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Ab initio rotational bands in medium and heavy nuclei

Calvin W. Johnson

"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"

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Robert Roth:

Open problem:
ab initio techniques for medium-mass open-shell nuclei

I will suggest an alternate approach

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This is the cosmic distance ladder.

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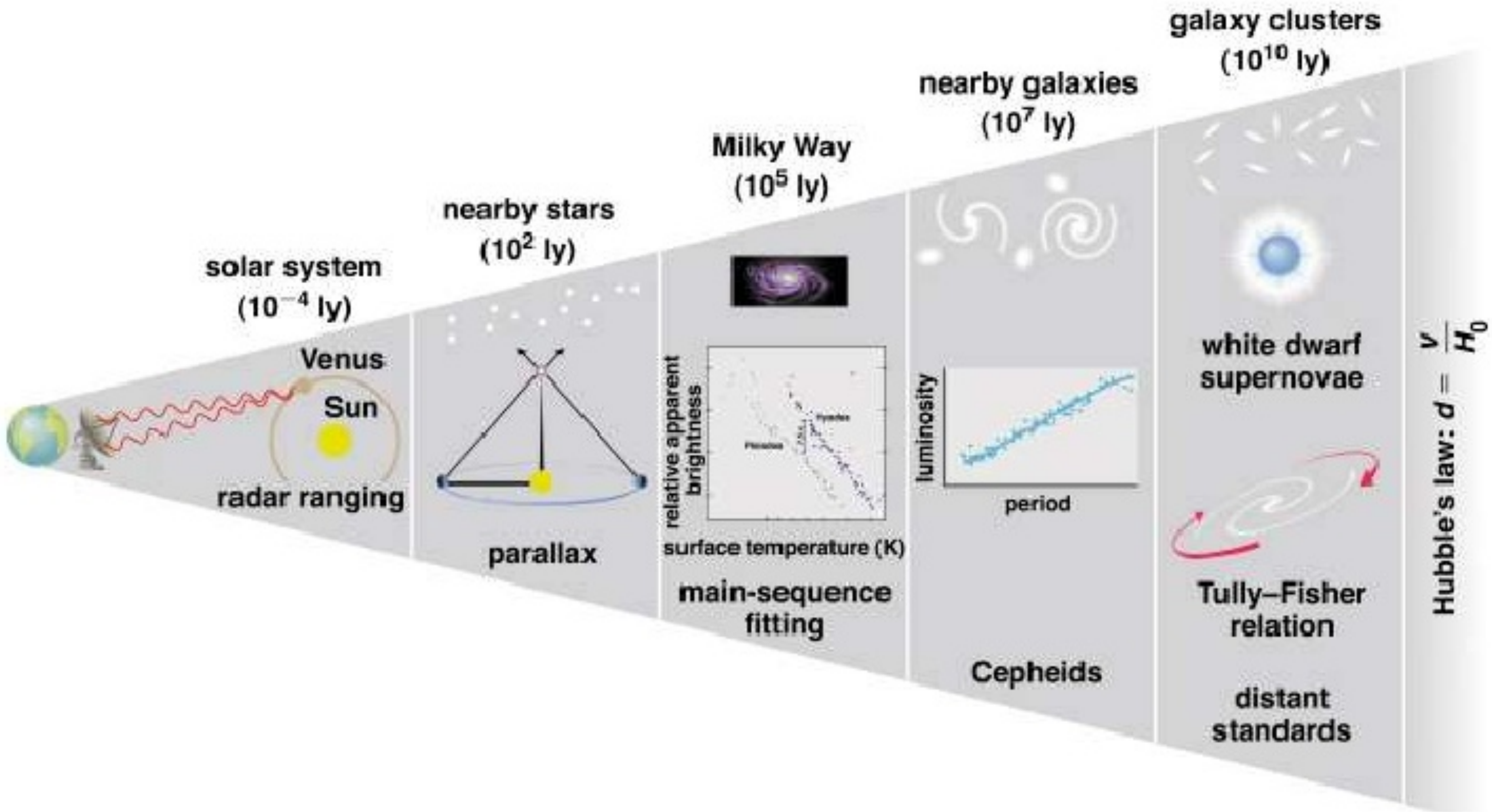
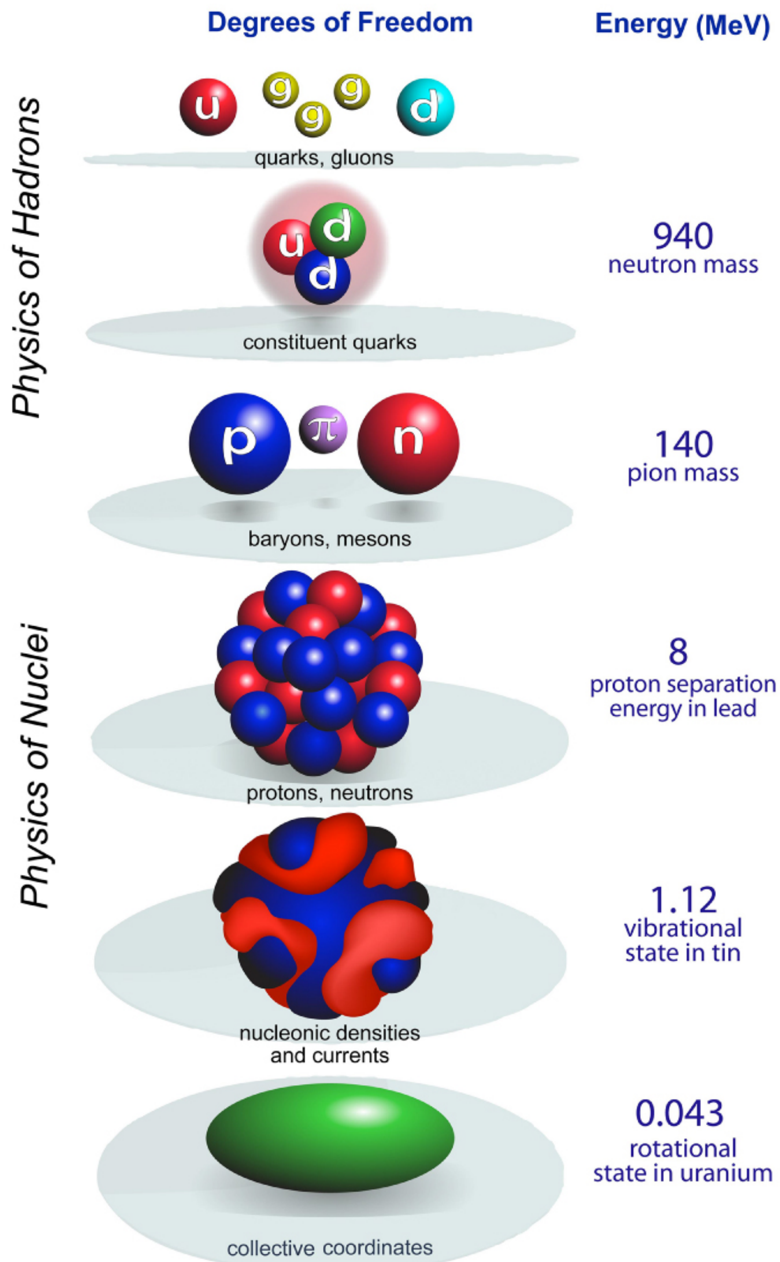


From "The Essential Cosmic Perspective", Bennett et al.



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The "nuclear ladder"

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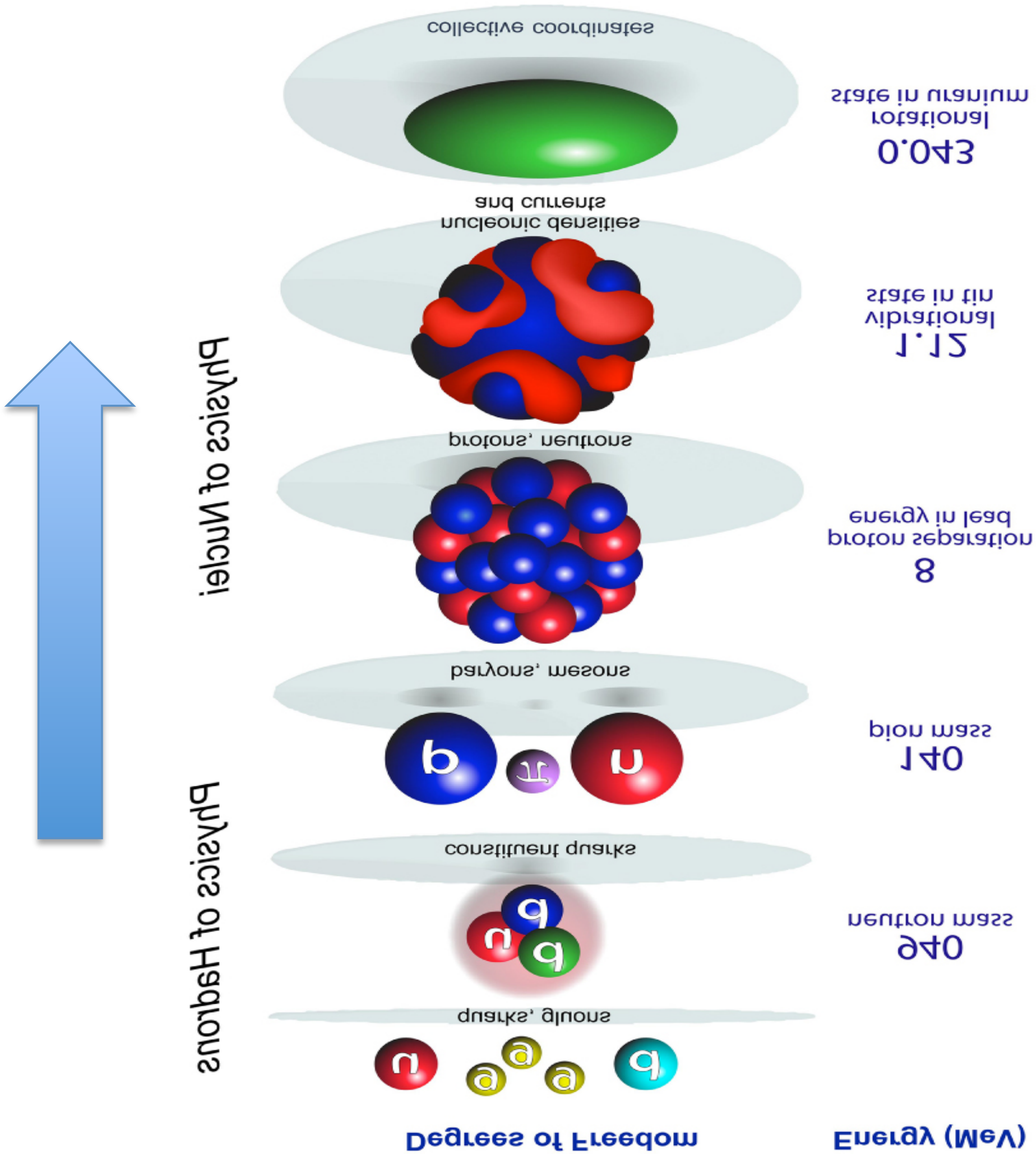
The "nuclear ladder"



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The old "nuclear ladder"

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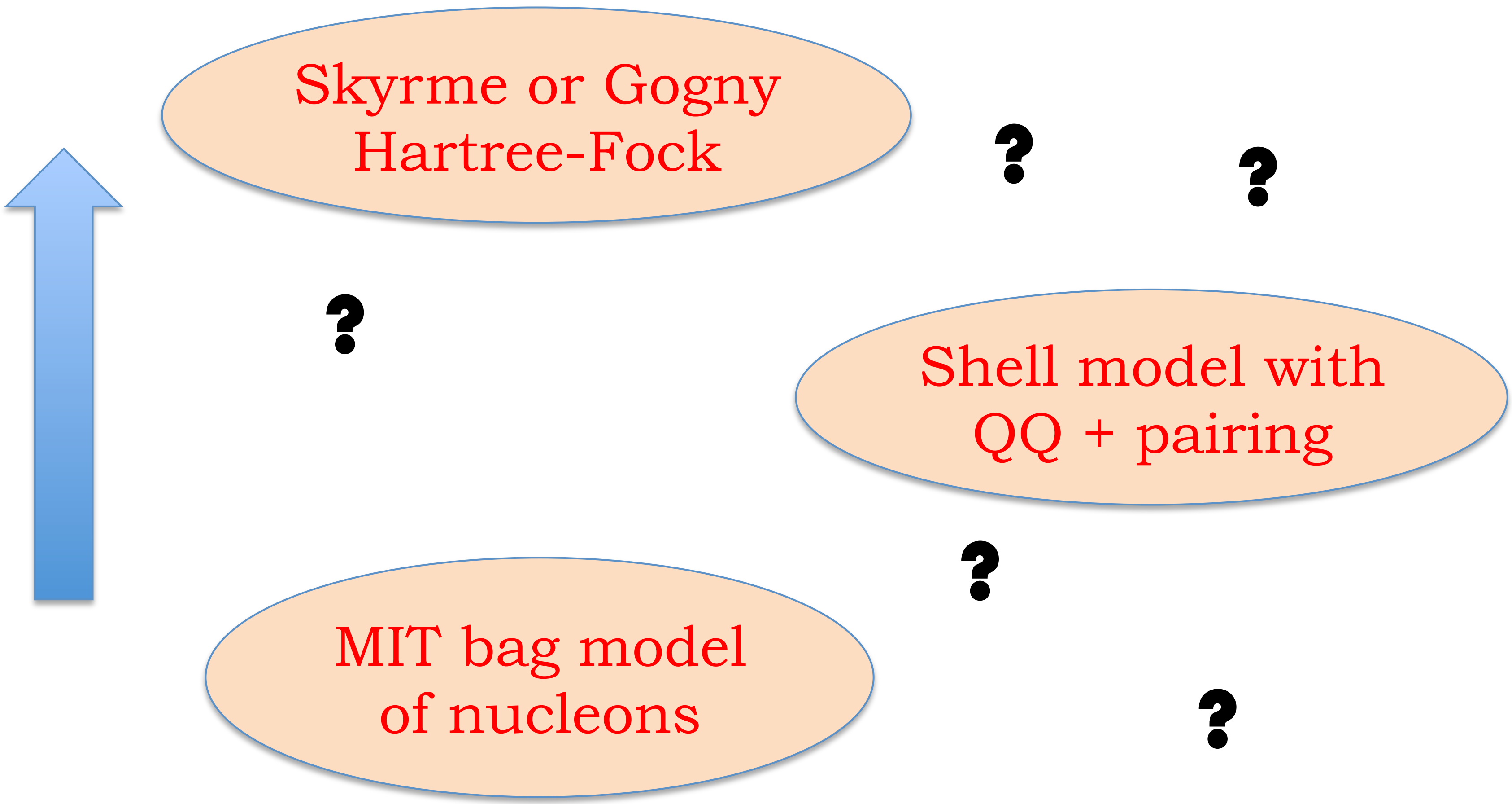

The old "nuclear ladder"

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Skyrme or Gogny
Hartree-Fock

?

?

"Nuclear forces are
short-ranged
blah blah blah"

Shell model with
QQ + pairing

?

MIT bag model
of nucleons

?

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Today's "nuclear ladder"

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Modern EDFs
e.g. UNEDF

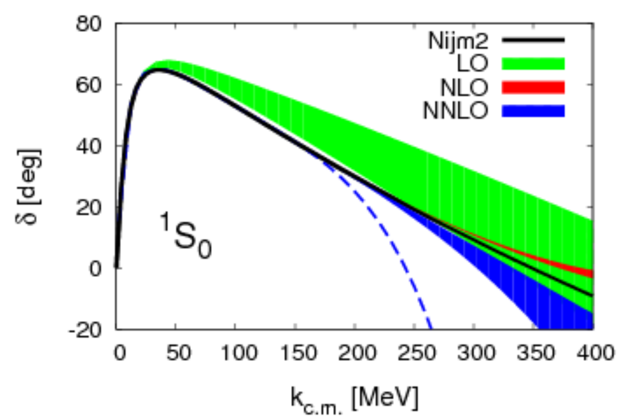
Powerful "exact" methods: GFMC, CC, NCSM

H.O. matrix elements

(SRG or other renormalization)

Chiral / Argonne/ other potentials

High precision expt phase shifts



Tomorrow's "nuclear ladder"

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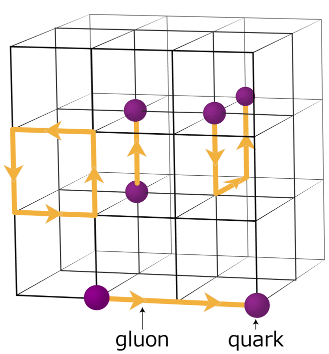
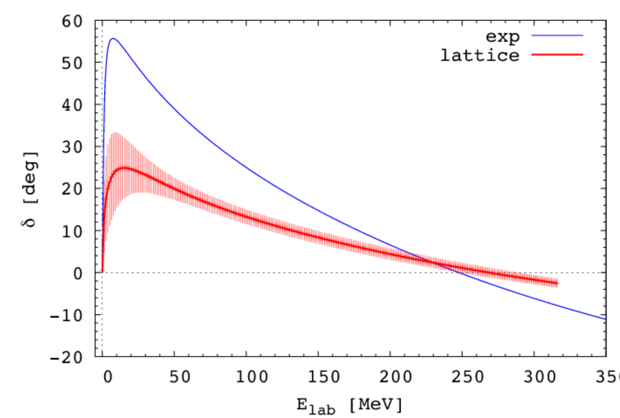
Modern EDFs
e.g. UNEDF

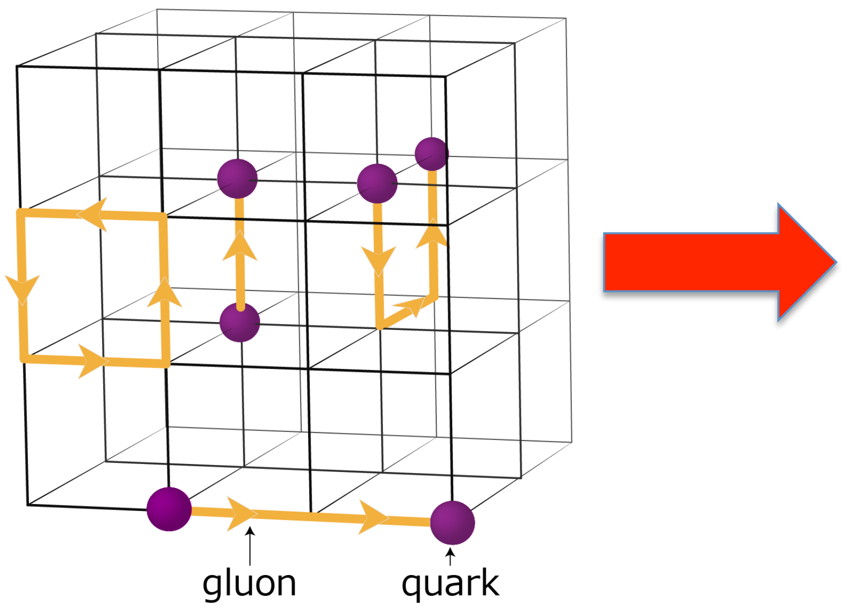
Powerful "exact" methods: GFMC, CC, NCSM

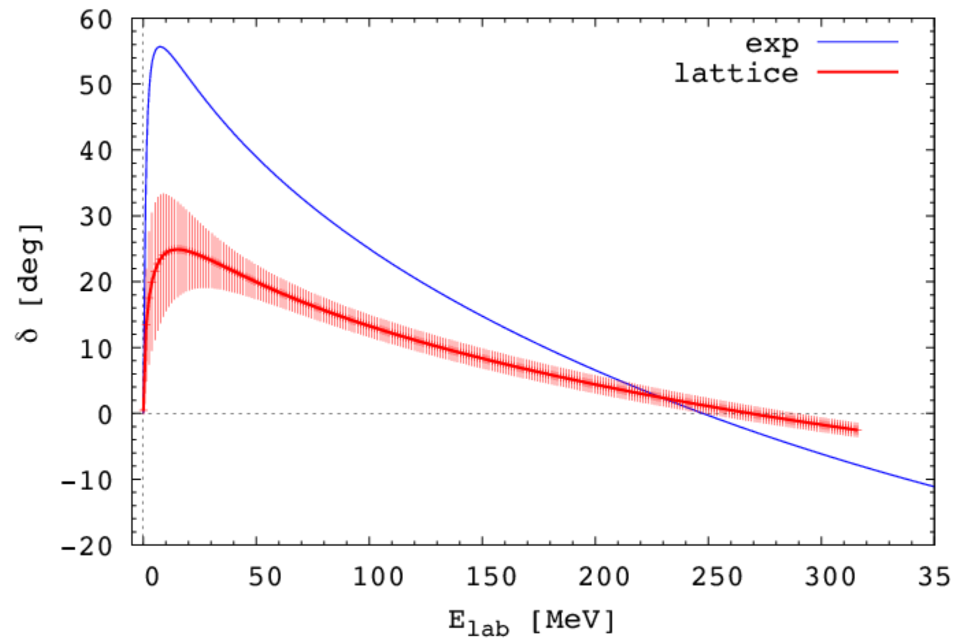
H.O. matrix elements





Lattice QCD phase shifts





Phase shifts directly from Lattice QCD

Beane et al Phys. Rev. Lett. 97, 012001 (2006)
Ishii et al, Phys. Rev. Lett. 99, 022001 (2007)

Interaction matrix elements in harmonic oscillator space directly from phase shifts:

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EFT approach
Stetcu et al Phys Lett B 653, 358 (2007)

J-matrix methods (starting from chiral EFT)
Shirokov et al Phys Lett B 644, 33 (2007) (JISP16)
Shirokov et al Phys Lett B 761, 87 (2016) (Daejeon16)

Haxton Phys. Rev. C 77, 034005 (2008) (HOBET)
McElvain and Haxton, arXiv:1607.06863

Binder et al Phys. Rev. C 93, 044332 (2016)
Yang Phys. Rev. C 94, 064004 (2016)

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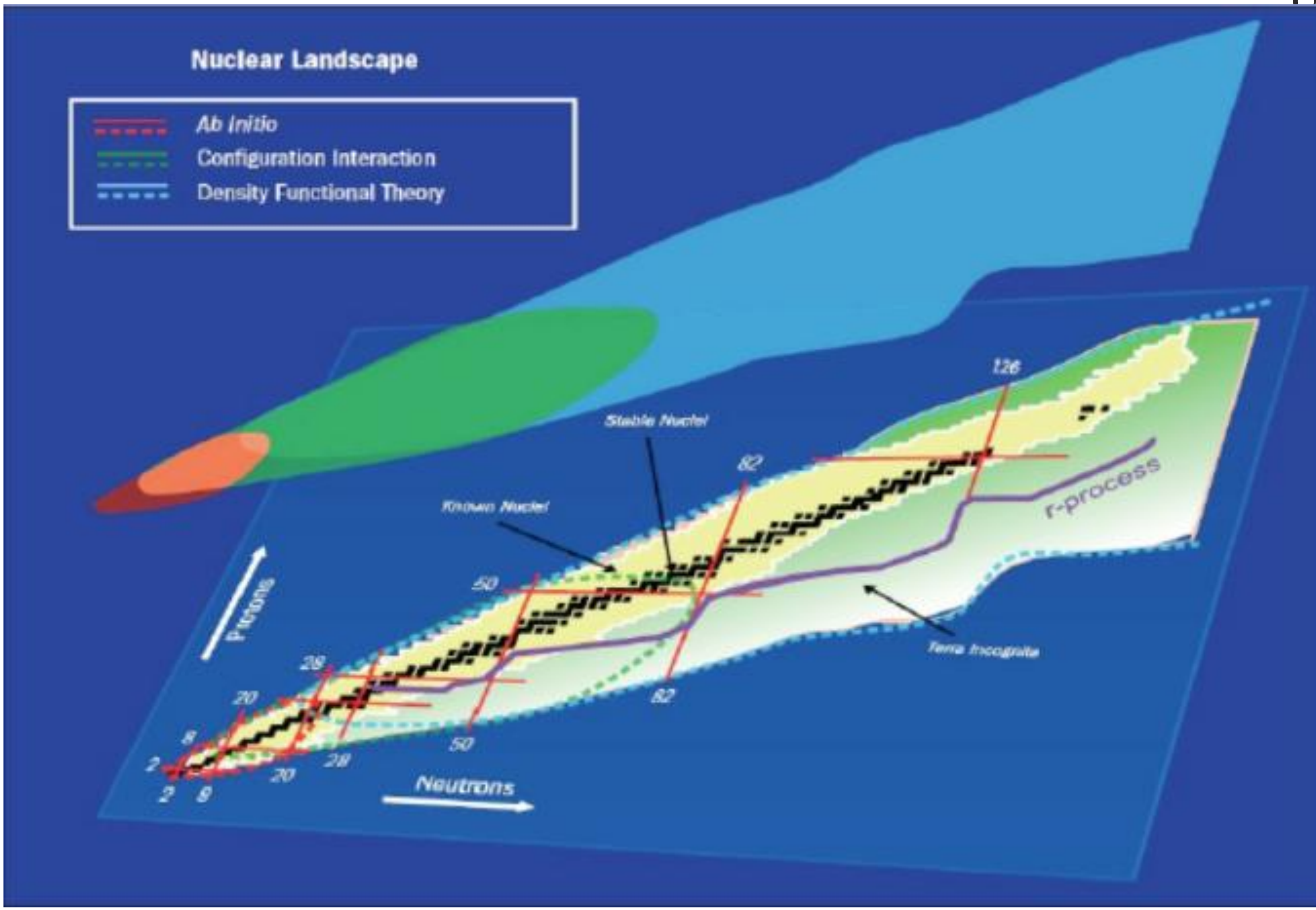

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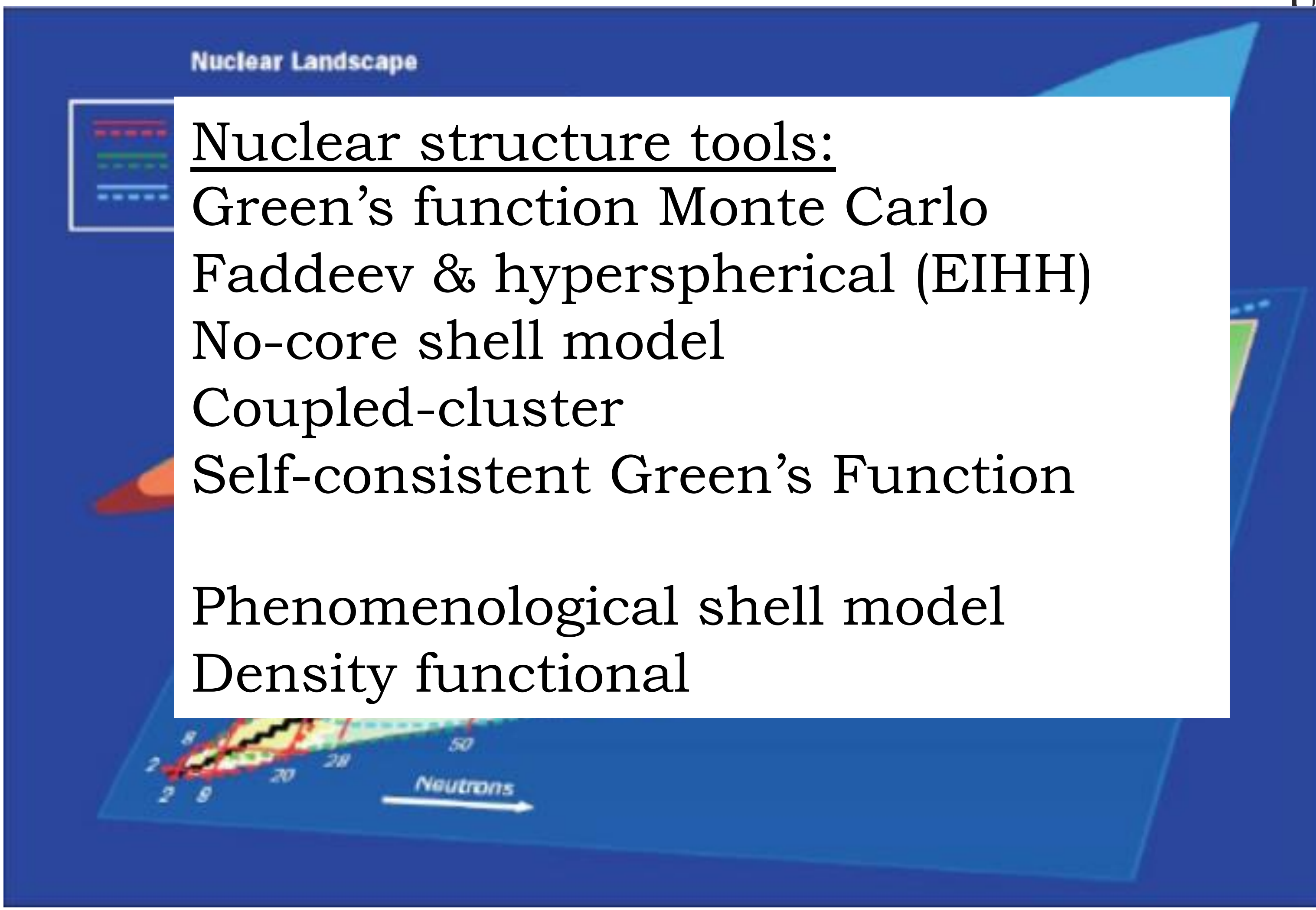
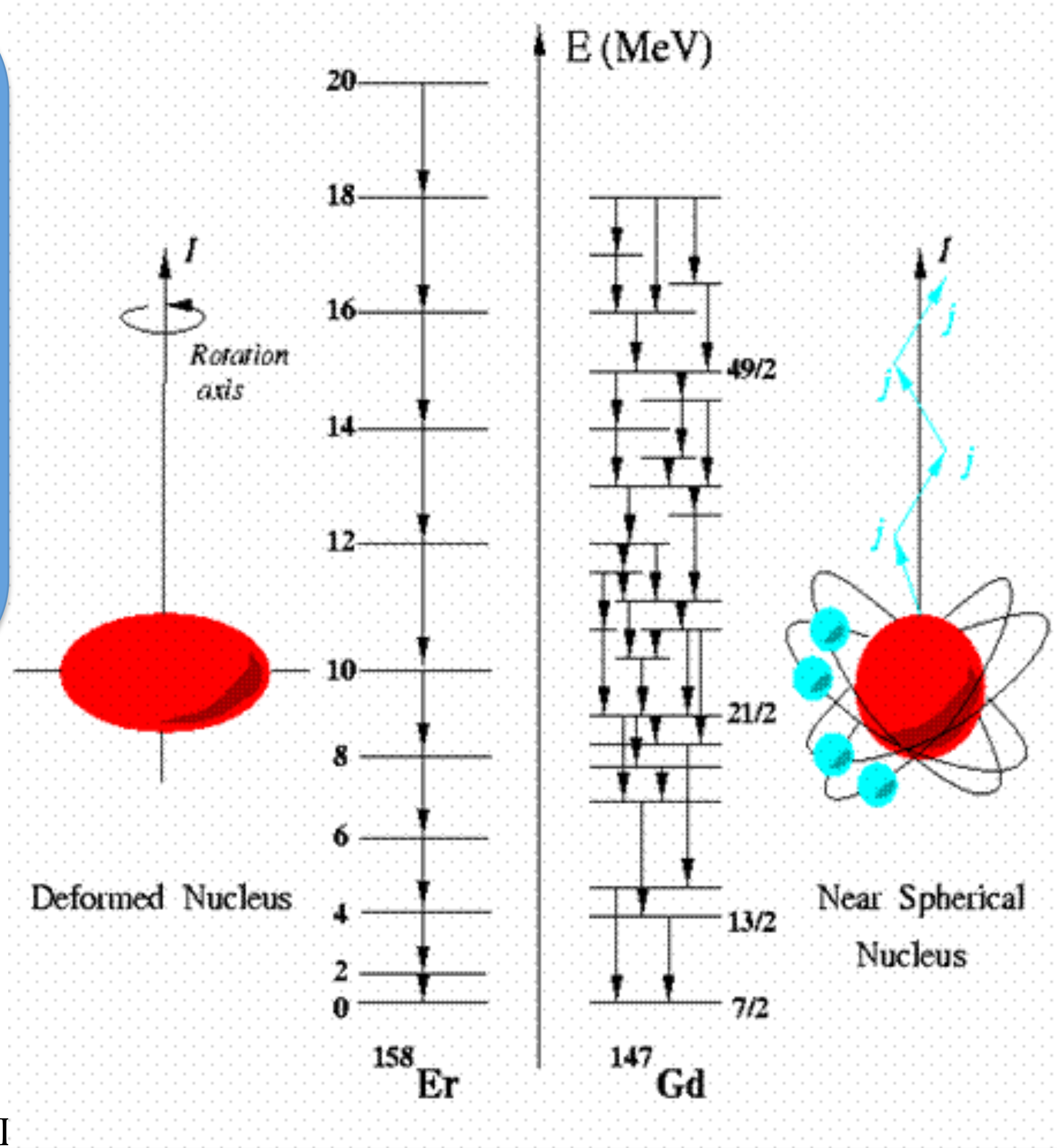


<u>Nuclear structure tools:</u>

Green’s function Monte Carlo
Faddeev & hyperspherical (EIHH)
No-core shell model
Coupled-cluster
Self-consistent Green’s Function

Phenomenological shell model
Density functional

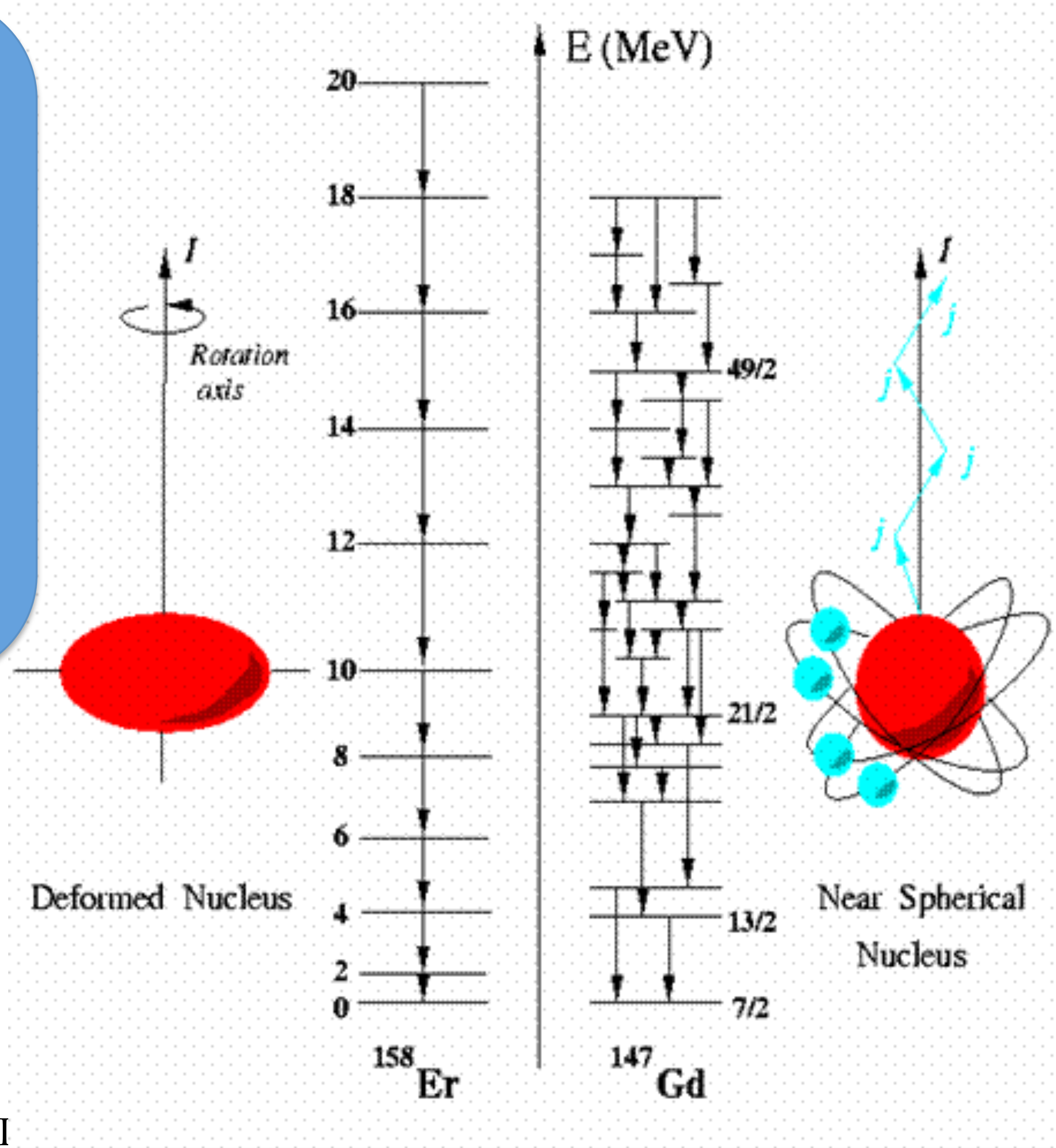
I'm going to focus on **rotational bands**: they are both a typical behavior but challenging to calculate



RE”

TRI

A “natural” way to describe rotations are through groups such as SU(3) and Sp(3,R) (see talks by M. Caprio and K. Launey



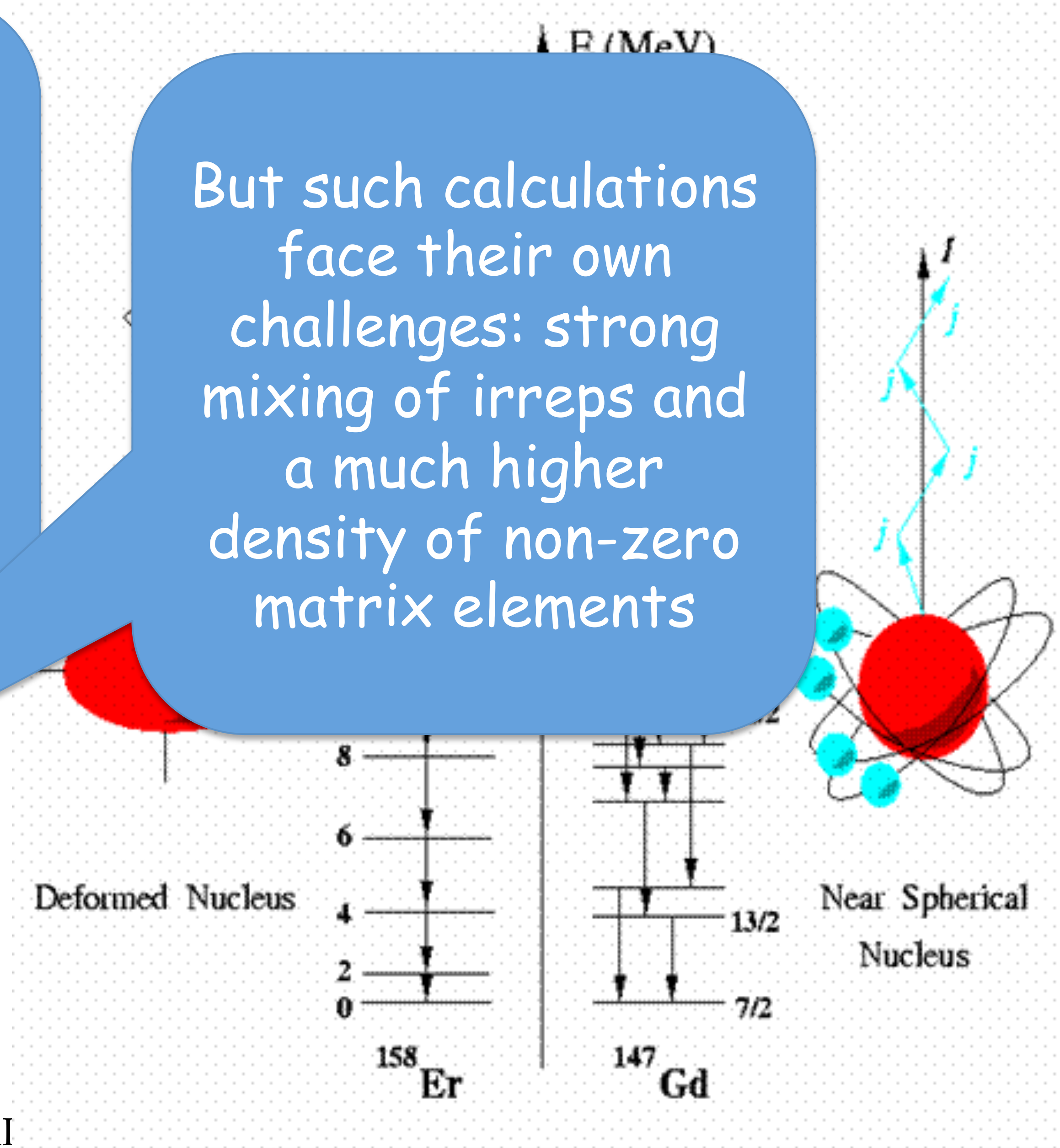
RE”

TRI

A "natural" way to describe rotations are through groups such as SU(3) and Sp(3,R) (see talks by M. Caprio and K. Launey

But such calculations face their own challenges: strong mixing of irreps and a much higher density of non-zero matrix elements

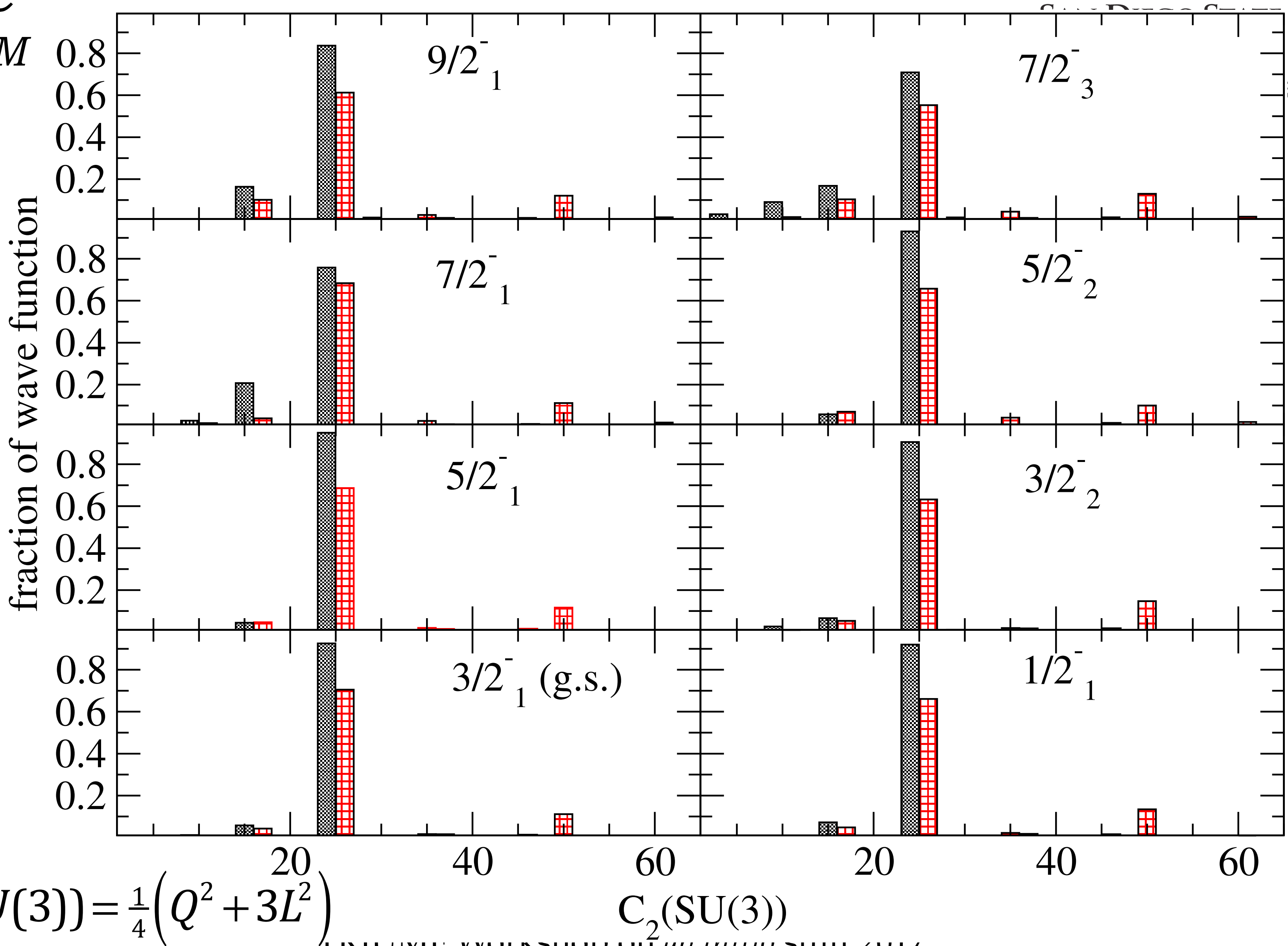
RE"



TRI

^{9}Be

NCSM



$$C_2(SU(3)) = \frac{1}{4}\left(Q^2 + 3L^2\right)$$

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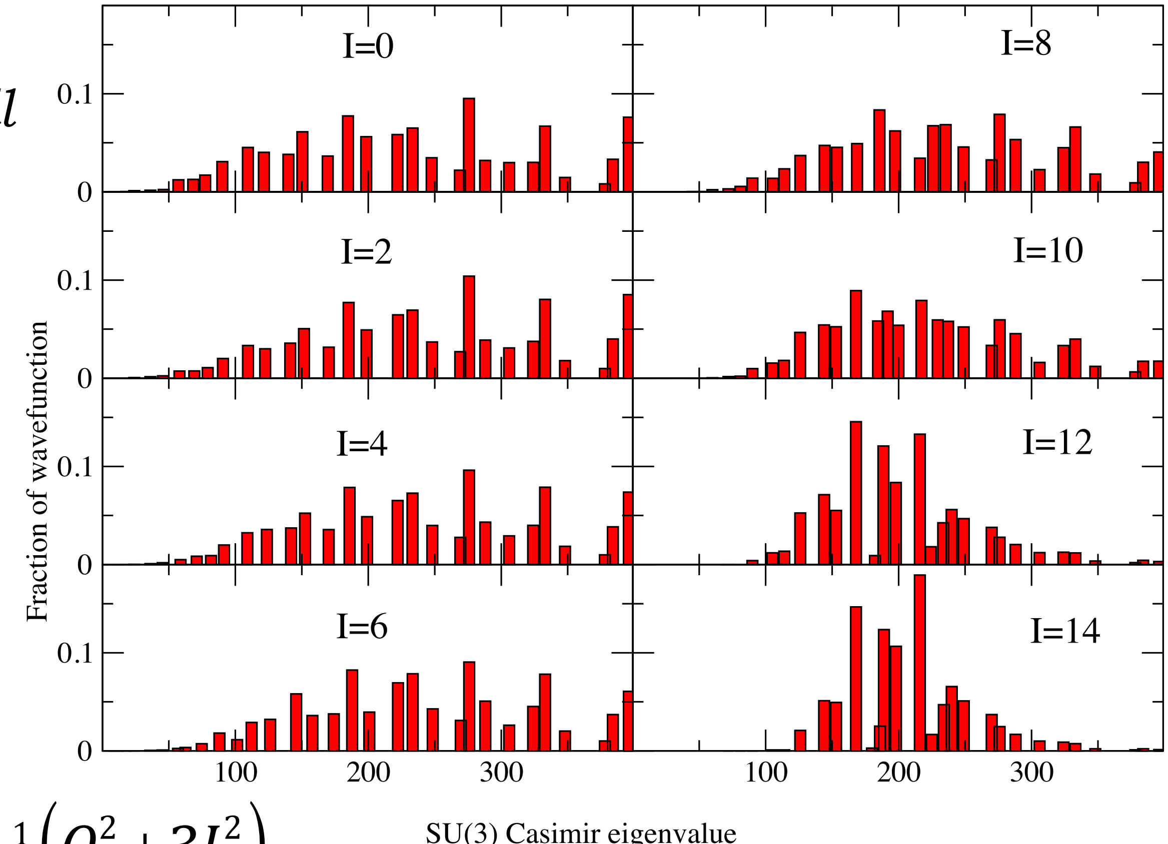
^{48}Cr
in *pf shell*



$$C_2(SU(3)) = \frac{1}{4}\left(Q^2 + 3L^2\right)$$

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Let me start with "standard" no-core shell model (NCSM) calculations:

That is, diagonalize the nuclear many-body Hamiltonian in a basis of Slater determinants built from h.o. s.p. states

with an "N_{max}" truncation

I do this with the BIGSTICK code

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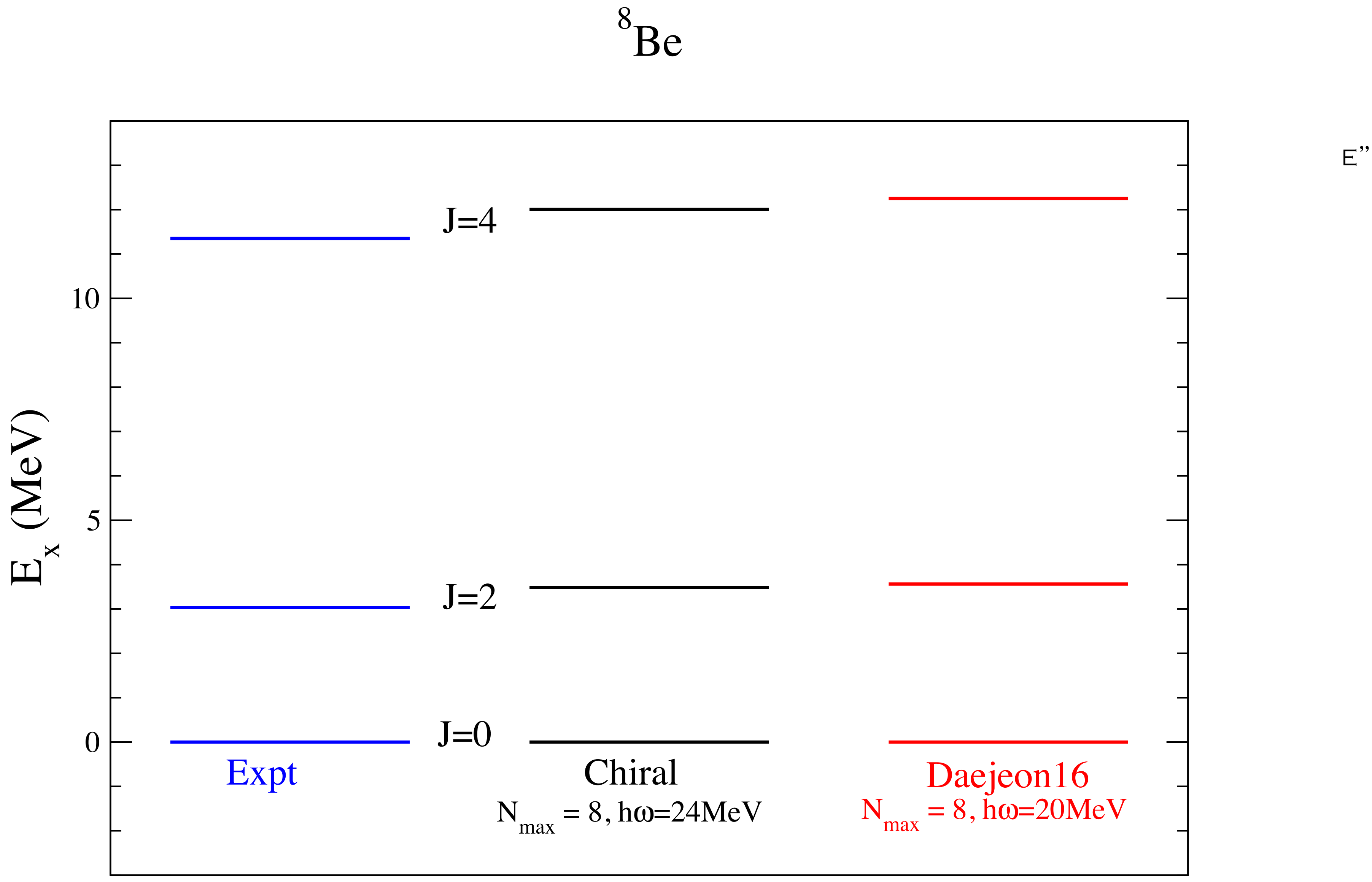
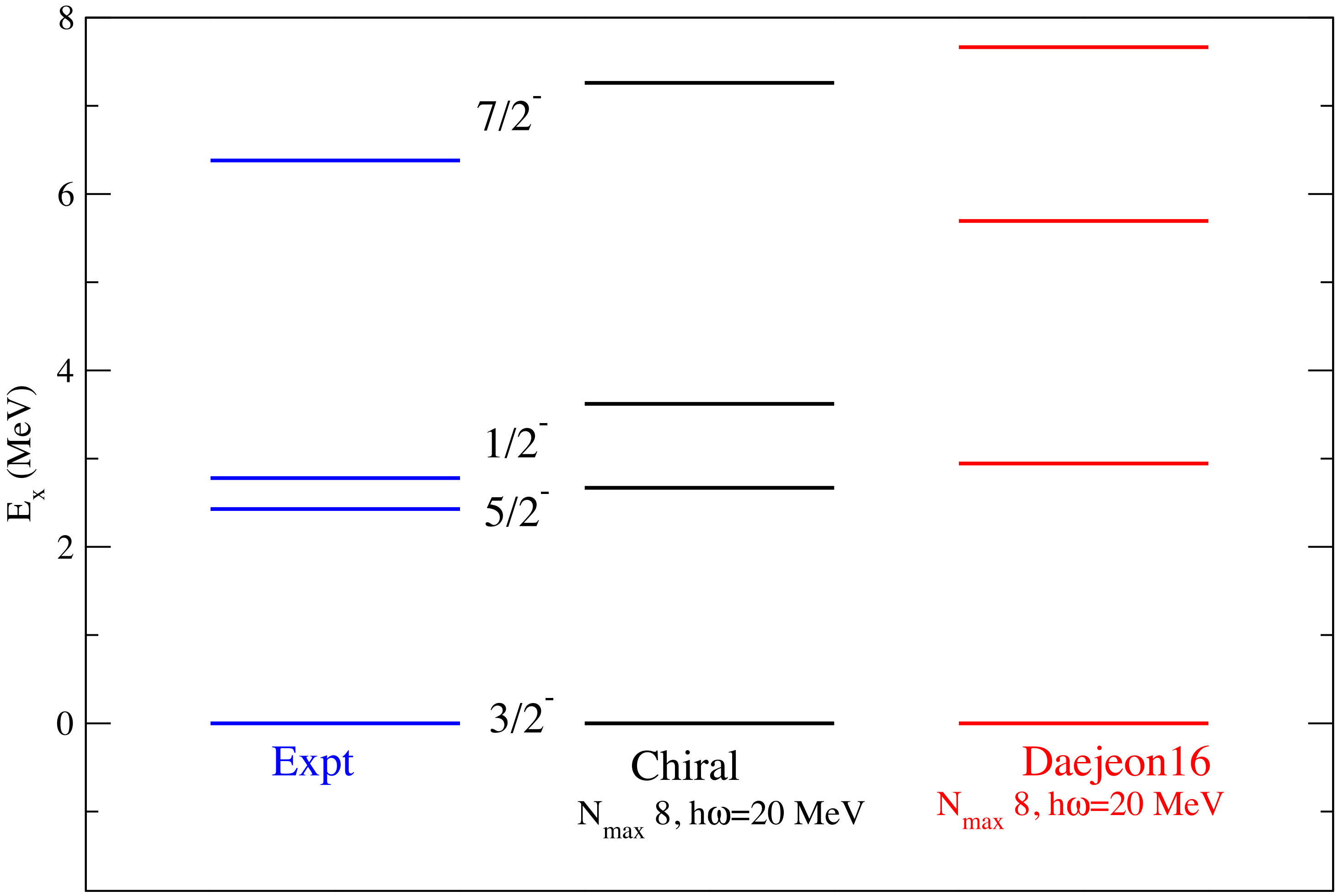
Let me start with beryllium isotopes
(see also pioneering studies of
Caprio, Maris, Vary, Phys Lett B 719, 179 (2013)
Maris, Caprio, Vary, Phys Rev C 91, 014310 (2015))

Used Entem & Machleidt N3LO Chiral, Daejeon16 interactions

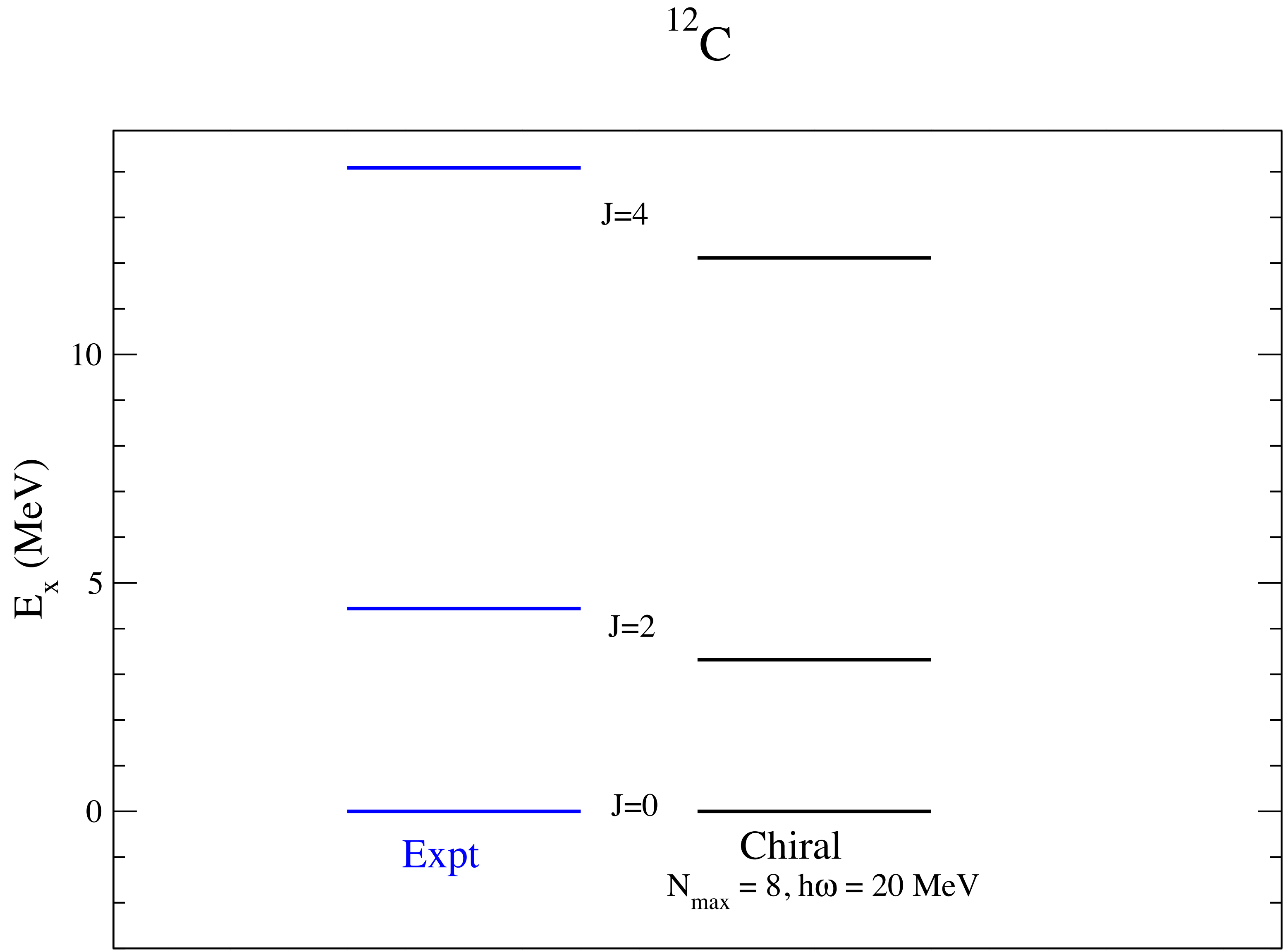


^{8}Be
E"
E_x (MeV)
10
5
0
J=4
J=2
J=0
Expt
Chiral
N_{max} = 8, hω=24MeV
Daejeon16
N_{max} = 8, hω=20MeV

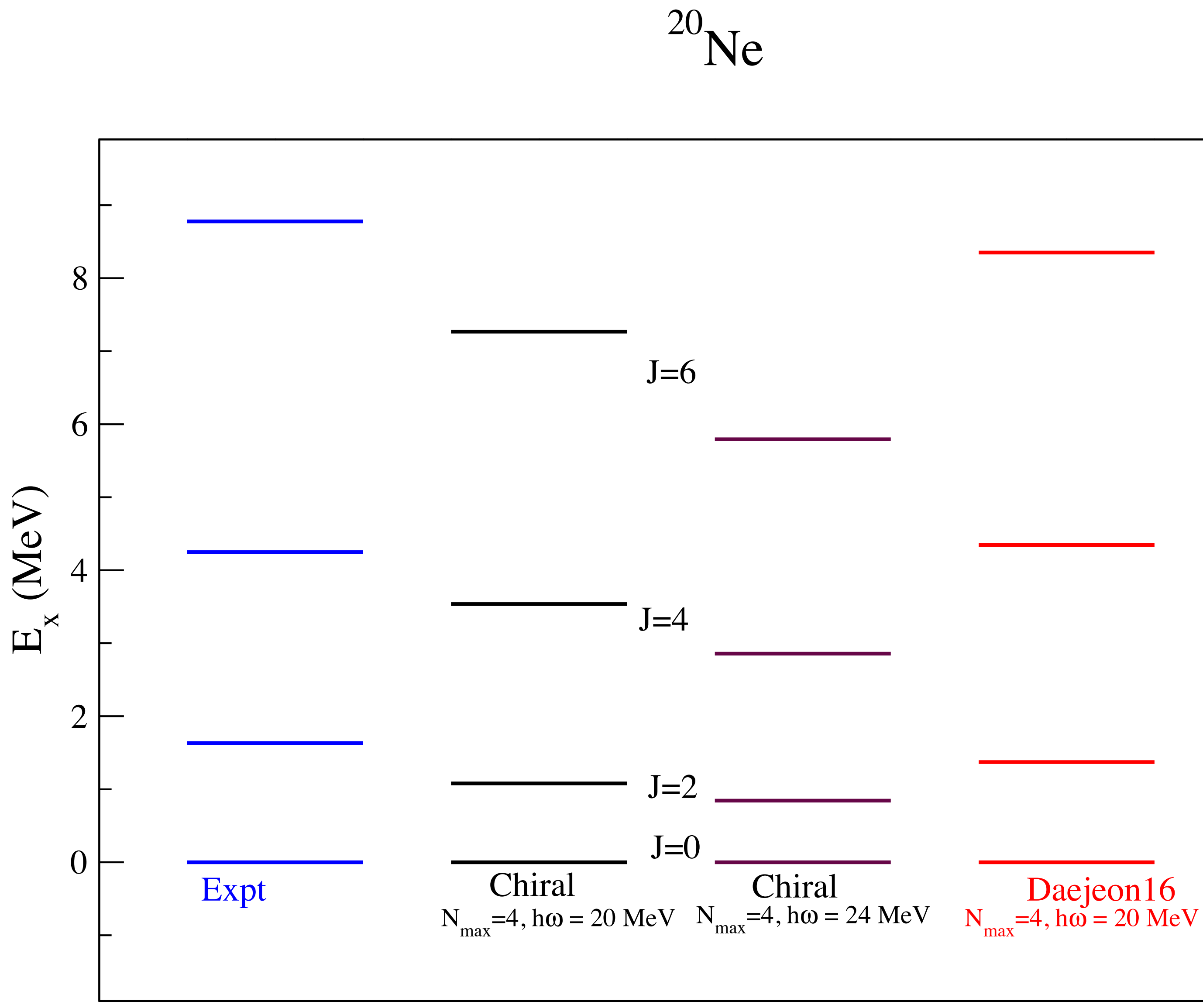
^{9}Be



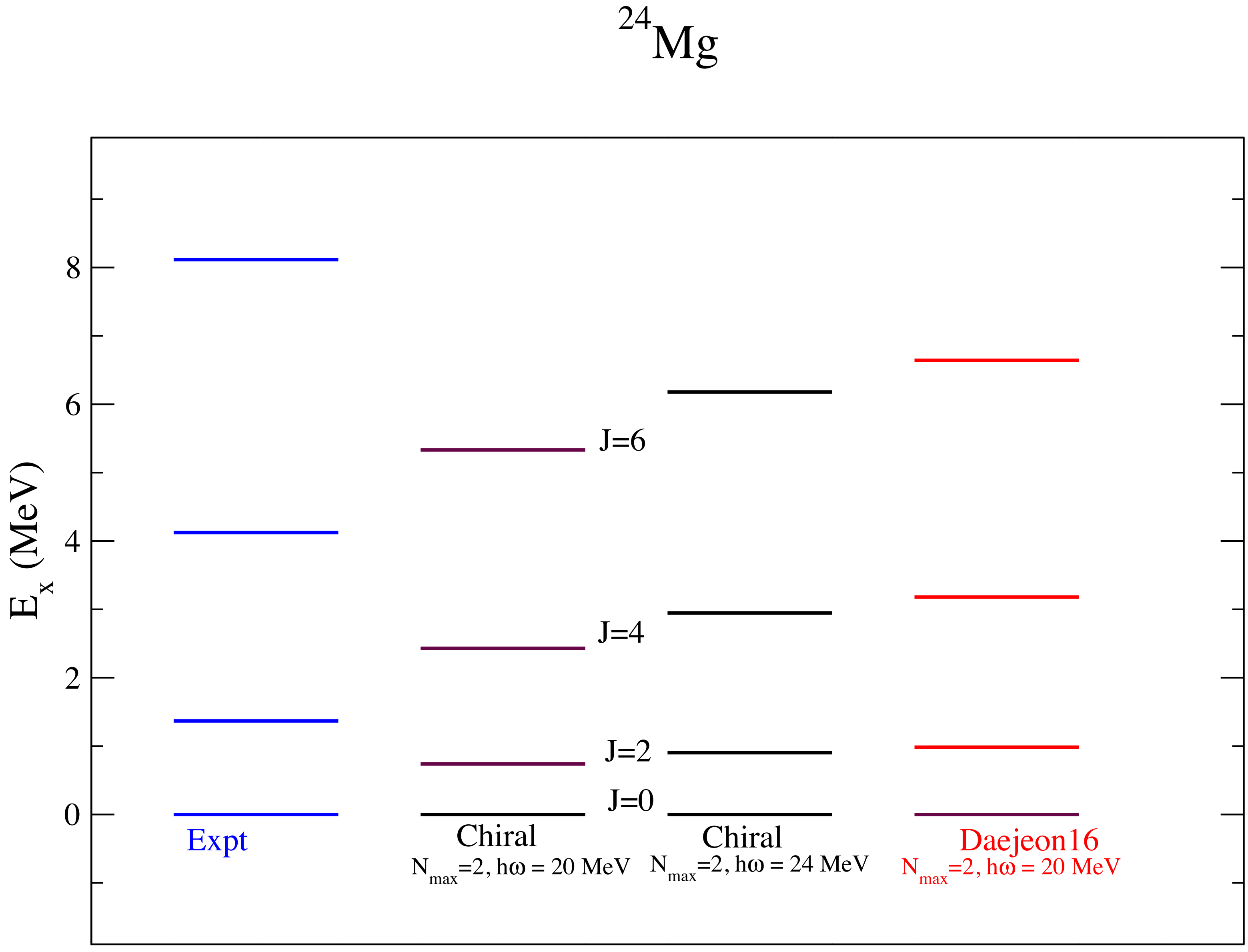
8
6
4
2
0
E_x (MeV)
7/2$^-$
1/2$^-$
5/2$^-$
3/2$^-$
Expt
Chiral
N_{max} 8, hω=20 MeV
Daejeon16
N_{max} 8, hω=20 MeV



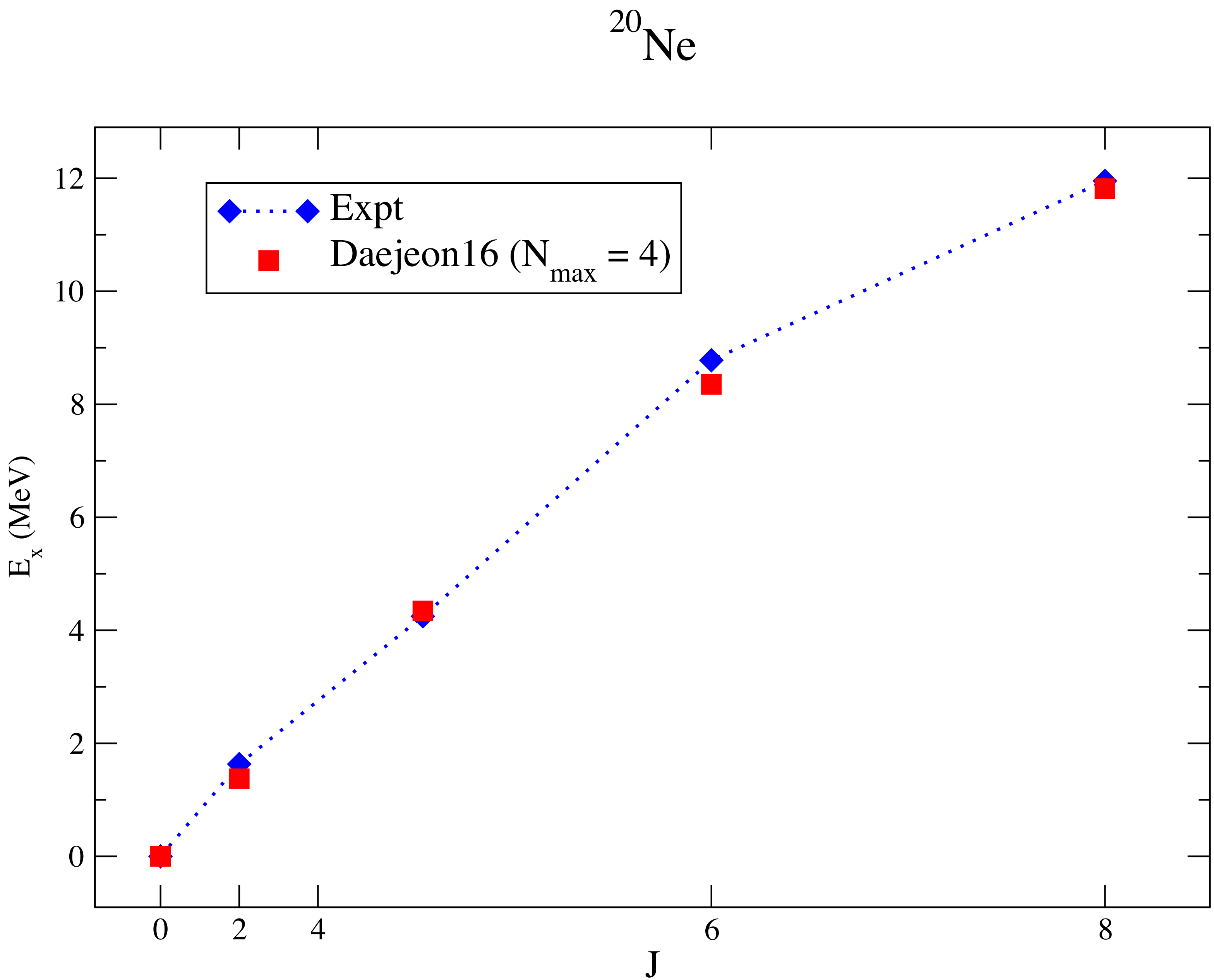
^{12}C
E_x (MeV)
10
5
0
J=4
J=2
J=0
Expt
Chiral
N_{max} = 8, hω = 20 MeV



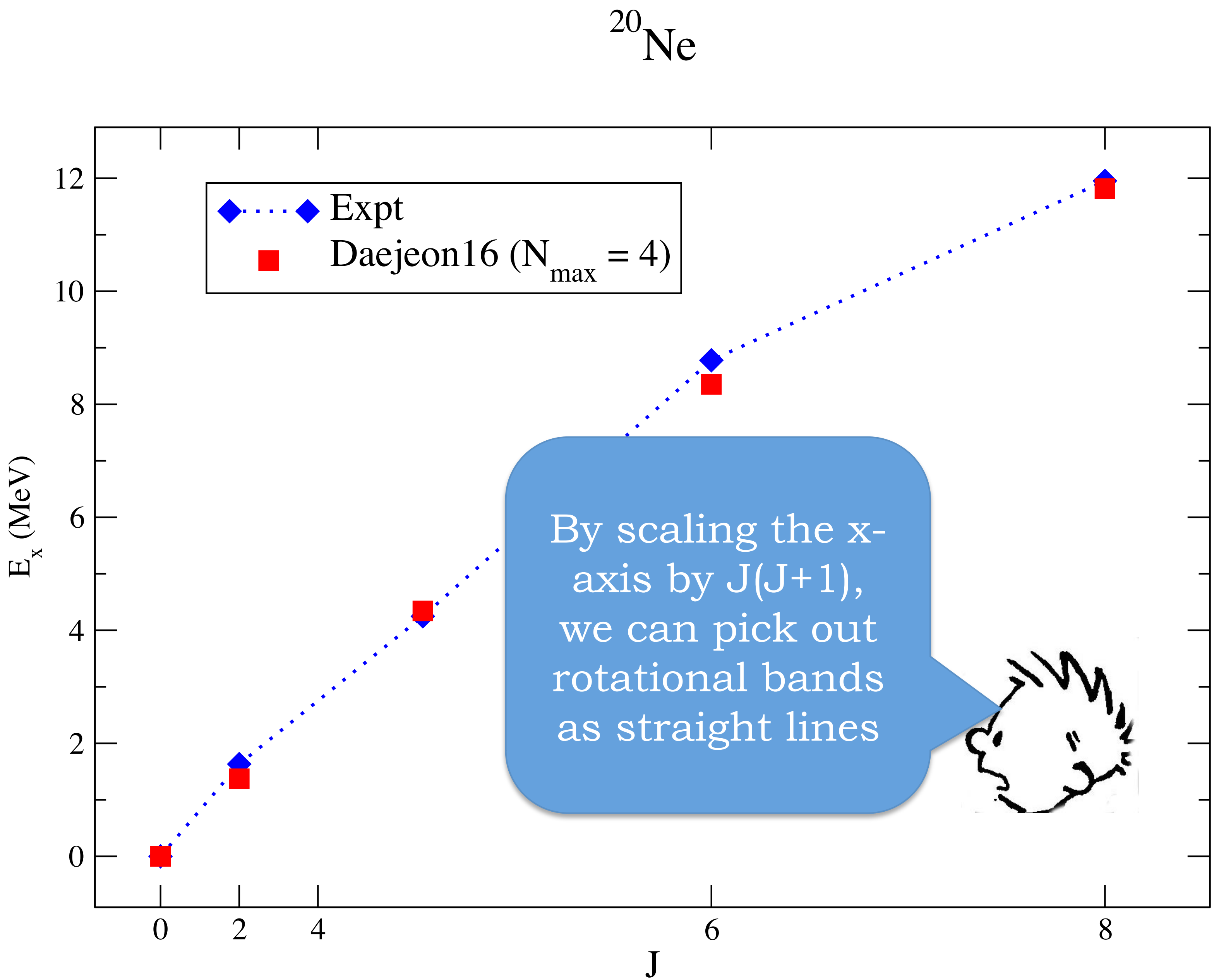
20Ne
Ex (MeV)
0
2
4
6
8
J=6
J=4
J=2
J=0
Expt
Chiral
Nmax=4, hω = 20 MeV
Chiral
Nmax=4, hω = 24 MeV
Daejeon16
Nmax=4, hω = 20 MeV



24Mg
Ex (MeV)
0
2
4
6
8
J=6
J=4
J=2
J=0
Expt
Chiral
Nmax=2, hω = 20 MeV
Chiral
Nmax=2, hω = 24 MeV
Daejeon16
Nmax=2, hω = 20 MeV



^{20}Ne
Expt
Daejeon16 (N_{max} = 4)
E_x (MeV)
J
0
2
4
6
8
10
12



^{20}Ne
Expt
Daejeon16 (N_{max} = 4)
By scaling the x-axis by J(J+1), we can pick out rotational bands as straight lines
E_x (MeV)
J
12
10
8
6
4
2
0
0
2
4
6
8

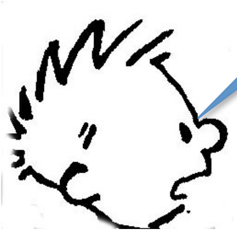
Beyond this point it becomes challenging to carry out NCSM calculations

And do we really need a full solution anyway?

If we imagine a liquid drop picture, then some mean-field approach should suffice

So I carry out Hartree-Fock and then project states of good angular momentum

This can be done using the same shell-model interactions as for those NCSM calculations



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- Hartree-Fock carried out using SHERPA code (Stetcu and Johnson, 2002)

* Found HF energy minimized by $\hbar\Omega$ ~ 20 MeV

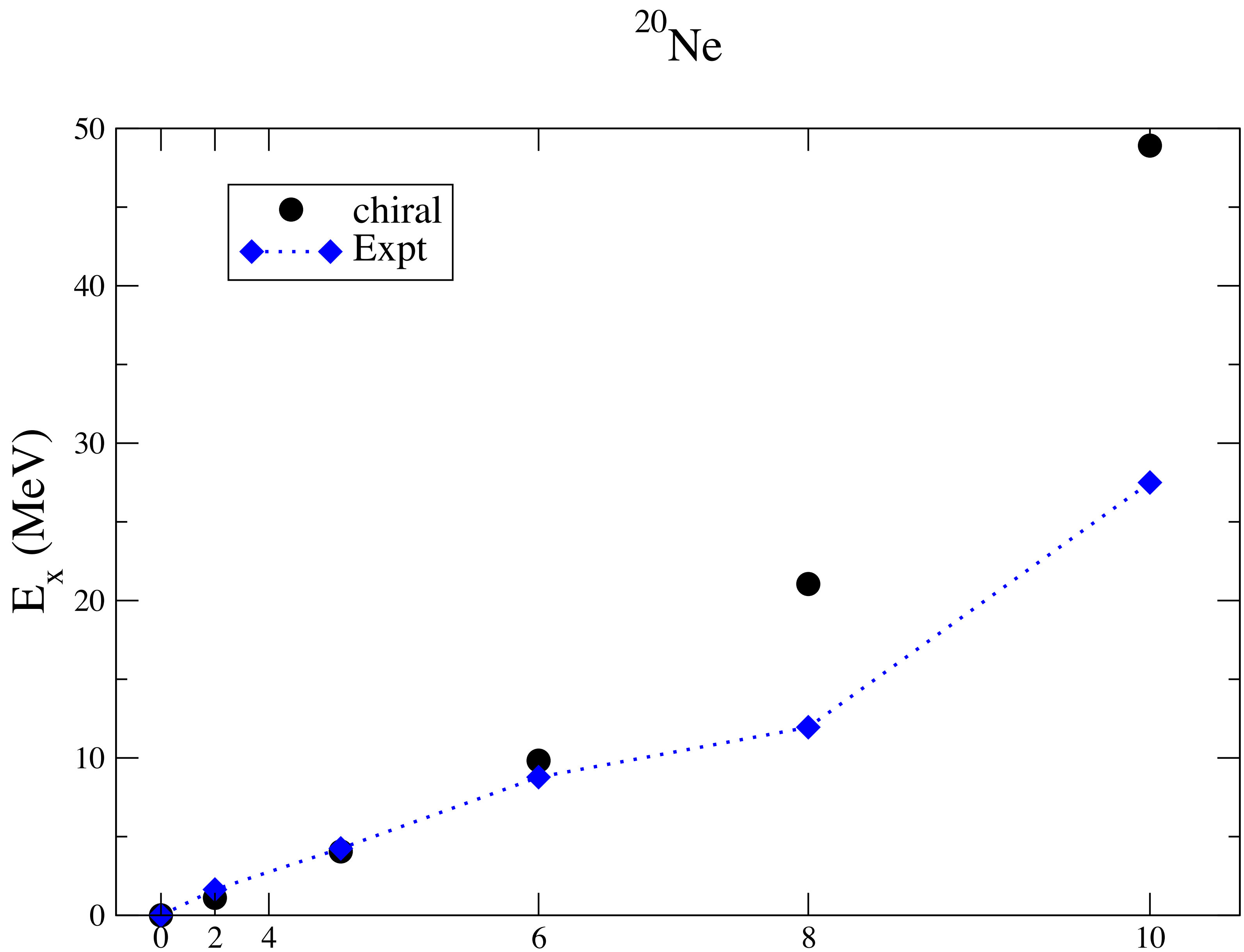
- For light to medium, added H_{cm},
- Found $< H_{cm} > \sim 1.51$ or $1.52\ \hbar\Omega$

- Also used Entem & Machleidt N3LO Chiral, Daejeon16 interactions

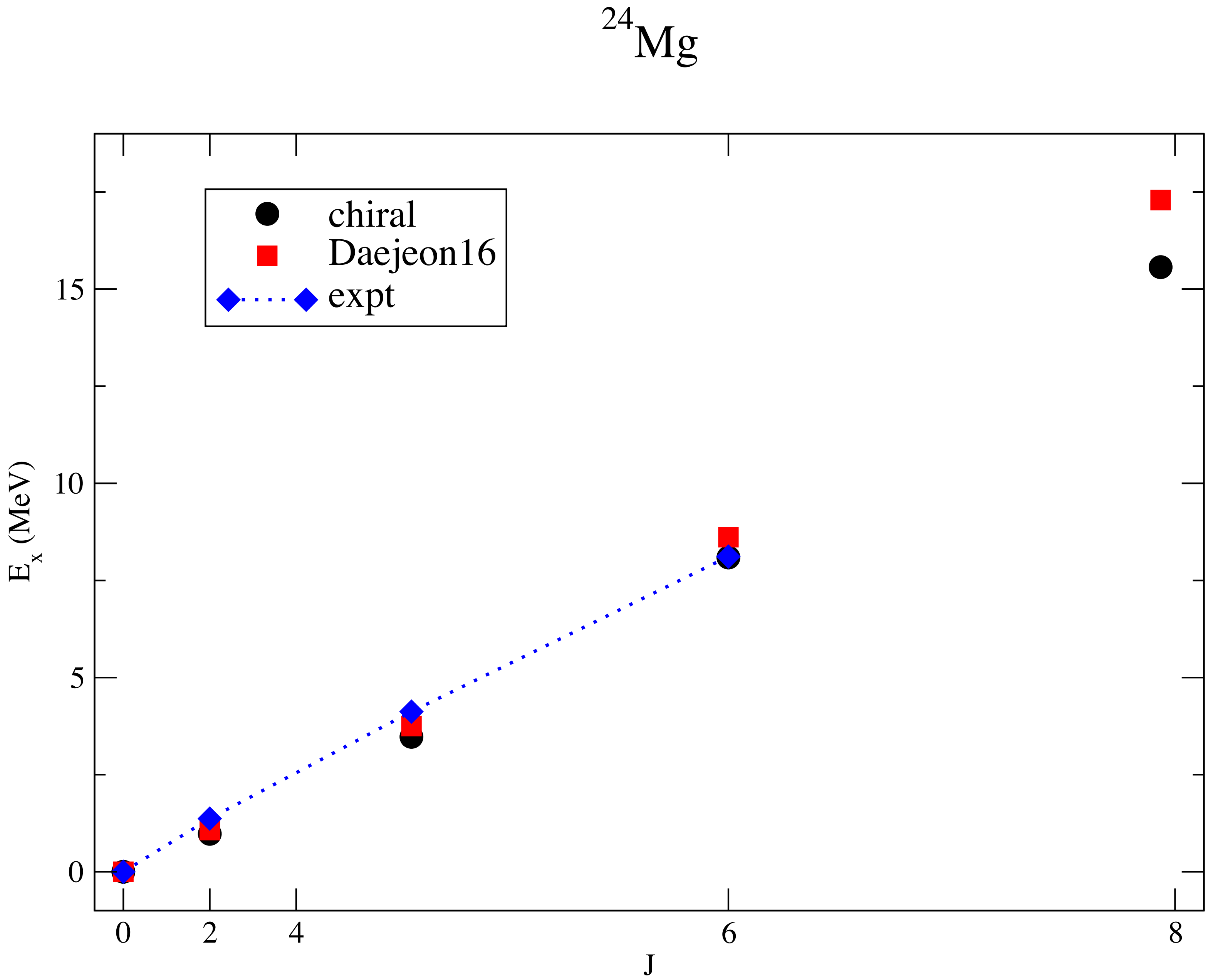
- Angular momentum projection done by novel linear algebra method which is more efficient than the standard integral when projecting out many value of J (not yet published)

Worked in "full configuration" space up to 10 h.o. shells.

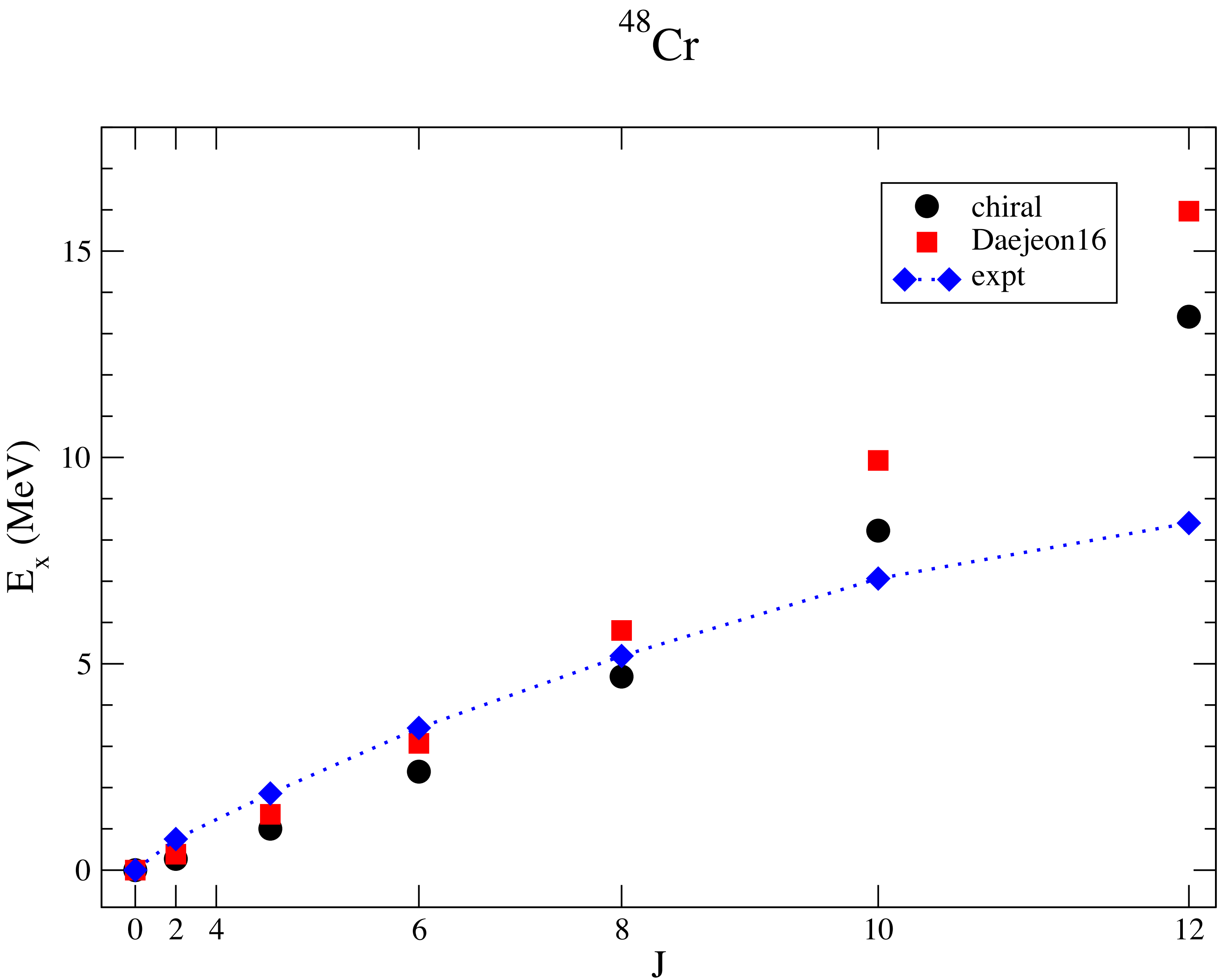
Method is approximate but forces are full *ab initio* – no adjustments!



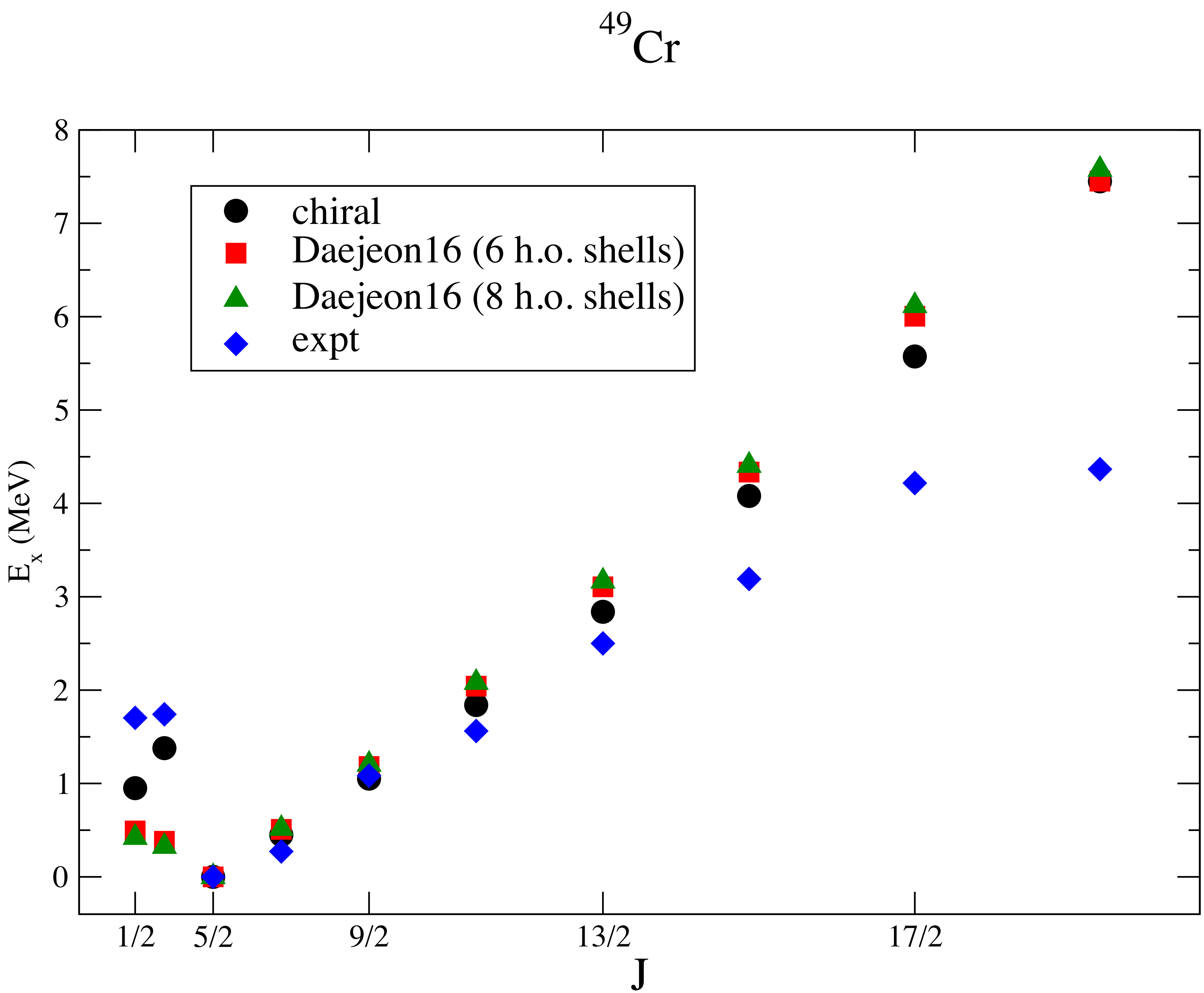
^{20}Ne
chiral
Expt
E_x (MeV)
0
10
20
30
40
50
0
2
4
6
8
10



^{24}Mg
chiral
Daejeon16
expt
E_x (MeV)
J
0
5
10
15
0
2
4
6
8

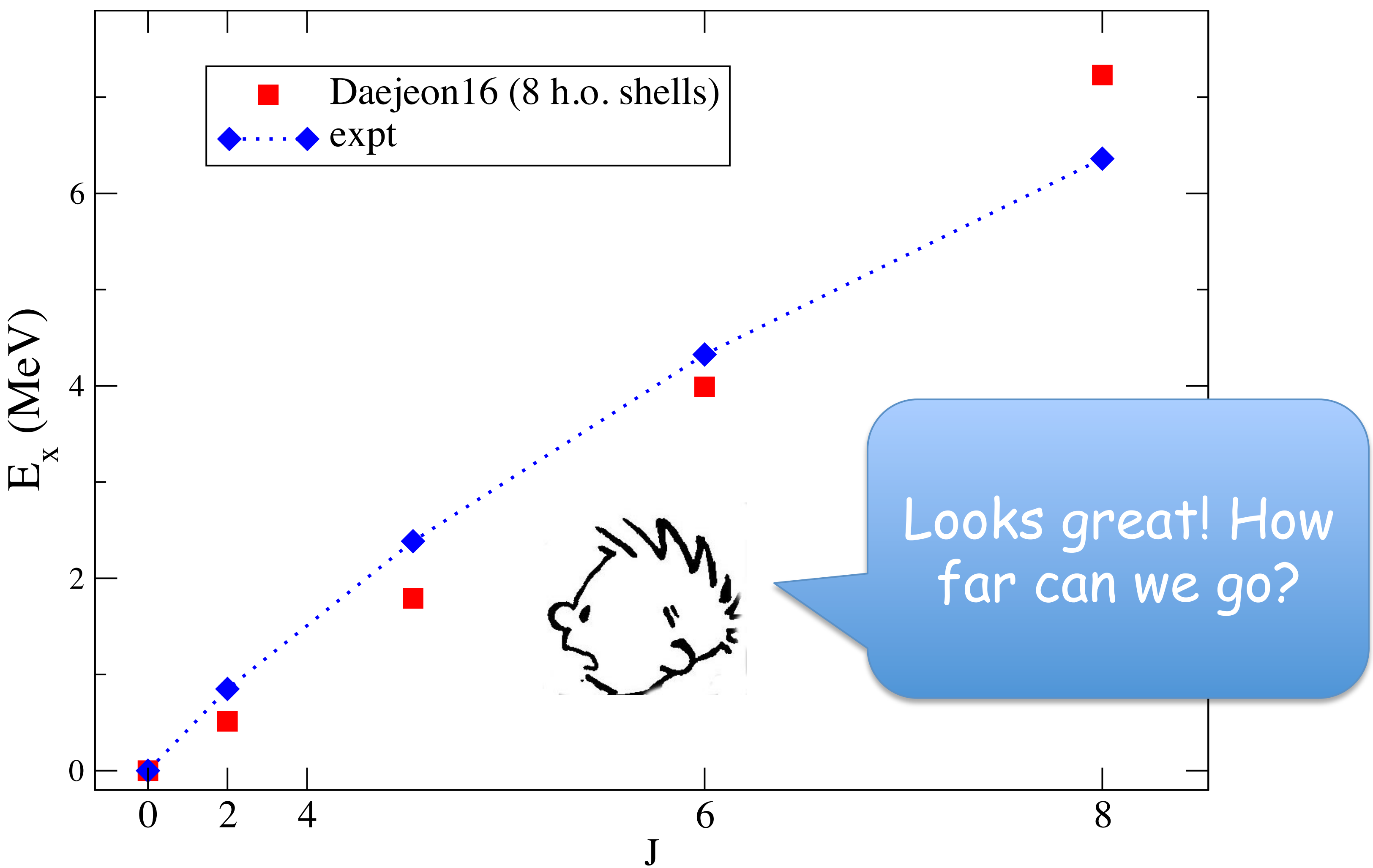


^{48}Cr
chiral
Daejeon16
expt
E_x (MeV)
J
0
5
10
15
0
2
4
6
8
10
12

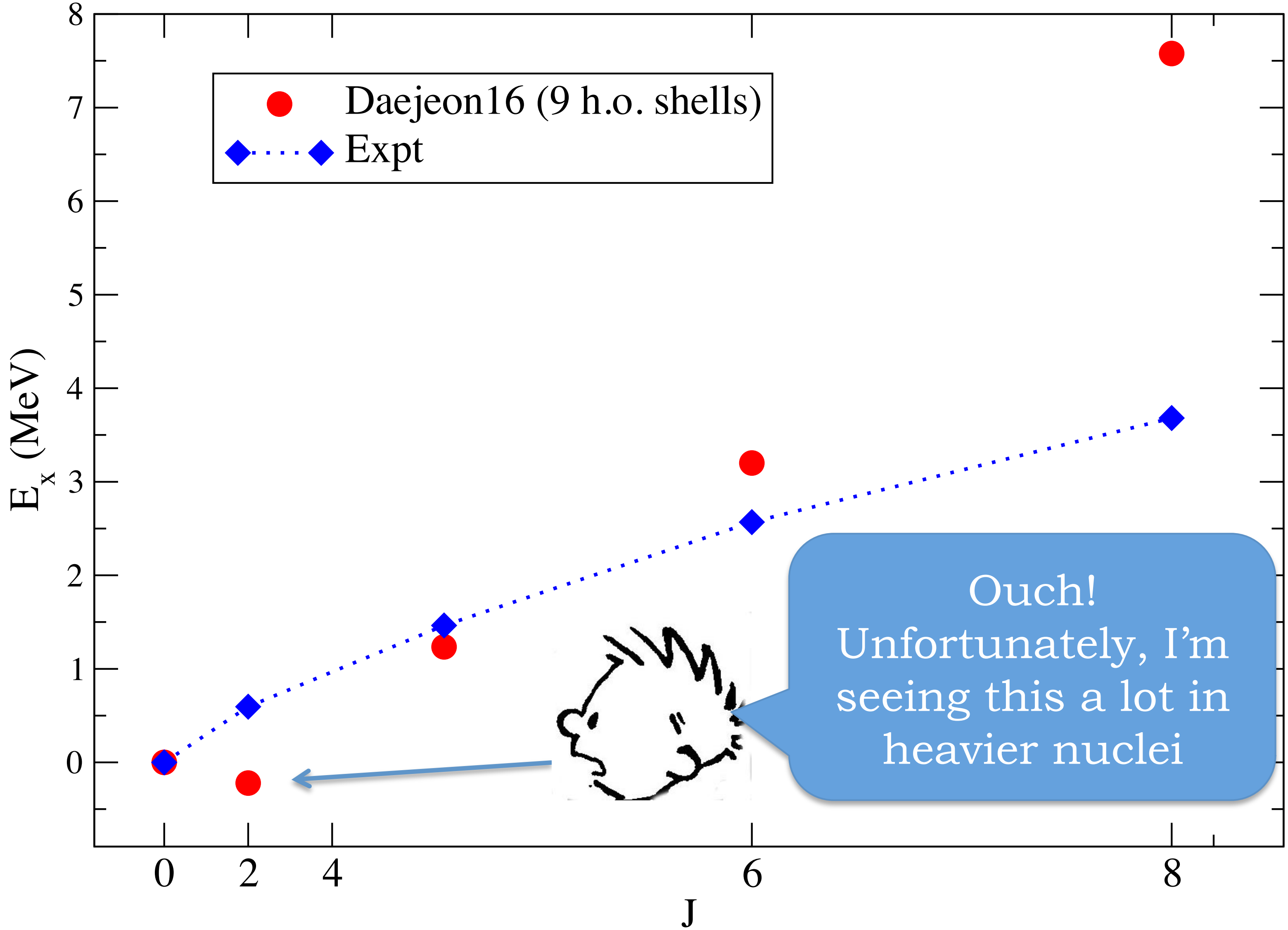


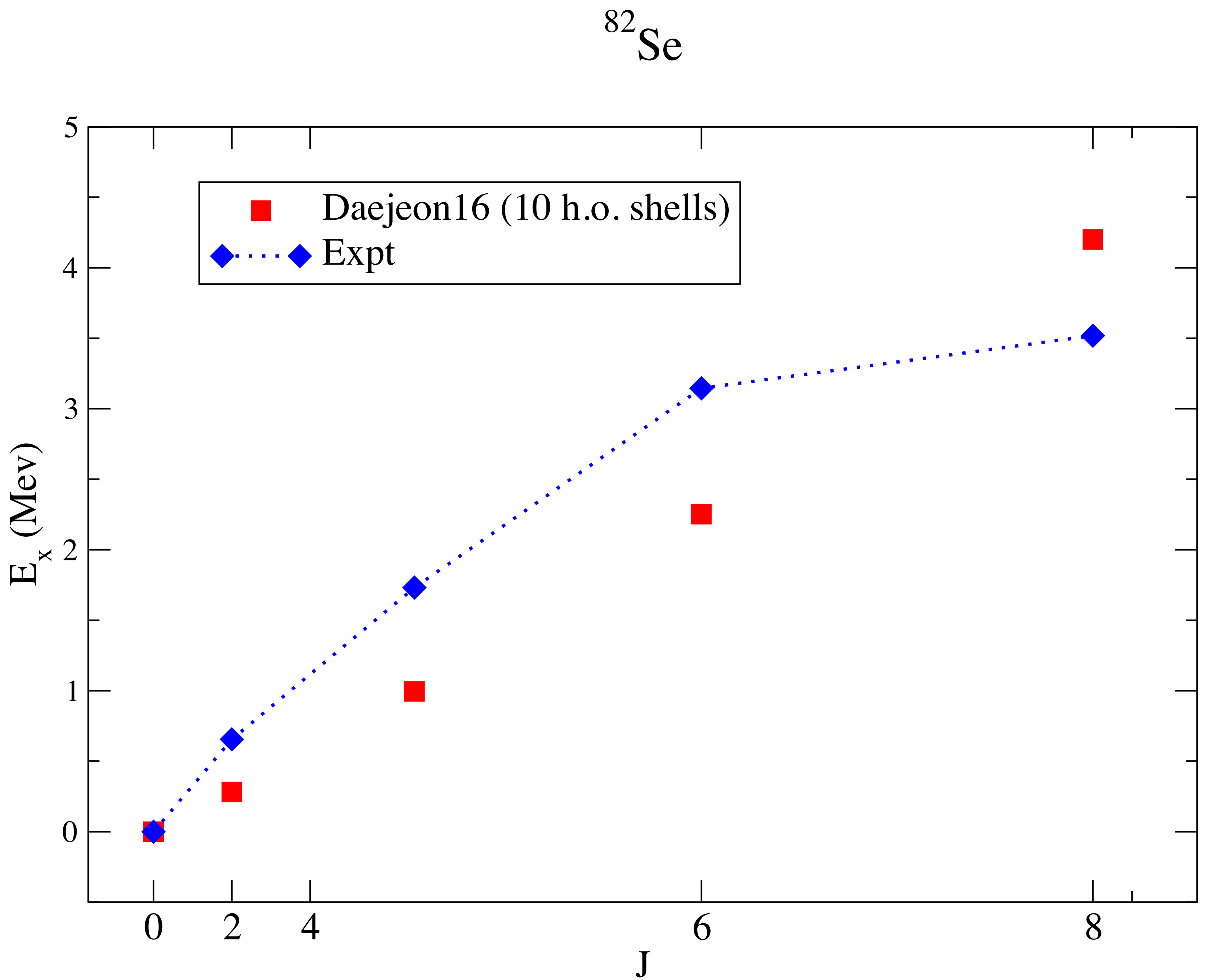
^{49}Cr
chiral
Daejeon16 (6 h.o. shells)
Daejeon16 (8 h.o. shells)
expt
E_x (MeV)
J
0
1
2
3
4
5
6
7
8
1/2
5/2
9/2
13/2
17/2

^{52}Fe

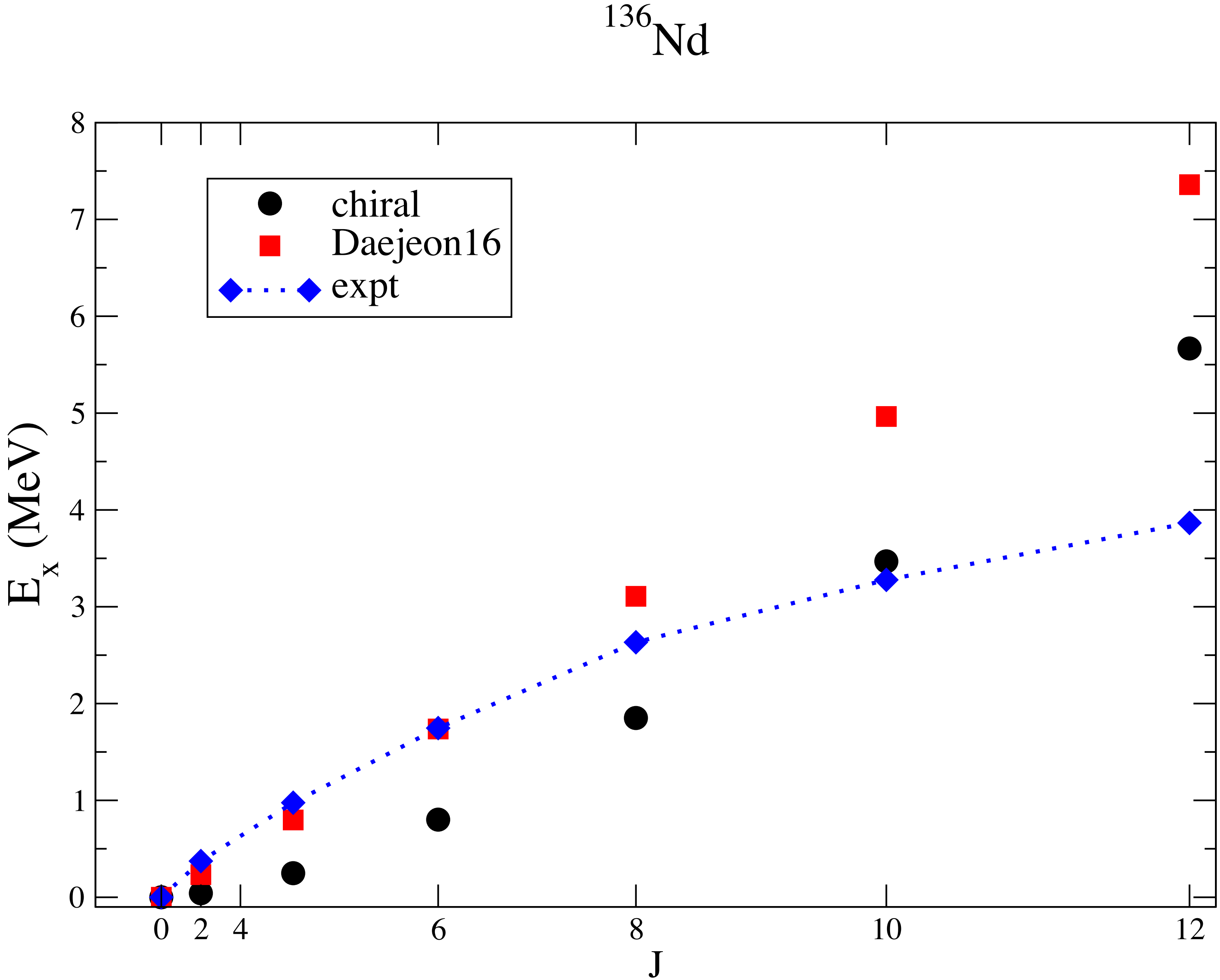

Daejeon16 (8 h.o. shells)
expt
E_x (MeV)
J
0
2
4
6
8
Looks great! How far can we go?

^{74}Ge

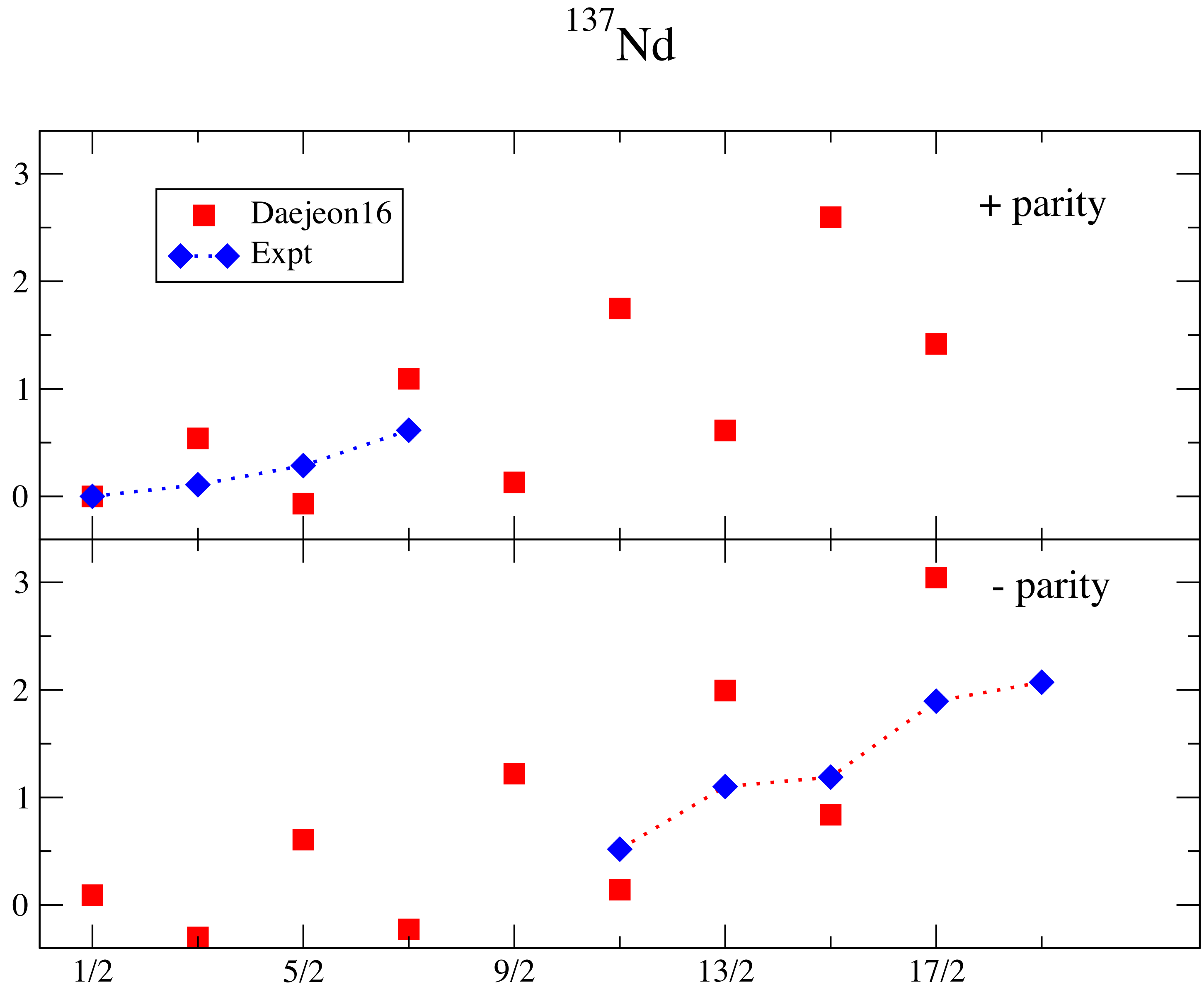

Daejeon16 (9 h.o. shells)
Expt
E_x (MeV)
J
0
1
2
3
4
5
6
7
8
0
2
4
6
8
Ouch!
Unfortunately, I'm
seeing this a lot in
heavier nuclei



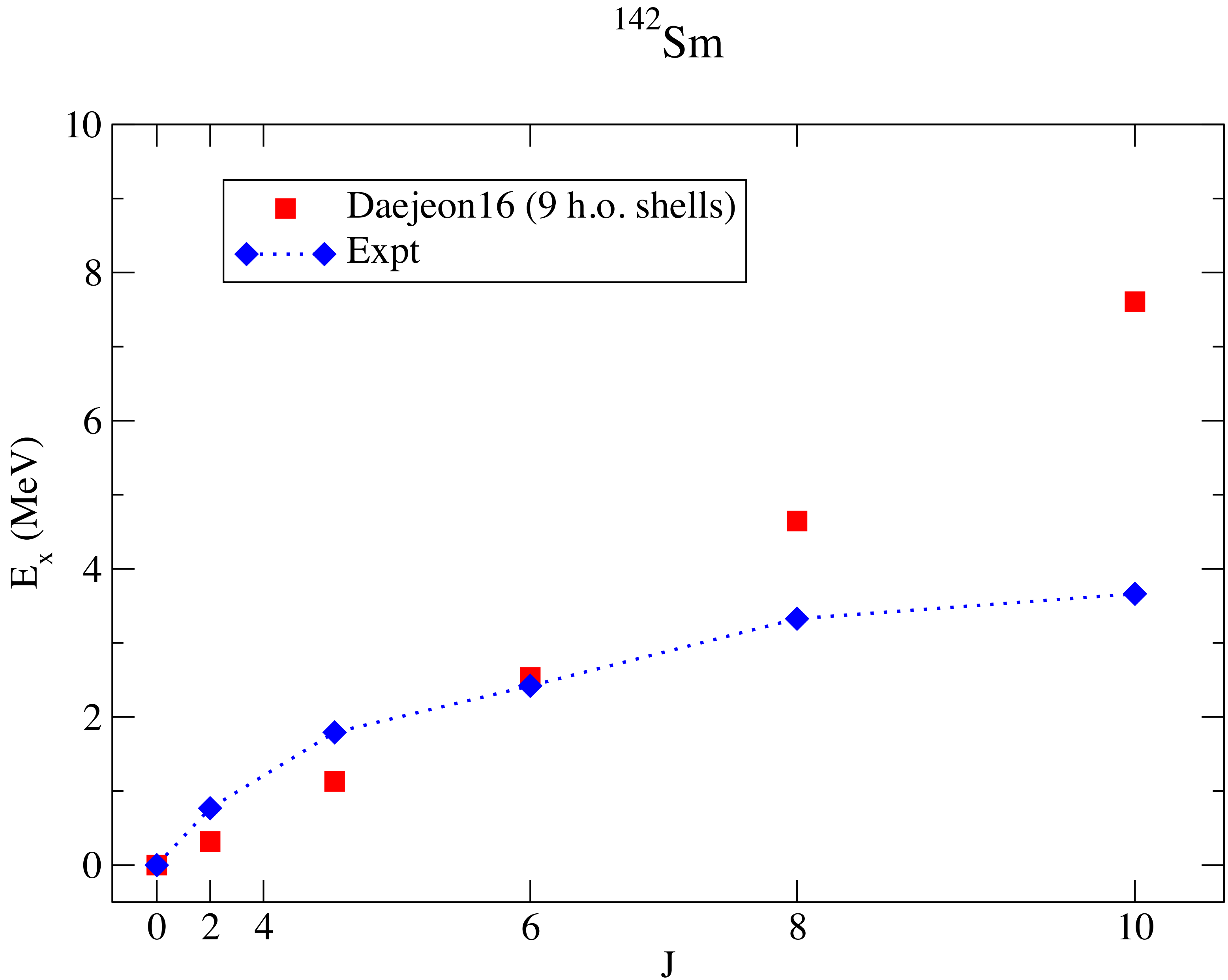
^{82}Se
Daejeon16 (10 h.o. shells)
Expt
E_x (Mev)
J
0
1
2
3
4
5
0
2
4
6
8



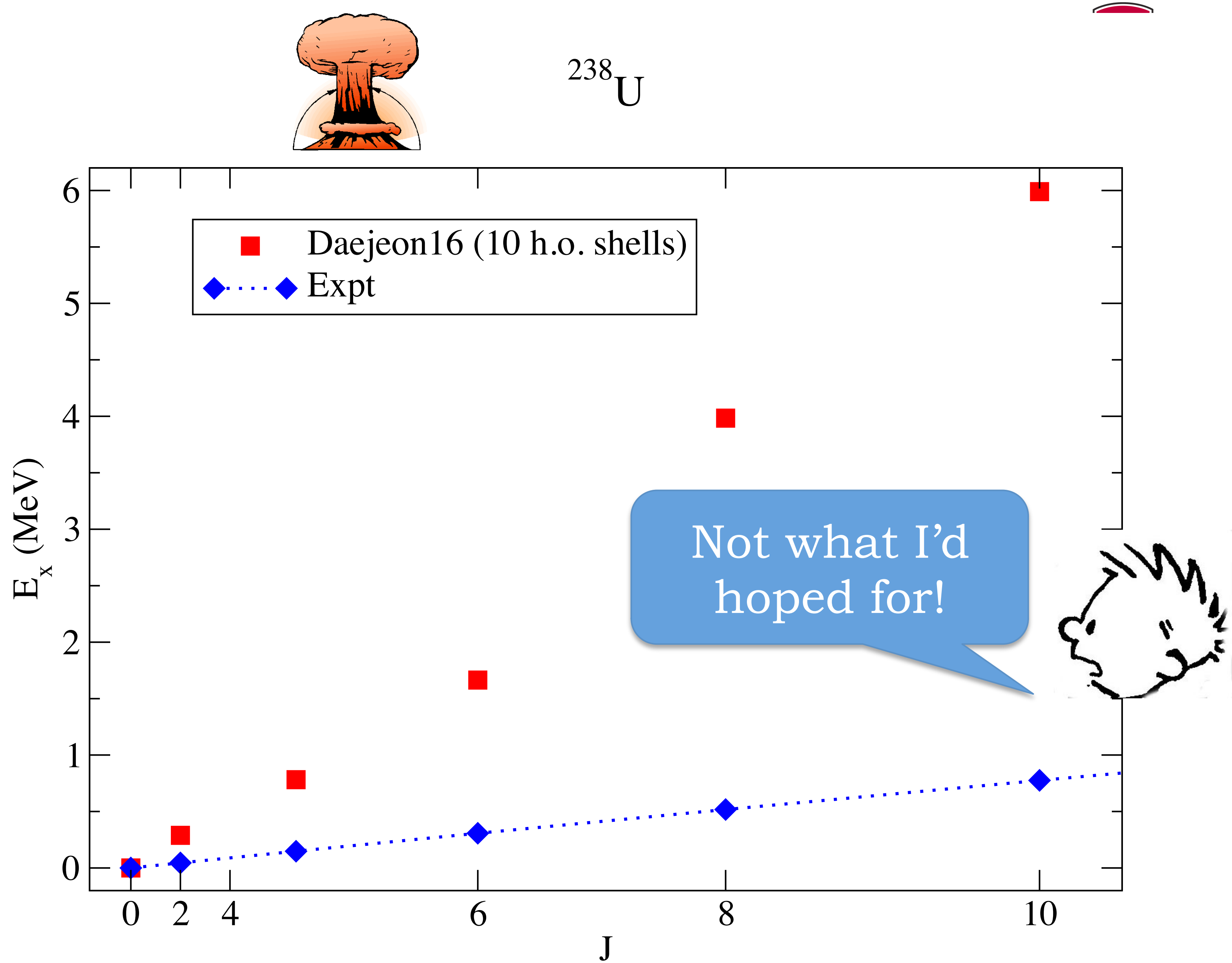
^{136}Nd
chiral
Daejeon16
expt
E_x (MeV)
J
0
1
2
3
4
5
6
7
8
0
2
4
6
8
10
12



^{137}Nd
Daejeon16
Expt
+ parity
- parity
3
2
1
0
3
2
1
0
1/2
5/2
9/2
13/2
17/2



^{142}Sm
Daejeon16 (9 h.o. shells)
Expt
E_x (MeV)
J
0
2
4
6
8
10



238U
Daejeon16 (10 h.o. shells)
Expt
Ex (MeV)
J
0
1
2
3
4
5
6
0
2
4
6
8
10
Not what I'd hoped for!

Summary

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We have strong evidence that

- Rotational motion is a robust phenomenon
- We can use a "classic" method: angular-momentum projected Hartree-Fock
- Works very well for medium-mass nuclei, may need to go to larger spaces for heavy nuclei
- Still, rare earths and actinides *may be in reach!*

While the *many-body method* is approximate, the force is full *ab initio*: no parameters were tuned!

What needs to be done:

- Calculate expectation values, e.g. of H_{cm}

- Calculate transition densities (requires double-projection),

What needs to be done:

- Improve codes to be more efficient in larger spaces, better parallelization (currently only OpenMP)

- Crank (implemented, not fully exploited) and/or add multiple Slater determinants (generator coordinate)

What I'd like to tackle

- Dark matter scattering
- (elastic) neutrino scattering
- Other properties of heavy nuclei

The Day after Tomorrow's "nuclear ladder"

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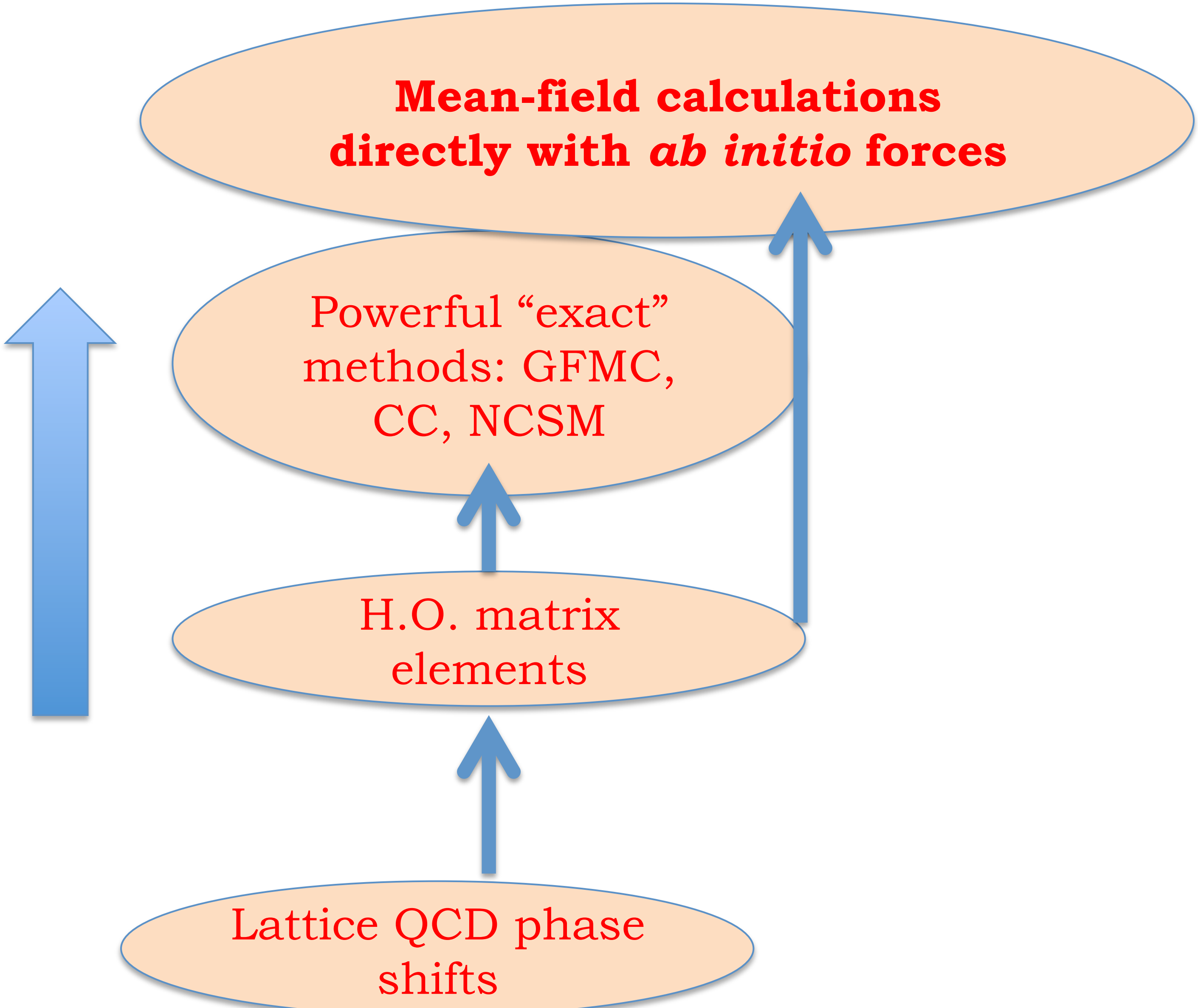

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Thanks to

Joshua Staker (MS/PhD)
Kevin O'Mara (undergrad)

CODE MONKEYS

Dillon Adams (undergrad)
Miguel Godinez (undergrad)