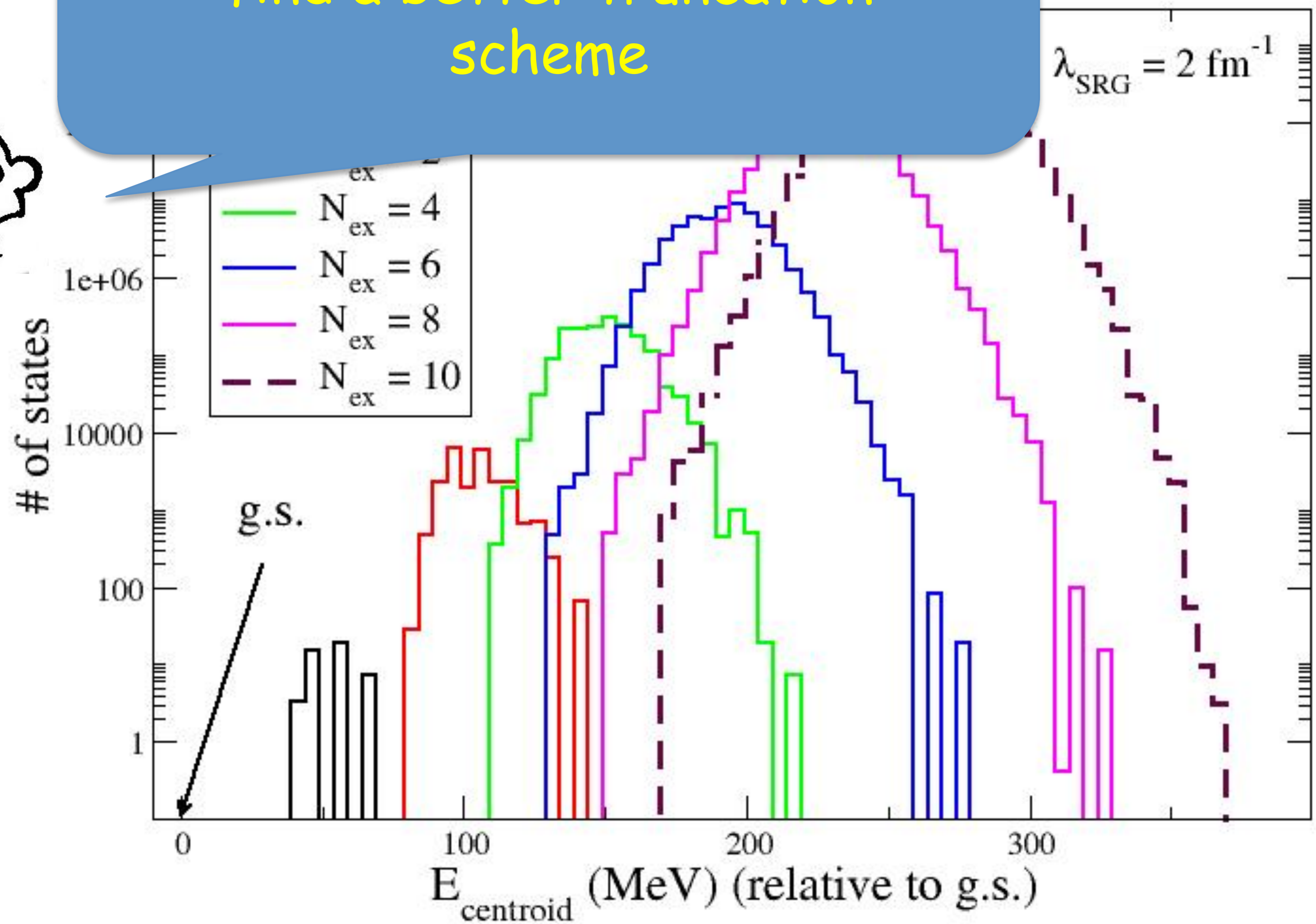


Spectral distribution theory and SRG……

SAN DIEGO STATE UNIVERSITY

Example
(chiral En

This suggest we might find a better truncation scheme



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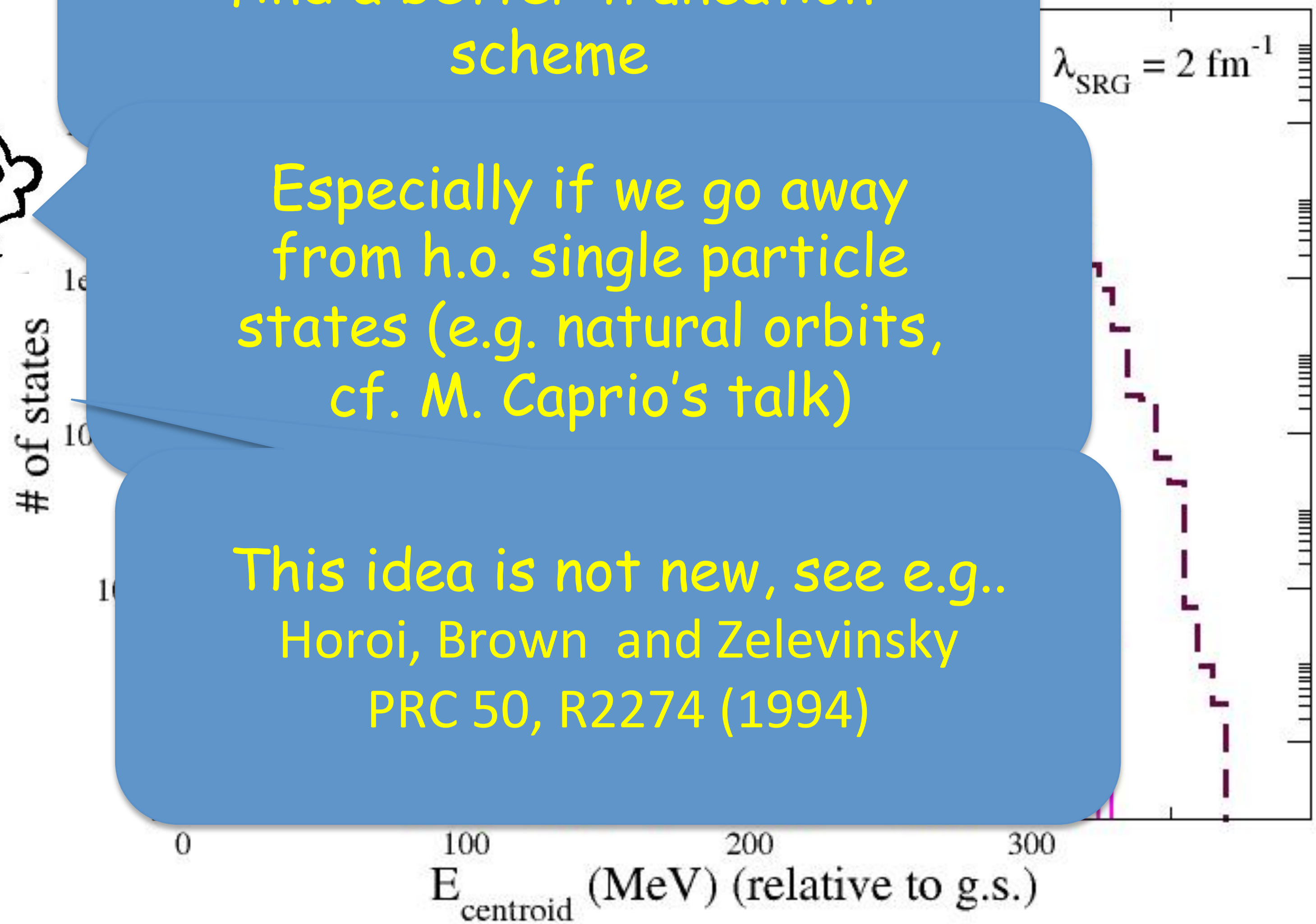
Example
(chiral En

This suggest we might find a better truncation scheme

Especially if we go away from h.o. single particle states (e.g. natural orbits, cf. M. Caprio's talk)

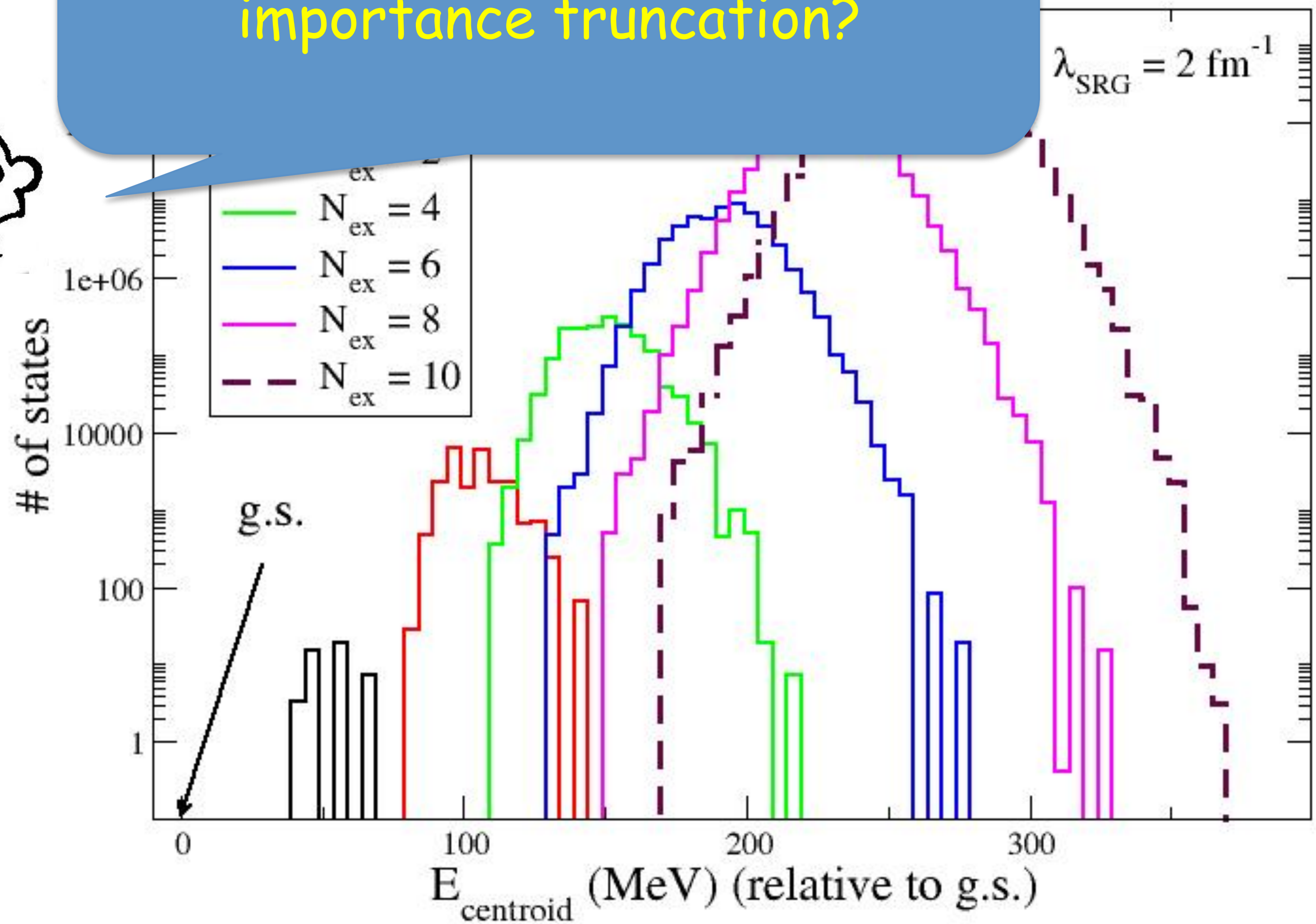
This idea is not new, see e.g..
Horoi, Brown and Zelevinsky PRC 50, R2274 (1994)



San Diego State University

Example:
(chiral En

Might it be of use in importance truncation?



Spectral distribution theory and my summary

Spectral distribution theory averages over many-body systems by traces, simpler than computing the entire matrix

The **main effect** of SRG is to shift the overall spectrum downward, with small (but probably non-perturbative) changes to **residual** and **monopole** pieces

Spectral distribution theory and THE END

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Spectral distribution theory averages over many-body systems by traces, simpler than computing the entire matrix

Possible applications for SDT include:

- **characterizing effect of SRG evolution**
- **Comparing different interactions (chiral vs. Argonne vs. JISP16, N3LO vs N2LO$_{sat}$ vs NXLO$_{yournamehere}$, CCEI vs IMSRG-EI vs phenomenology....)**

- **Can we find simplify the effects of SRG? especially for higher-rank (N-body) parts?**

- **What happens to operators (e.g. R^2)**

- **Aid in improving single-particle basis**
- **Aid in truncation of many-body basis/ importance truncation**