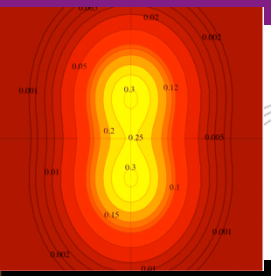
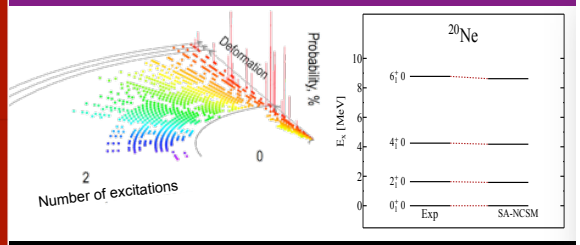
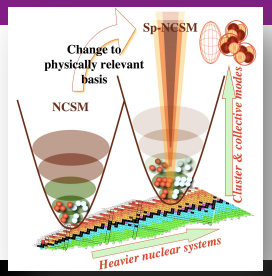
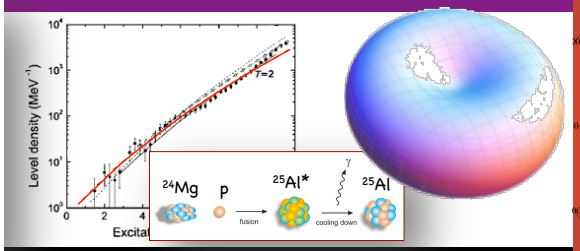
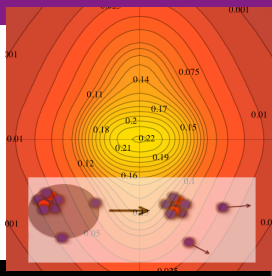









Lessons from the ab initio symmetry-adapted no-core shell model: collectivity, clustering, sum rules and scattering

Kristina Launey **... LSU Team ...** **Jerry Draayer, Tomas Dytrych,**
Alexis Mercenne
Robert Baker, Ali Dreyfuss,
David Kekejian, Grigor Sargsyan,
Madeleine Miora

In collaboration with

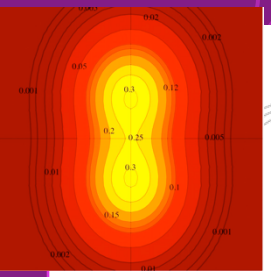
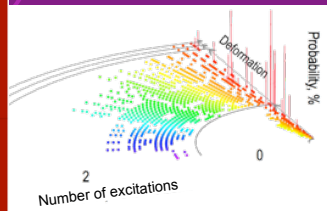
Ohio U. – Ch. Elster
Mainz/TRIUMF – S. Bacca
Czech Republic – D. Langr & T. Oberhuber
Princeton U. – W. Tang & B. Wang

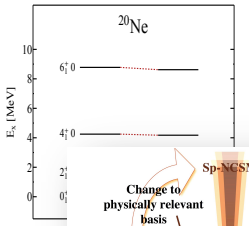
HPC Resources

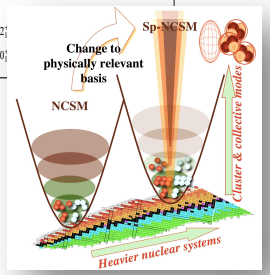
NSF/U. of Illinois ...*BlueWaters*
LSU...*SuperMike-II*

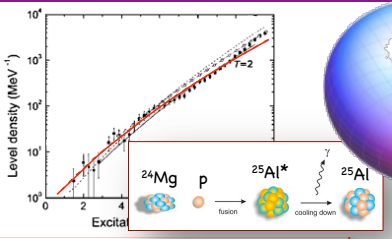
Supported by NSF & DOE

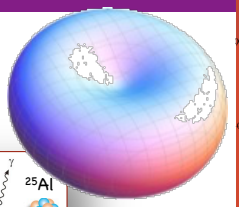
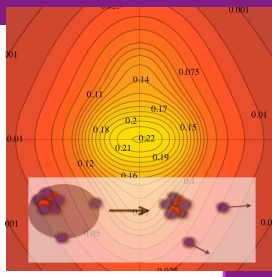
LSU

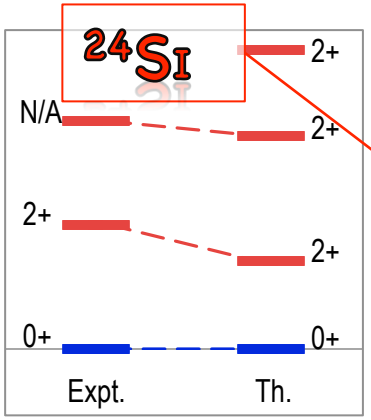


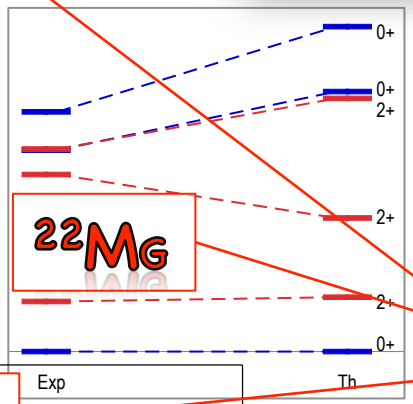


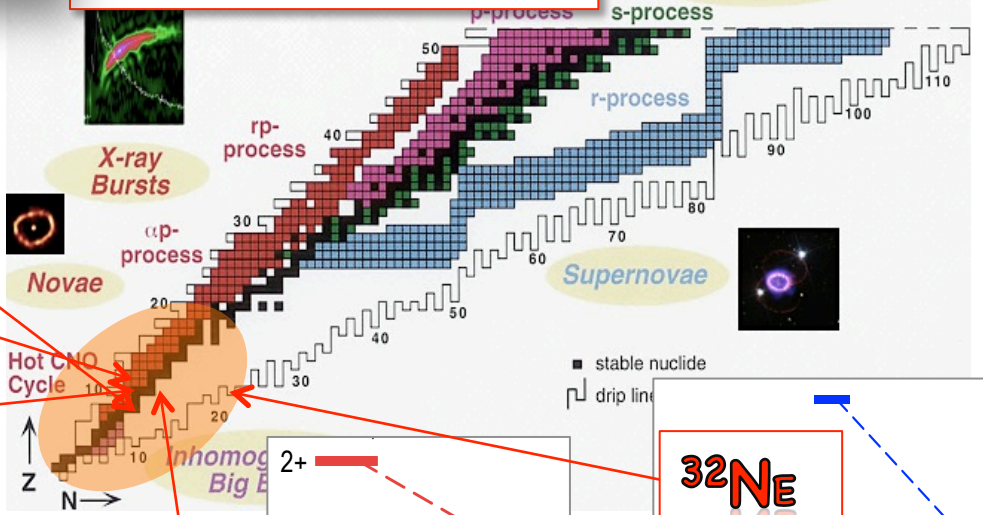


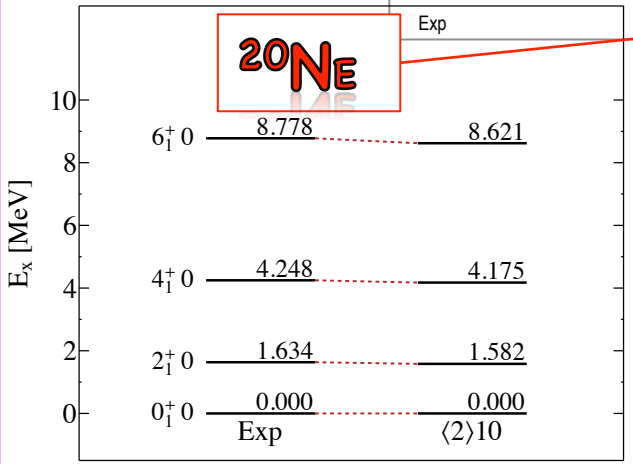



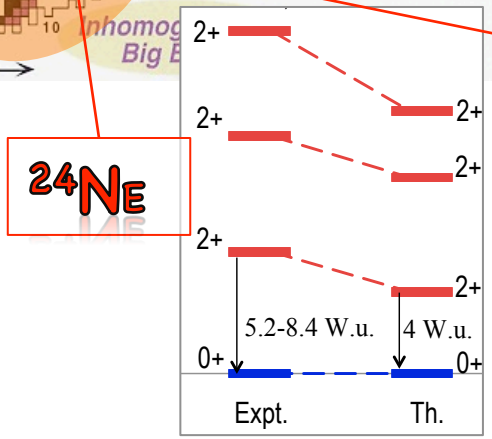
Symmetry-adapted No-core Shell Model (SA-NCSM)

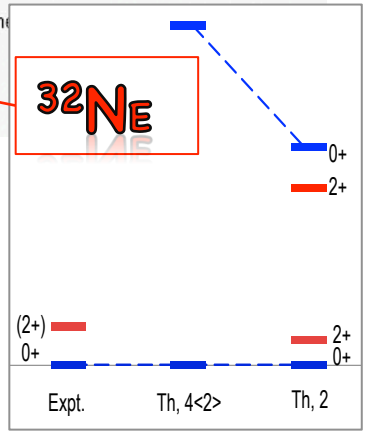


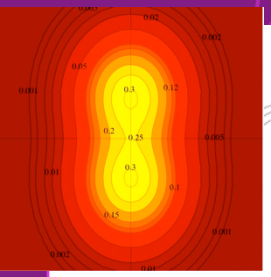


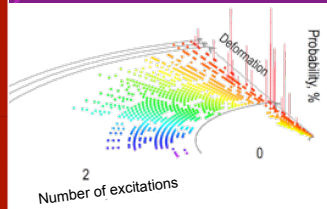


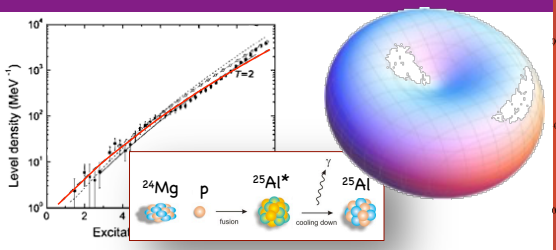


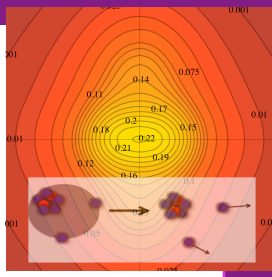


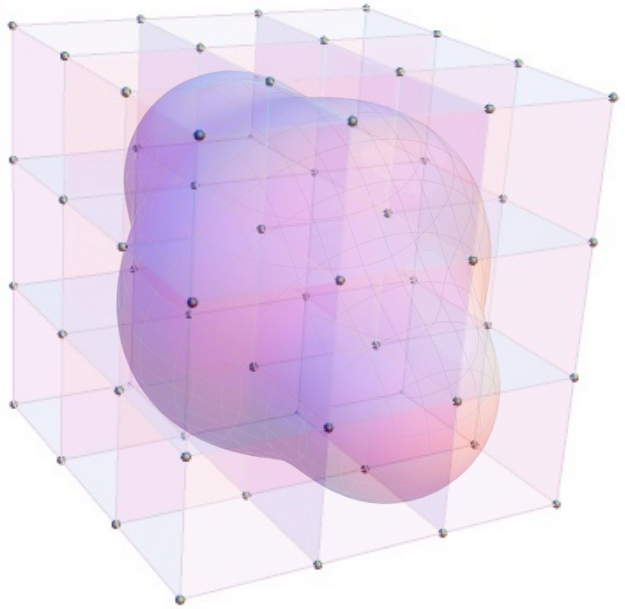






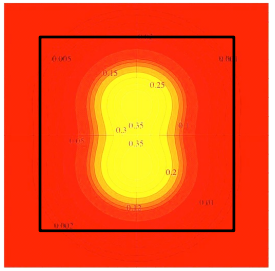






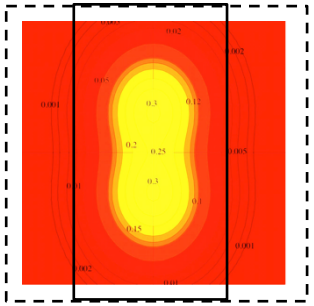
NCSM

Total HO quanta
N_{max}



SA-NCSM

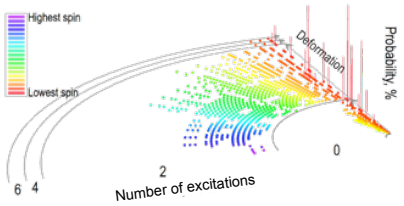
Total HO quanta
N_{max}
+
Distribution:
z, x, y

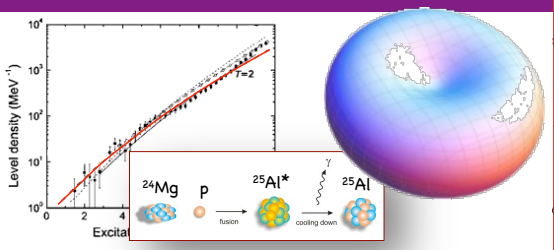


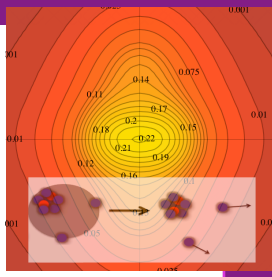
LSU code (LSU3shell): sourceforge.net/projects/lsu3shell

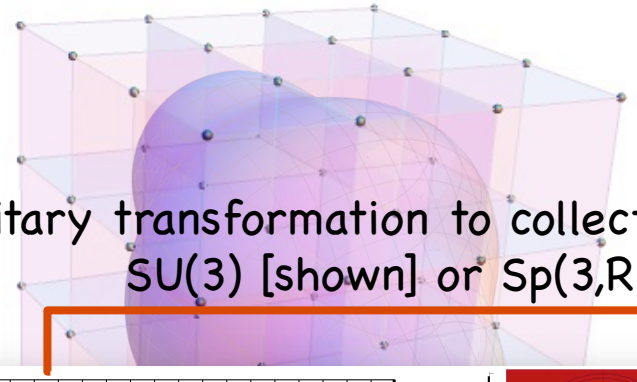
Dytrych et al., Phys. Rev. Lett. 111 (2013) 252501

Launey et al., Prog. Part. Nucl. Phys. 89 (2016) 101





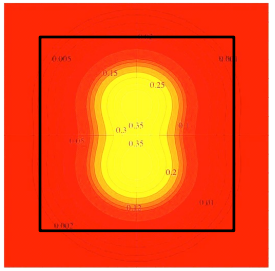




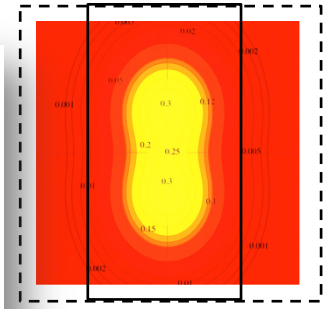
Unitary transformation to collective basis,
SU(3) [shown] or Sp(3,R)

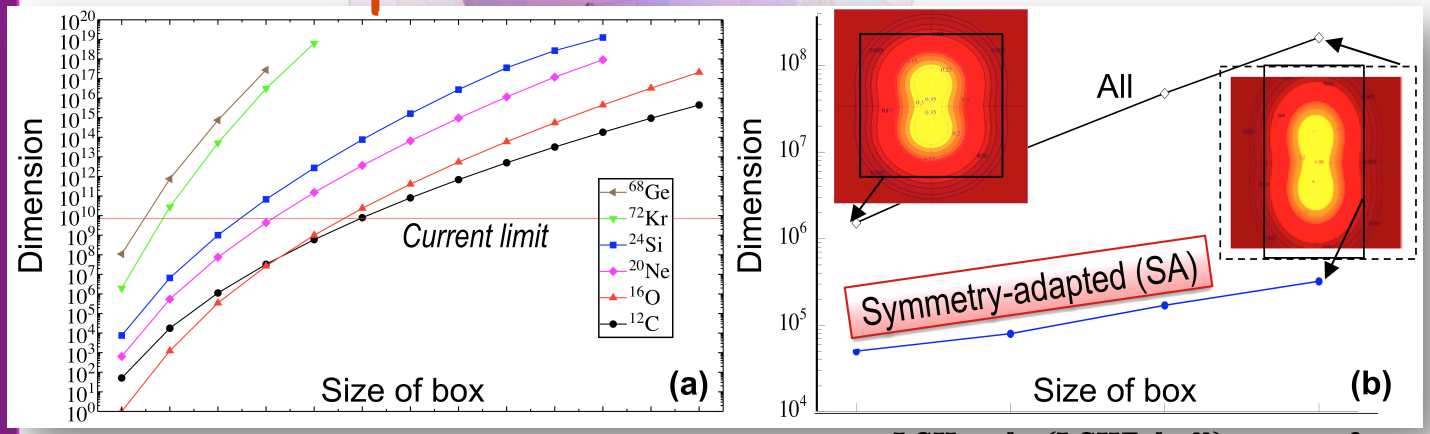
NCSM

Total HO quanta
N_{max}



SA-NCSM





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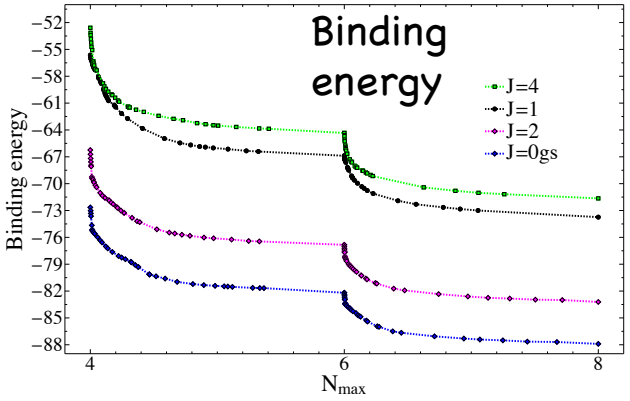
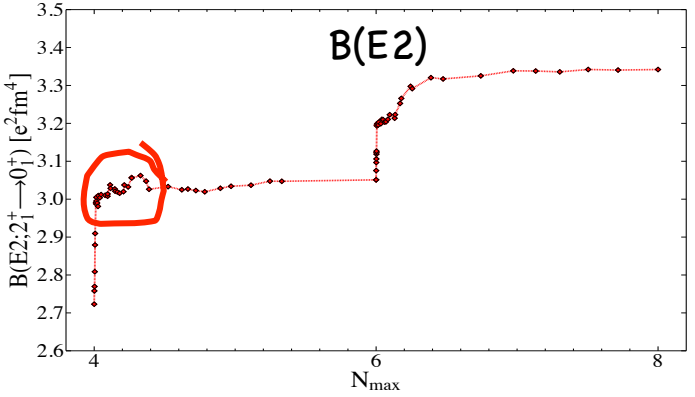
Dytrych et al., Phys. Rev. Lett. 111 (2013) 252501

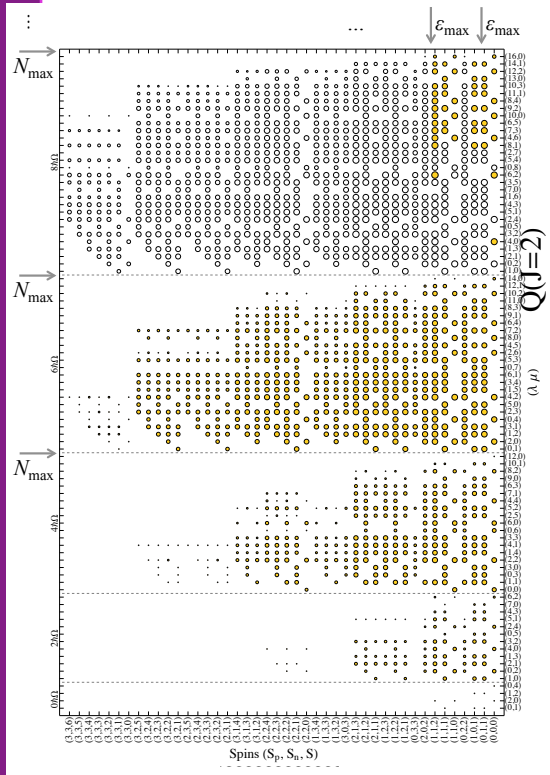
Launey et al., Prog. Part. Nucl. Phys. 89 (2016) 101

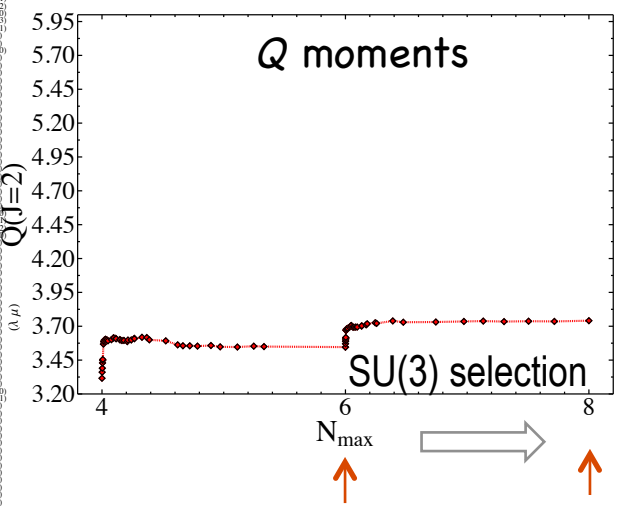
SU(3) Selection

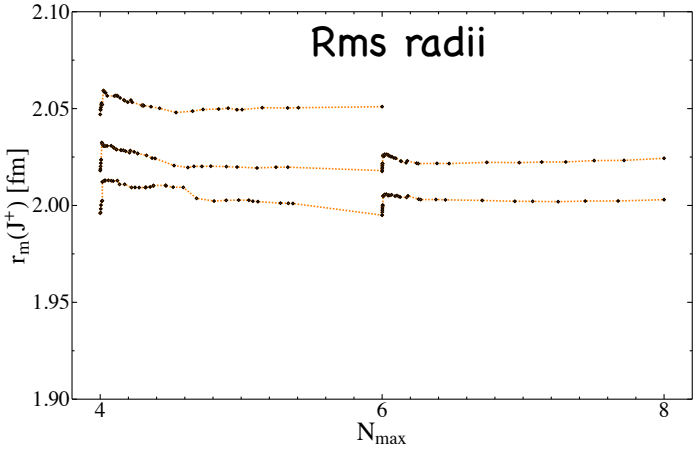
^{12}C



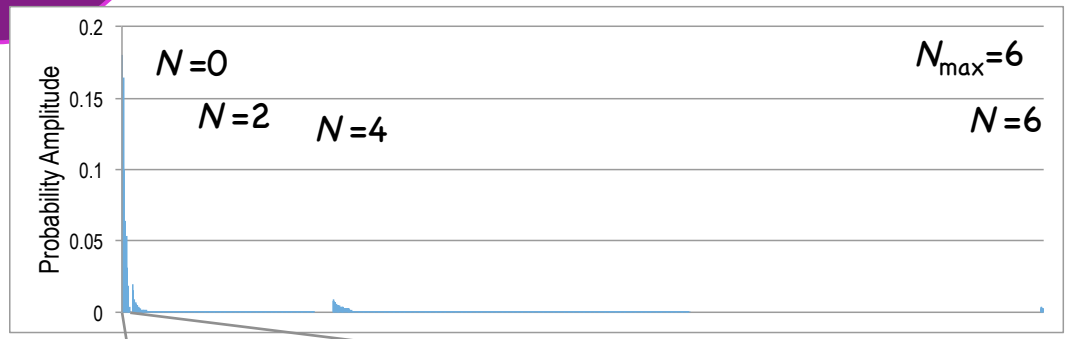


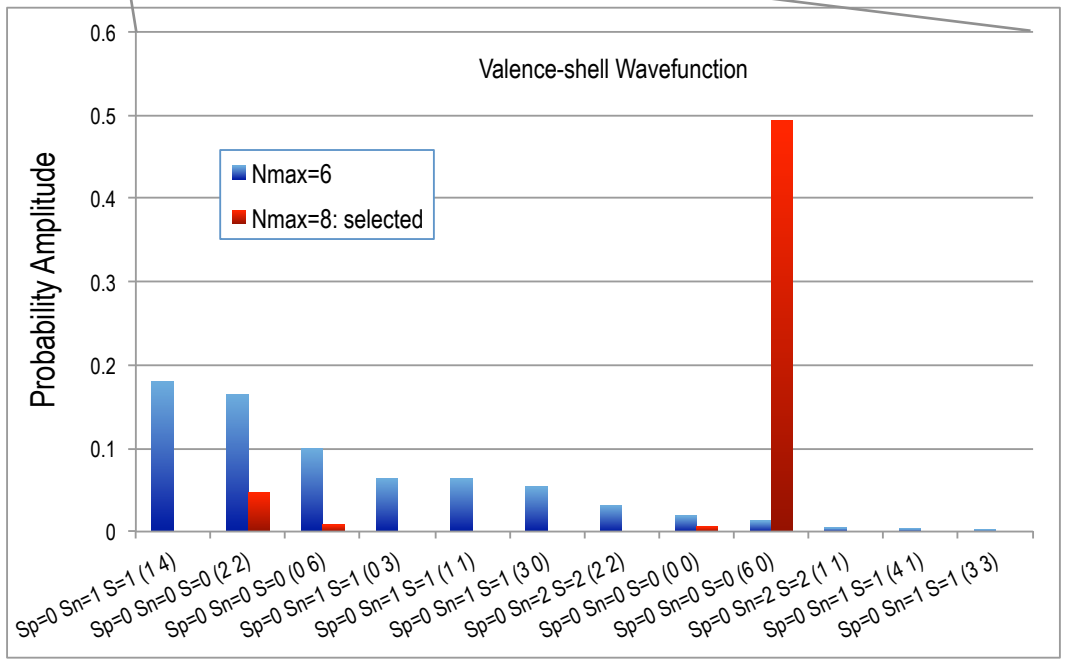


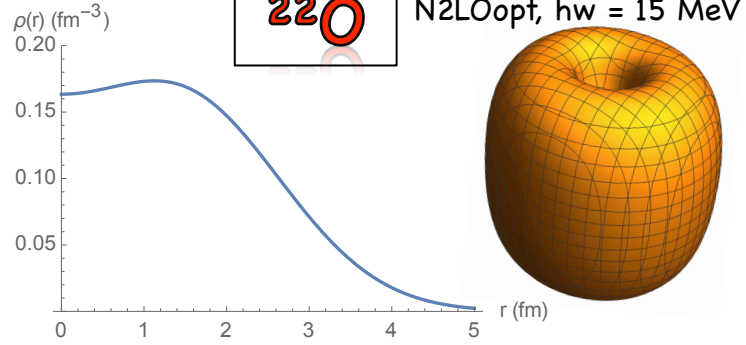


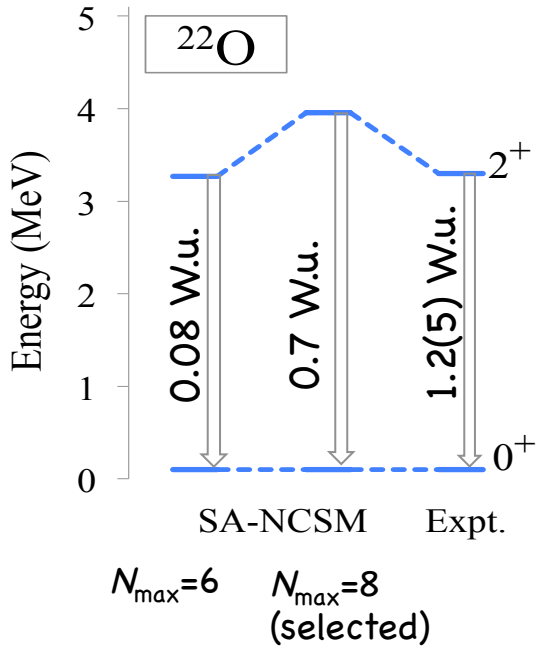


Oxygen isotopes



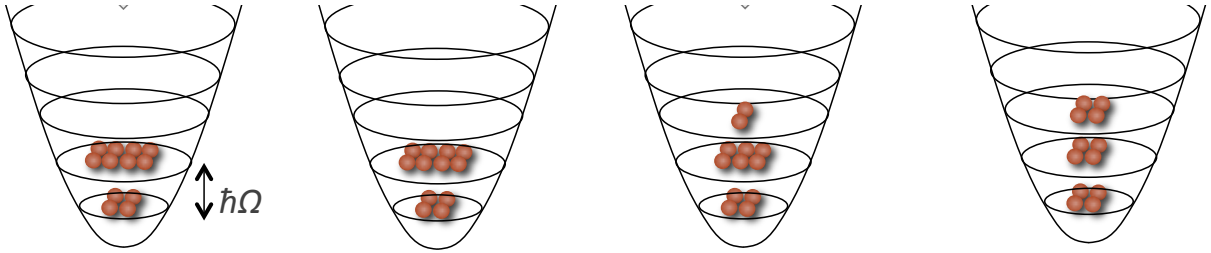






Grigor Sargsyan, PhD student, LSU

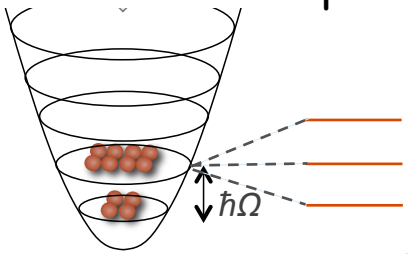
Symmetry-adapted Bases: SU(3)-coupled



- Spherical harmonic oscillator basis
- Distributions of nucleons over shells

e.g.: p shell, single particle

spatial dof (nlm) × spin dof (ss_z)



m = 0,+1,-1

n = 1, l = 1
3 states

spatial dof (nlm) × spin dof (ss_z)

0 0 1
0 1 0
1 0 0

n_z n_x n_y
3 states

Degenerate 3 states … U(3)=U(1) × SU(3) symmetry

$n = n_z + n_x + n_y$ $\quad \lambda = n_z - n_x$, $\mu = n_x - n_y$ $\leftrightarrow (\lambda\ \mu)$

1 0 0 <-> (1 0)

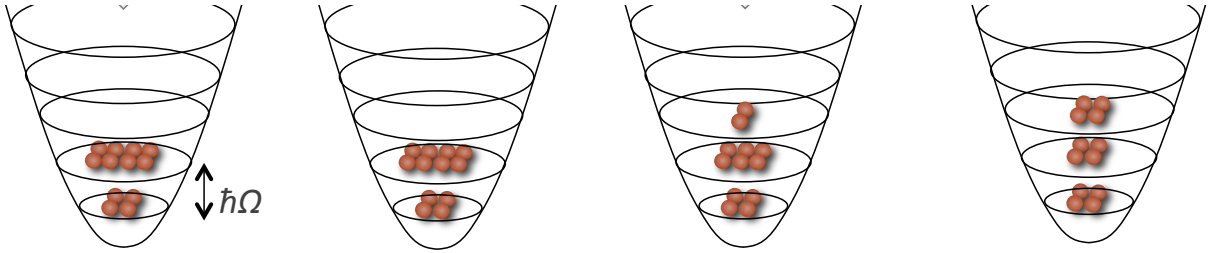
n_z -> n_x

n_x -> n_y

SU(3) generators

All we need to know: a_n^+ is (n 0) SU(3) tensor

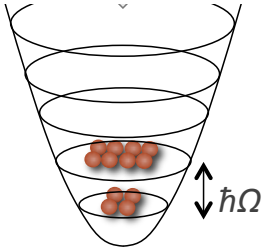
Symmetry-adapted Bases: SU(3)-coupled



- Spherical harmonic oscillator basis
- Distributions of nucleons over shells

e.g.: C-12 (4 protons and 4 neutrons above s shell)

1 possible configuration



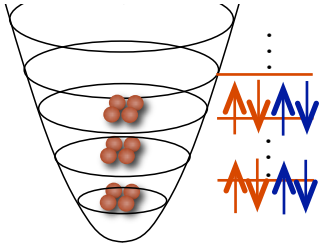
n_z n_x n_y	Total excitations
0 0 1	0 0 0
0 1 0	0 4 0
1 0 0	4 0 0
4 4 0	
or	
$(\lambda\ \mu) = (0\ 4)$	

3 states

…Ground state: built on it

Oblate shape

1 possible configuration



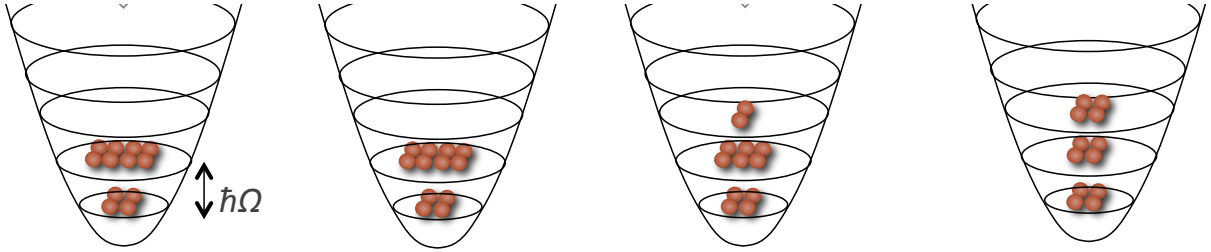
n_z n_x n_y	Total excitations
1 1 0	0 0 0
2 0 0	8 0 0
1 0 0	4 0 0
12 0 0	
or	
$(\lambda\ \mu) = (12\ 0)$	

3 states

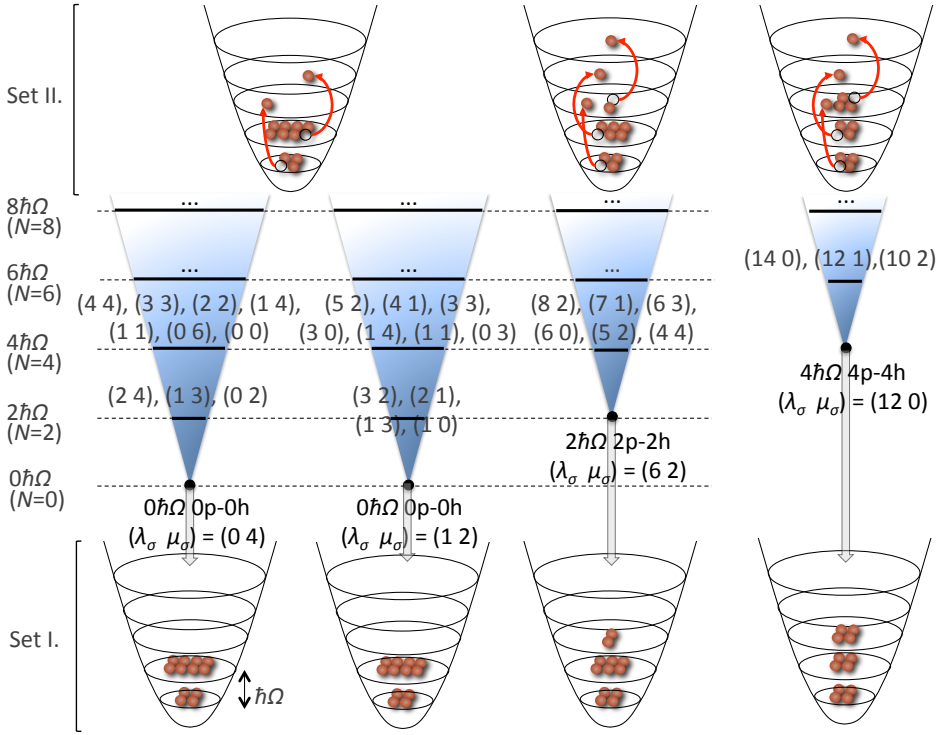
…Hoyle state: built on it

Prolate shape

Symmetry-adapted Bases: Sp(3,R)-coupled

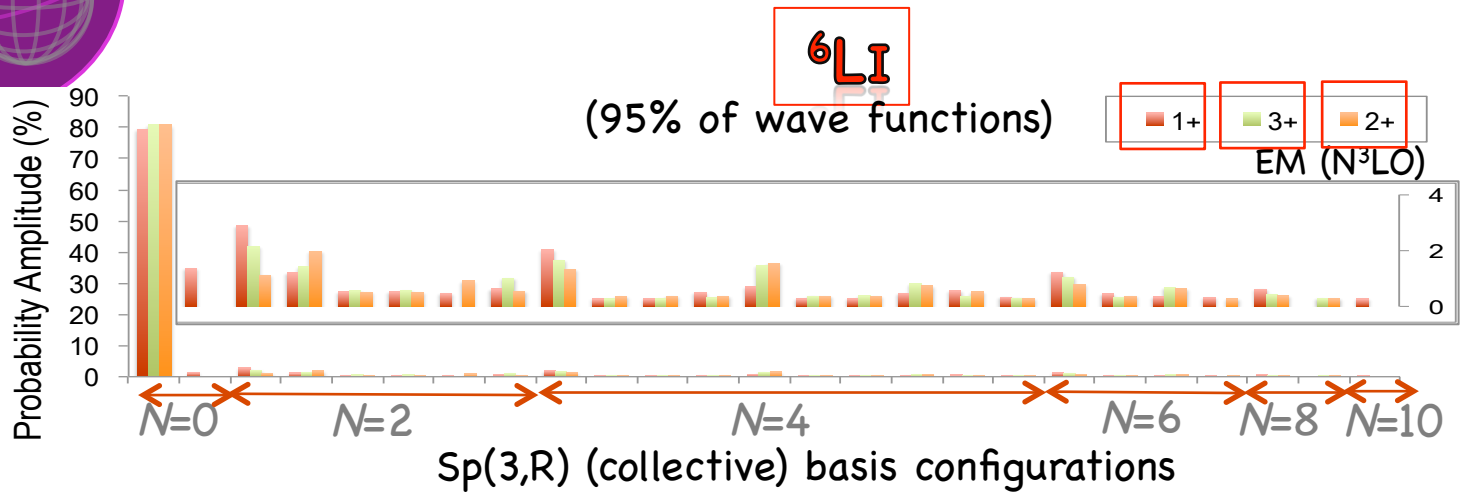


- Spherical harmonic oscillator basis
- Distributions of nucleons over shells



Excitations driven by:
r^2 (L=0) [or kinetic energy, T]
Q (L=2)

Preference of Nature

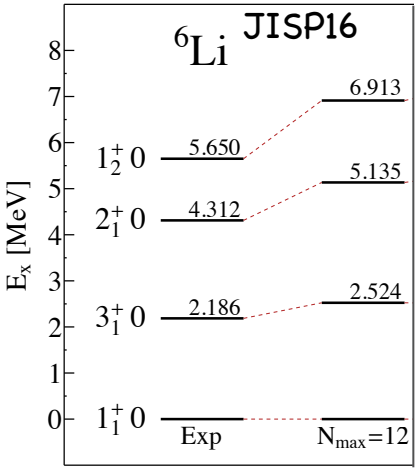


^{6}Li, Nmax=12

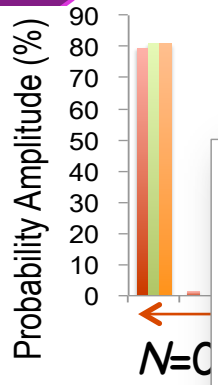
J=1,2,3 states……2×10^7

Sp configurations……528

Sp configurations with P>0.2%……25



SA-NCSM with Sp(3,R) basis



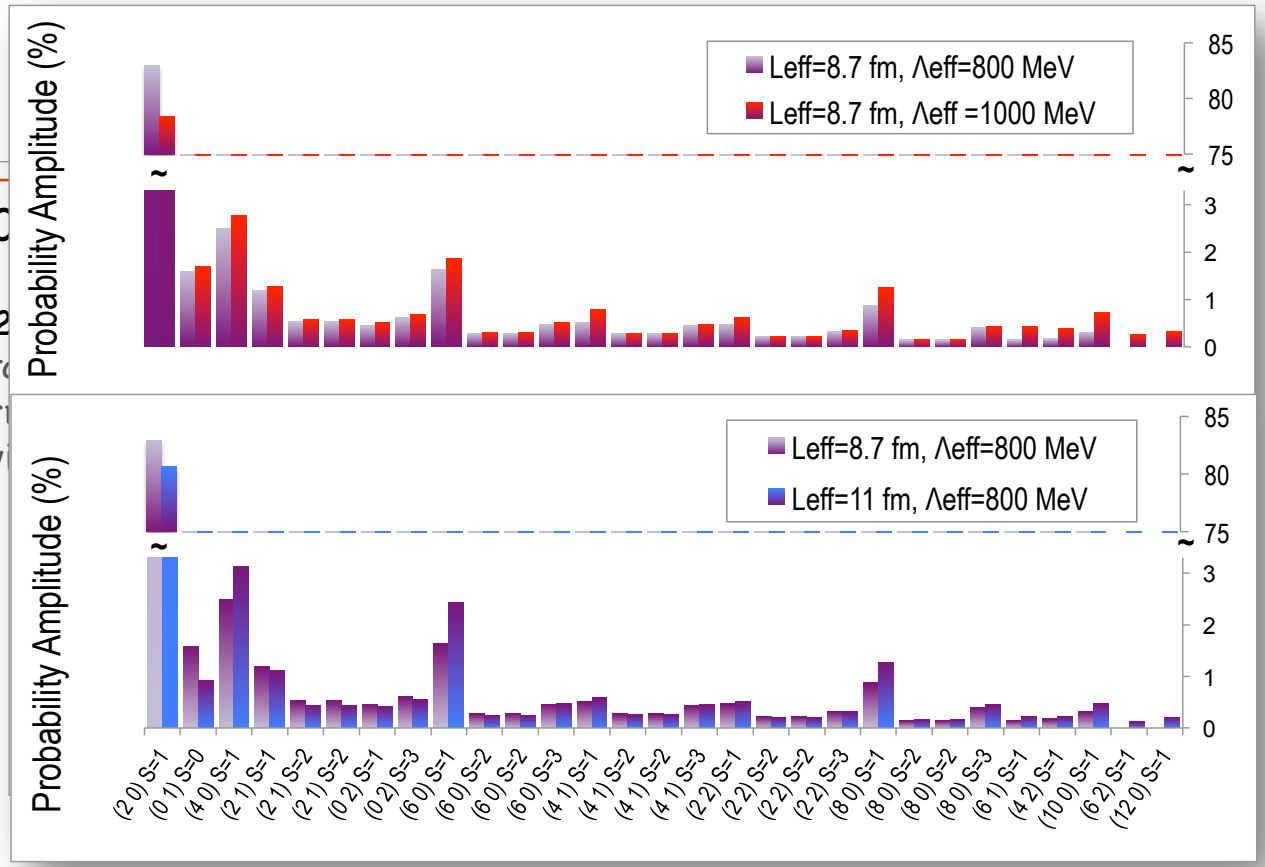
^{6}Li, Nmax=12
J=1,2,3 st
Sp(3,R) ir
Sp(3,R) w

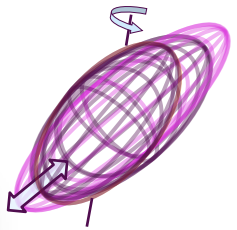
^{6}Li

(95% of wave functions)

1+ 3+ 2+

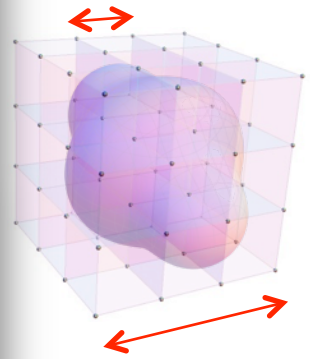
EM (N^{3}LO)





"resolution"

$1/\Lambda_{eff}$

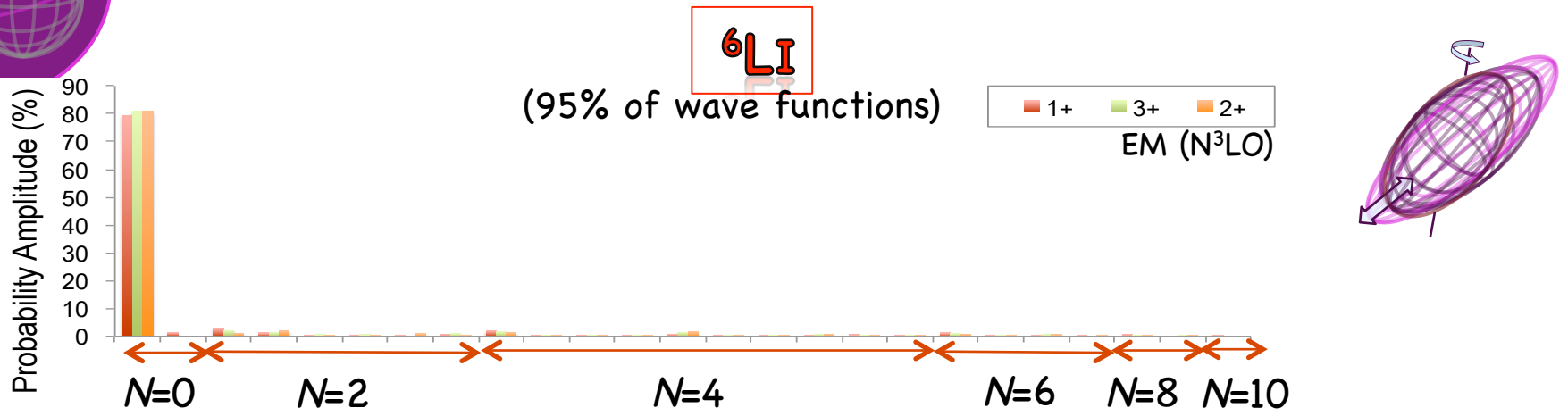


L_{eff}

"box size"

L_{eff} & Λ_{eff} based on: Wendt, Forssén, Papenbrock, & Sääf, Phys. Rev. C 91, 061301(R)

SA-NCSM with Sp(3,R) basis



^{6}Li, Nmax=12

J=1,2,3 states……..2x10^7

Sp(3,R) irreps……..528

Sp(3,R) with P>0.2%…….25

Reproducing B(E2)?

$$B(E2) = \frac{1}{2J_i+1}\frac{5}{16\pi}\left(\frac{\hbar}{m\omega}\right)^2 |\langle J_f \| Q_2 \| J_i \rangle|^2$$

$$Q_{2M} = \sqrt{3}\left(A^{(20)}_{2M} + C^{(11)}_{2M} + B^{(02)}_{2M}\right)$$

Symplectic generators –
do not mix Sp basis configurations

=> Significance of dominant Sp configuration

Symplectic Sp(3,R) Symmetry!

Formal definition

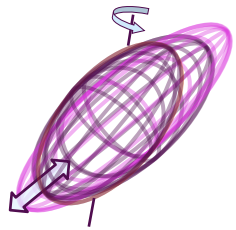
All linear canonical transformations of the single-particle phase-space observables

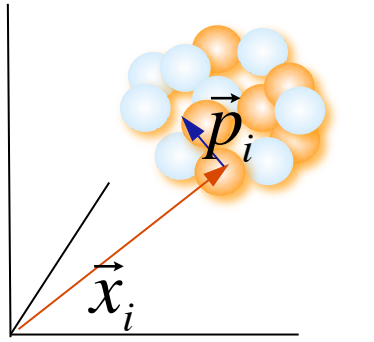
$$x_{i\alpha} \rightarrow \sum_{\beta=x,y,z} a_{\alpha\beta} x_{i\beta} + b_{\alpha\beta} p_{i\beta}$$

$$p_{i\alpha} \rightarrow \sum_{\beta=x,y,z} c_{\alpha\beta} x_{i\beta} + d_{\alpha\beta} p_{i\beta}$$

that preserve the canonical commutation relation

$$\left[x_{i\alpha}, p_{j\beta} \right] = i\hbar \delta_{ij} \delta_{\alpha\beta}$$





Generators:

$$Q_{ij} = \sum_n x_{ni} x_{nj},$$

$$S_{ij} = \sum_n (x_{ni} p_{nj} + p_{ni} x_{nj}),$$

$$L_{ij} = \sum_n (x_{ni} p_{nj} - x_{nj} p_{ni}),$$

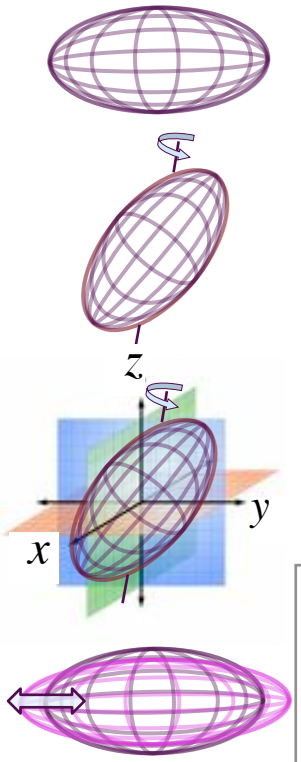
$$K_{ij} = \sum_n p_{ni} p_{nj},$$

SU(3) in a HO shell (Elliott, 1958)

Rowe, Rosensteel, Draayer, Hecht, Suzuki, Escher, Bahri, ….

What physics can we learn from Sp basis?

Sp (collective) basis configuration:



one equilibrium deformation (``shape")

rotations

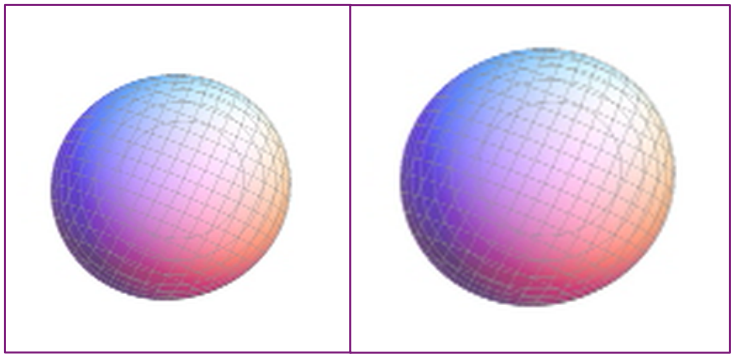
space orientation

Vibrations

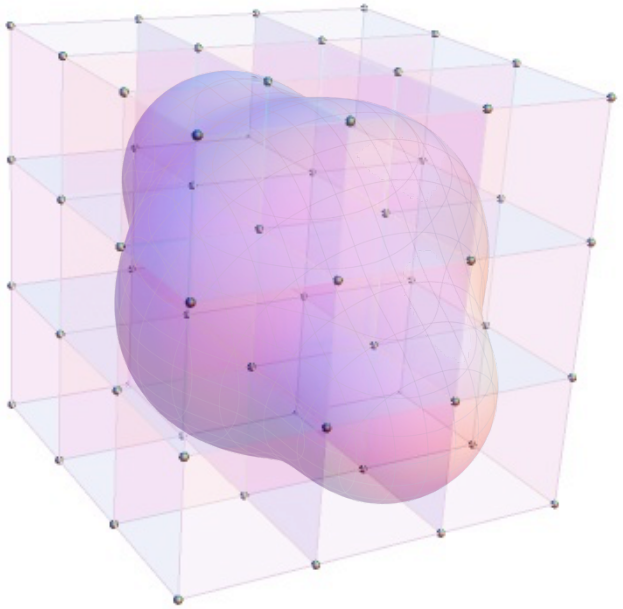
(of the giant resonance monopole (r^2)/ quadrupole (Q) type)

All states preserve the equilibrium shape...

Symmetry?

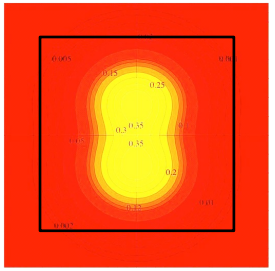


Connecting Bound States to the Continuum



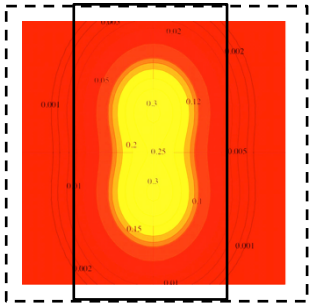
NCSM

Total HO quanta
N_{max}

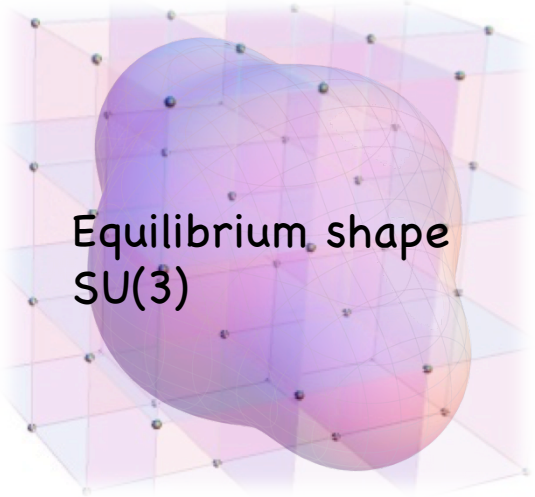


SA-NCSM

Total HO quanta
N_{max}
+
Distribution:
z, x, y

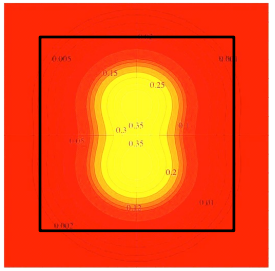


Connecting Bound States to the Continuum



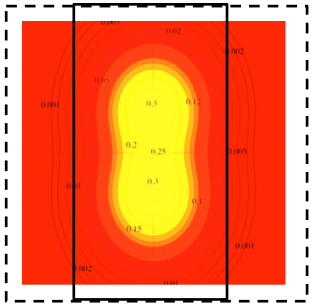
NCSM

Total HO quanta
N_{max}

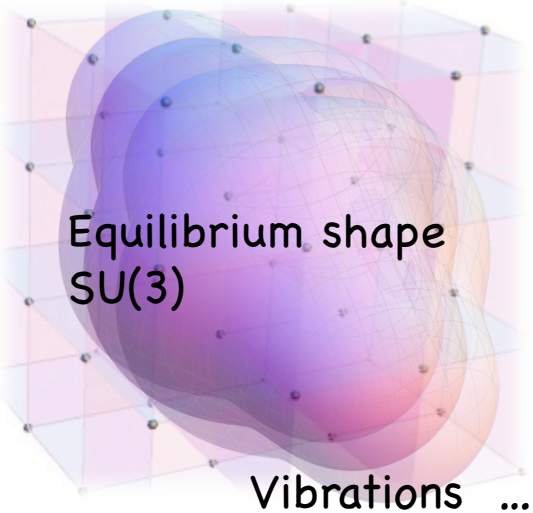


SA-NCSM

Total HO quanta
N_{max}
+
Distribution:
z, x, y



Connecting Bound States to the Continuum



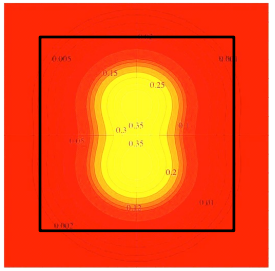
Equilibrium shape
SU(3)

Vibrations
Sp(3,R)

...coupling to
the continuum

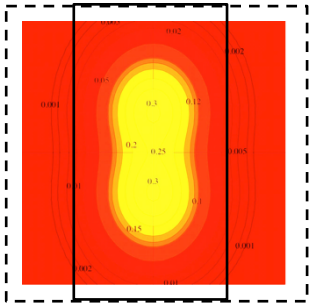
NCSM

Total HO quanta
N_{max}



SA-NCSM

Total HO quanta
N_{max}
+
Distribution:
z, x, y



"Inside": wave functions coupled to the continuum (no widths)

Widths + reactions:

"Outside": exact solution (Coulomb functions)

(SA-NCSM/RGM + *R*-matrix)

See Alexis Mercenne's talk

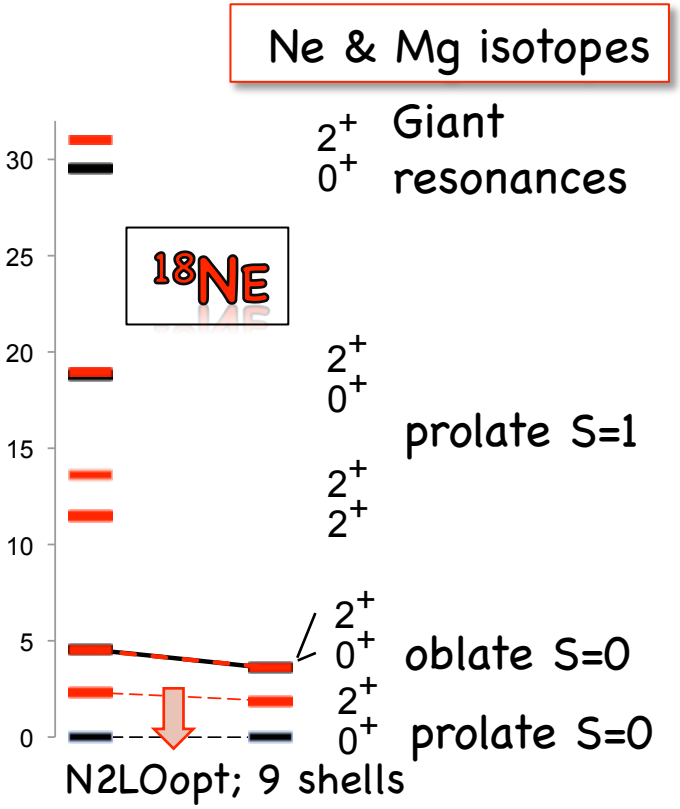
Collectivity & clustering up to medium mass

^{18}Ne, B(E2: $2^+ \rightarrow 0^+$)

Experiment…… 17.7(18) W.u.

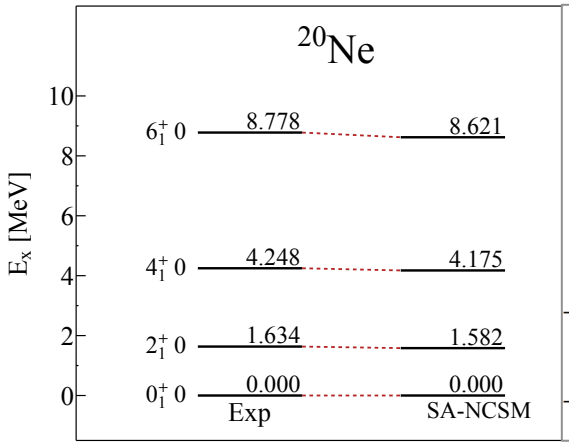
9 shells …… 1.13 W.u.

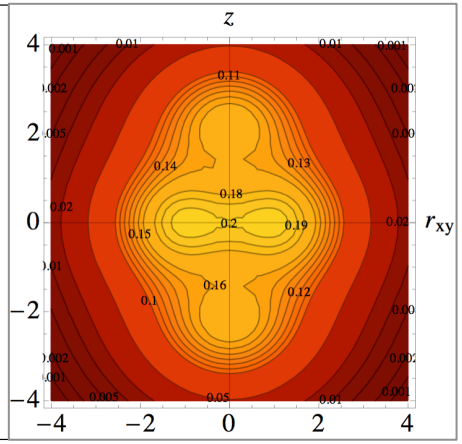
33 shells …… 13.0(7) W.u.
(no effective charges)

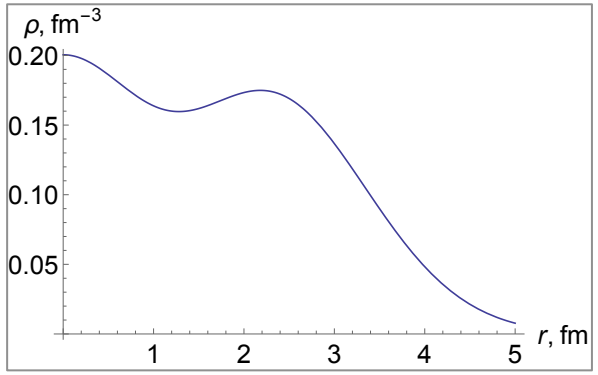


Grigor Sargsyan, PhD student, LSU

Collectivity & clustering up to medium mass



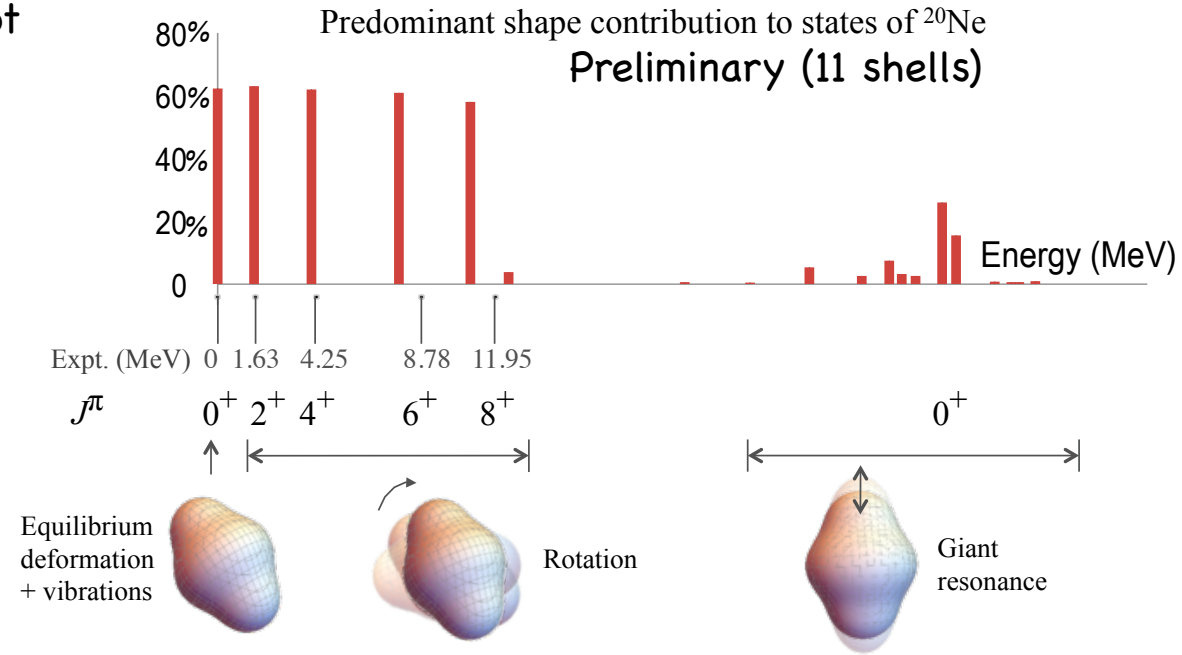




SA-NCSM, 13 shells, N2LOopt

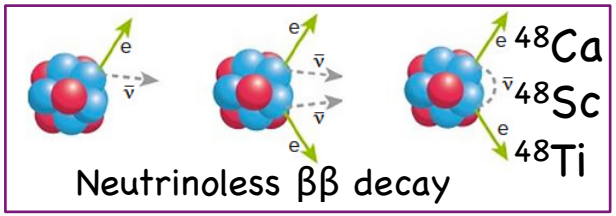
SA model space:
50 million states

Complete model space:
1000 billion states
(currently not feasible)



Structure of Ca-48 and Ti-48

^{48}Ca



Neutrinoless ββ decay

^{48}Ti

8 shells, N2LOopt

0^+

SA-NCSM (selected): ……966,152

Complete model space: ……3,162,511,819

2^+

SA-NCSM (selected): ……3,055,554

Complete model space: …14,522,234,982

8 shells, N2LOopt

0^+

SA-NCSM (selected): ……602,493

Complete model space: …..24,694,678,414

2^+

SA-NCSM (selected): ……1,178,834

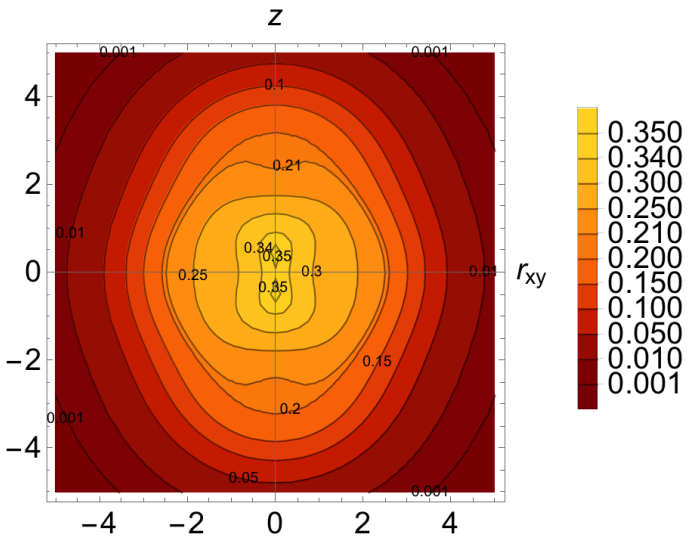
Complete model space: …113,920,316,658

^{48}Ti, $Q(2^+)$ [e fm^2]

Experiment…… -17.7

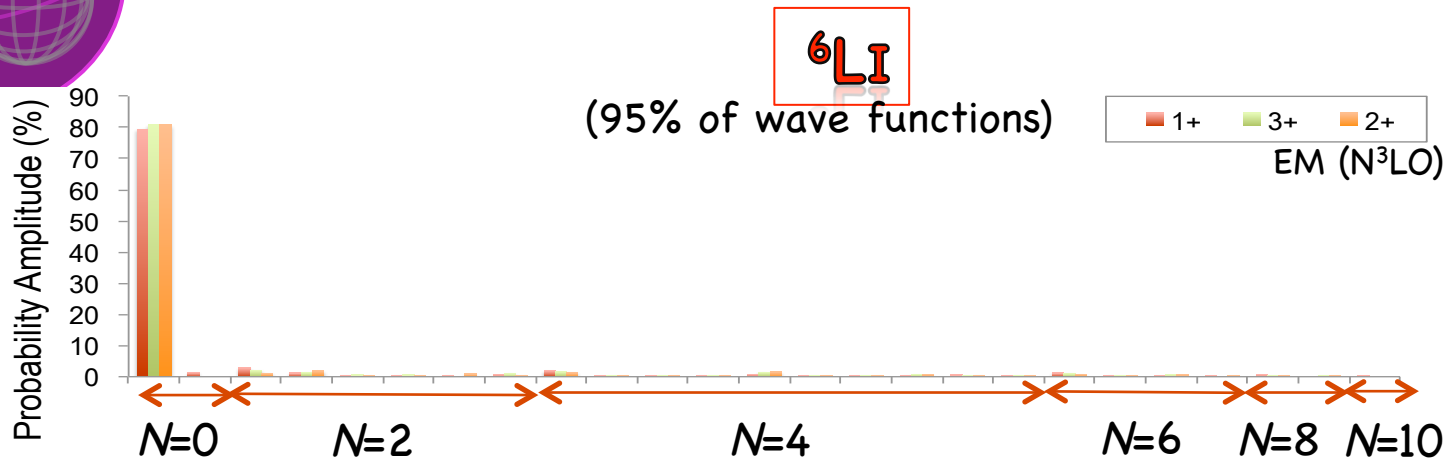
8 shells …… -19.3

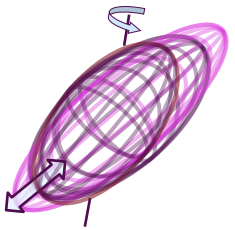
(no effective charges)



Grigor Sargsyan, PhD student, LSU

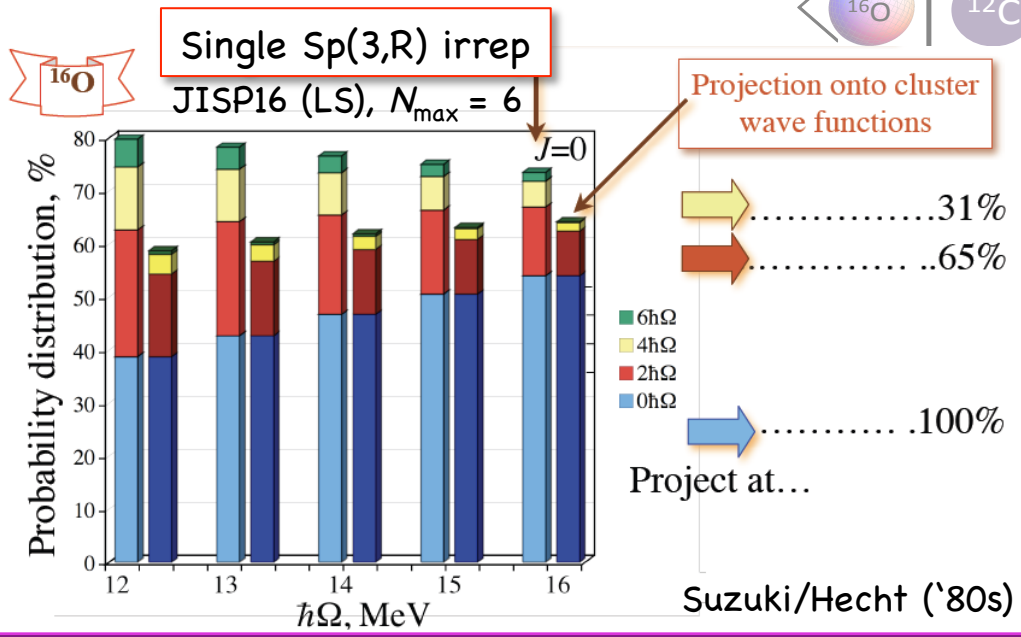
SA-NCSM with Sp(3,R) basis





^{6}Li, Nmax=12
J=1,2,3 states……2x10^7
Sp(3,R) irreps……528
Sp(3,R) with P>0.2%….25

Relation to alpha clustering?

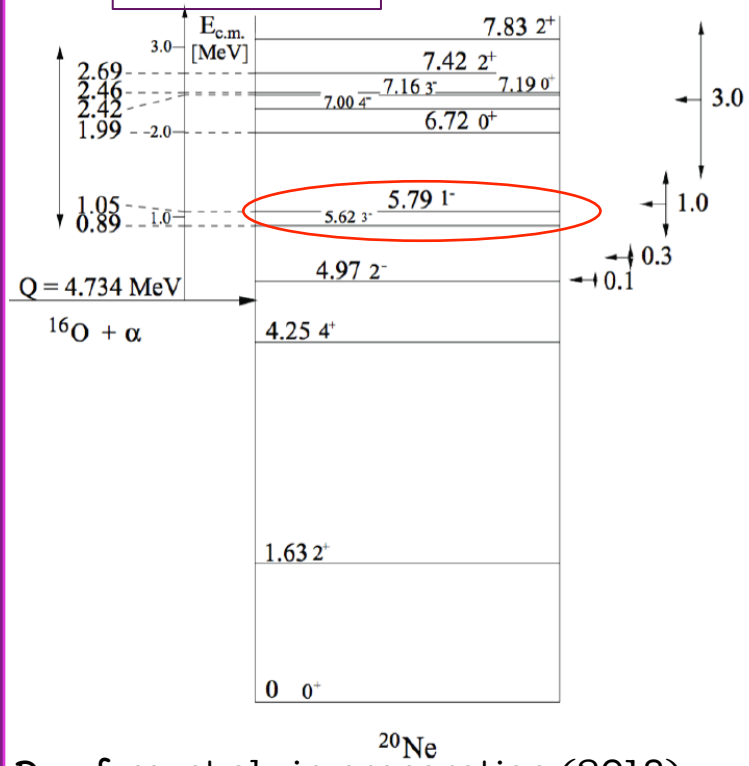


XRB nucleosynthesis abundances from *ab initio* wave functions

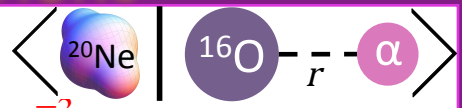
SA-NCSM:
- N2LOopt
- Sp(3,R)-preserving microscopic interaction (single adjustable parameter)

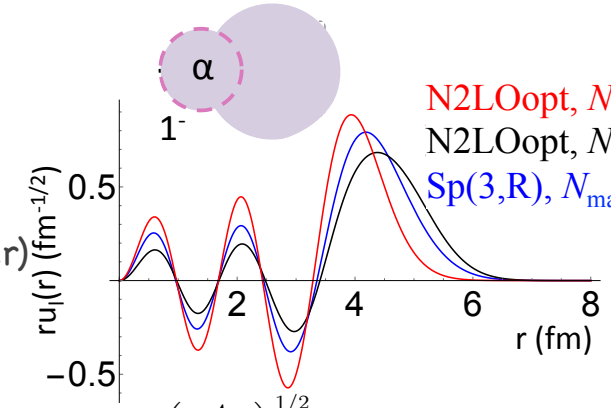
Alpha capture reactions

$^{16}\mathrm{O}(\alpha,\gamma)^{20}\mathrm{Ne}$



Dreyfuss, et al., in preparation (2018)





Wave functions from *ab initio* SA-NCSM with N2LOopt

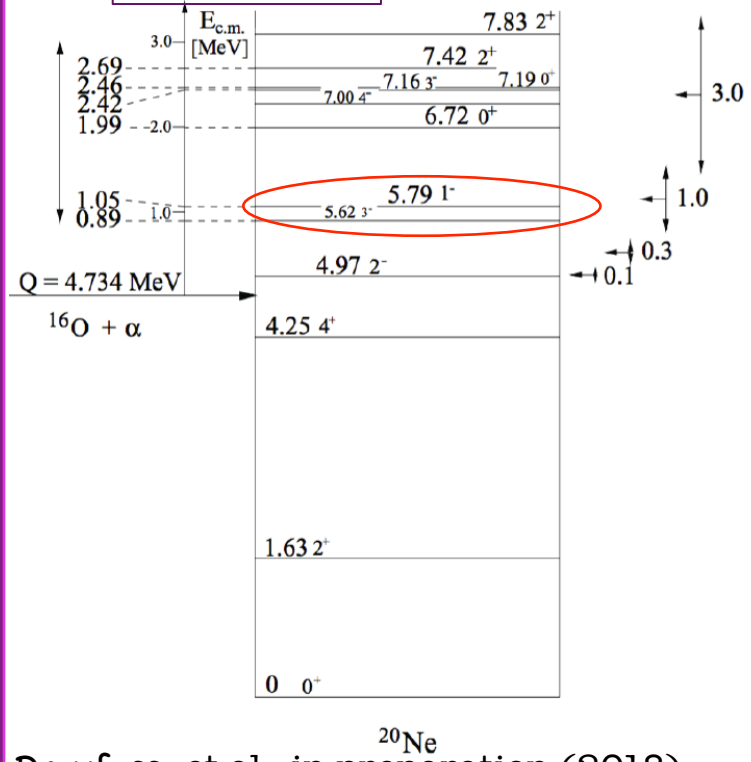
$$u_l(r) = \sum_Q \binom{A}{A-a}^{1/2} R_{Q,l}(r)\; c_Q \langle Q[\gamma(\lambda\mu)] \mid \{\{(\lambda_c\mu_c)\times(0\;0)\}^{(\lambda_c\mu_c)}\times(Q\;0)\}_l^{(\lambda\mu)}\rangle$$

XRB nucleosynthesis abundances from *ab initio* wave functions

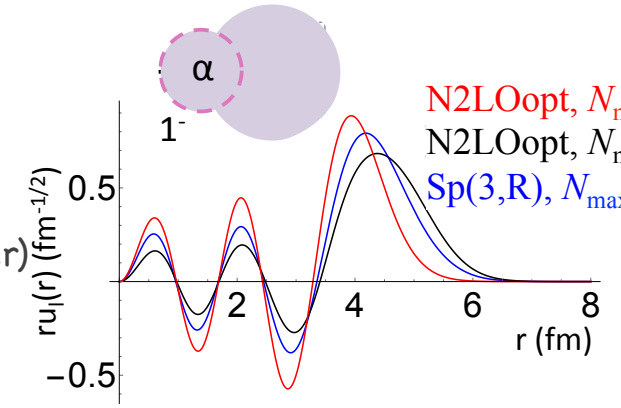
SA-NCSM:
- N2LOopt
- Sp(3,R)-preserving microscopic interaction (single adjustable parameter)

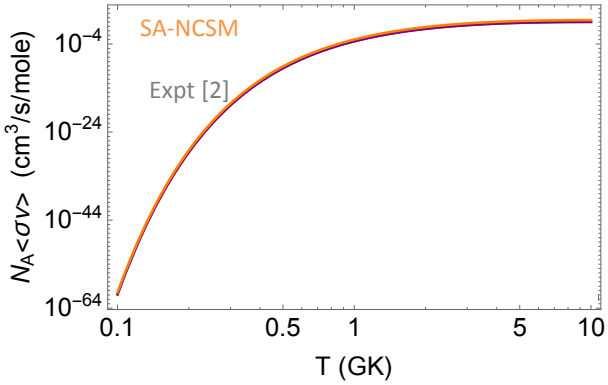
Alpha capture reactions

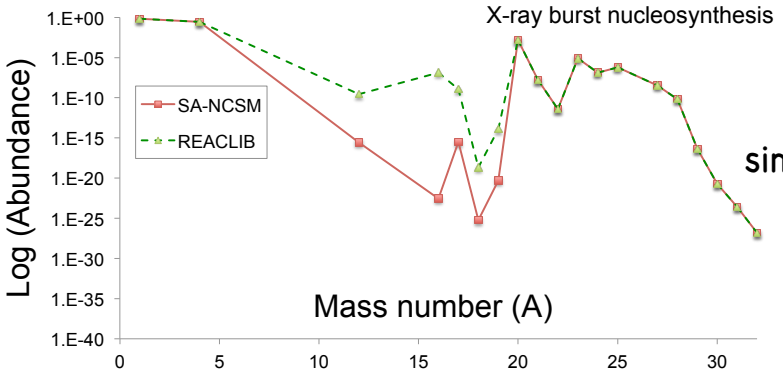
$^{16}O(\alpha,\gamma)^{20}Ne$



Dreyfuss, et al., in preparation (2018)







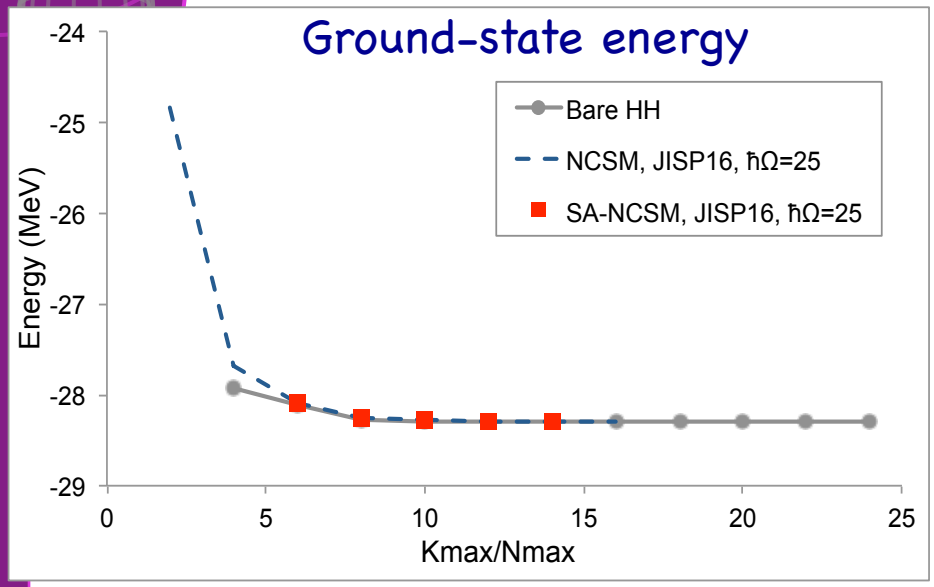
Wave functions from *ab initio* SA-NCSM with N2LOopt

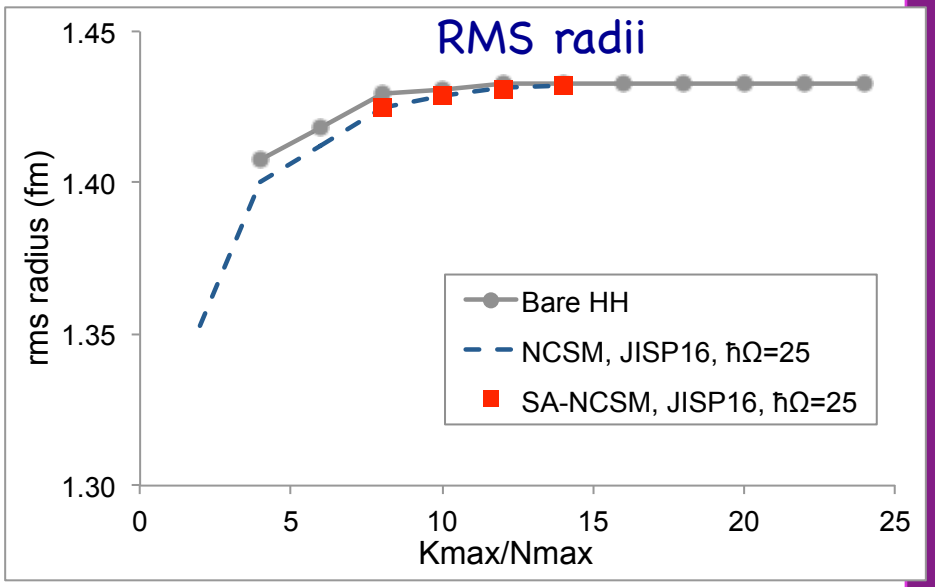
Γ_α width

Reaction rates

Nucleosynthesis simulations (Xnet): XRB abundance pattern

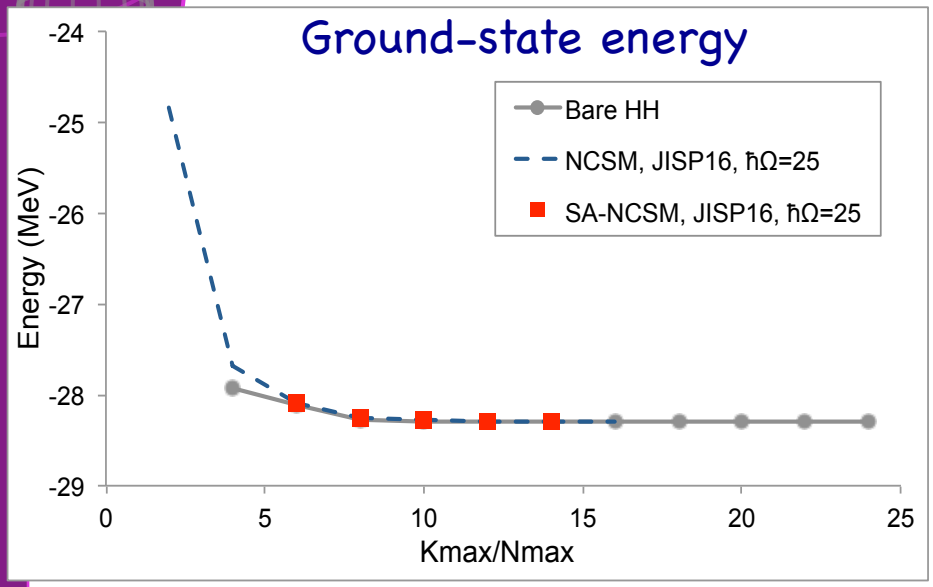
Lorentz Integral Transform (LIT): ^{4}He benchmark

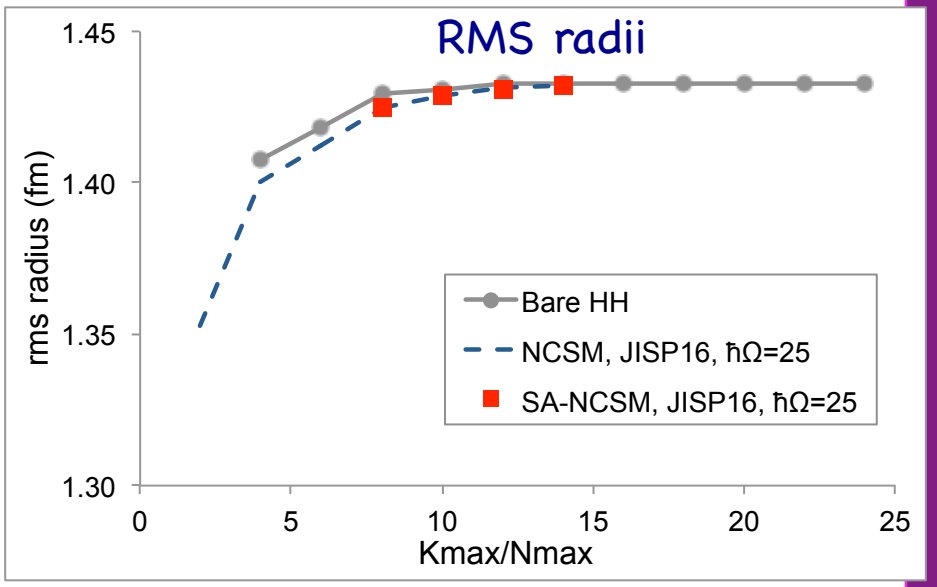


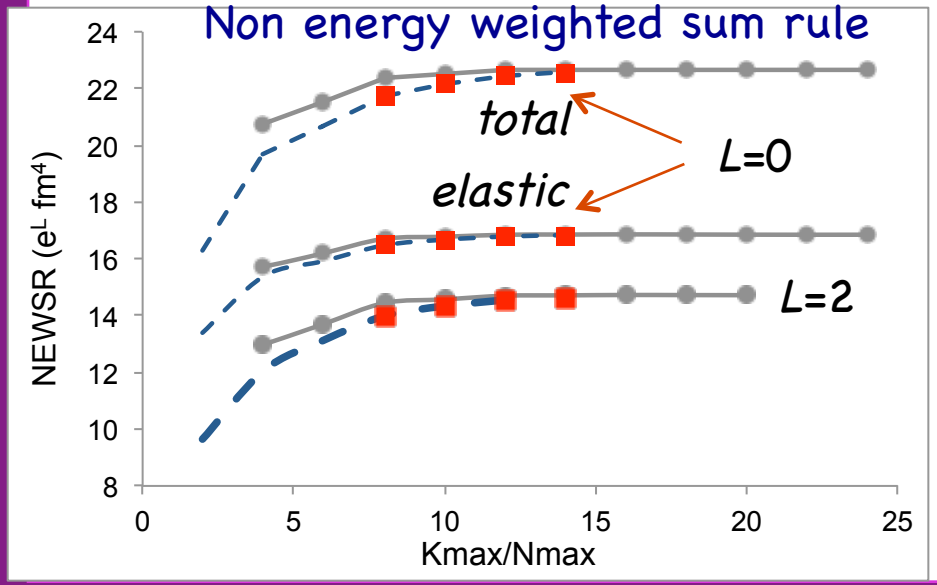


Baker et al., in preparation (2018)

Sum rules for ^{4}He: HH and SA-NCSM benchmark







Response function

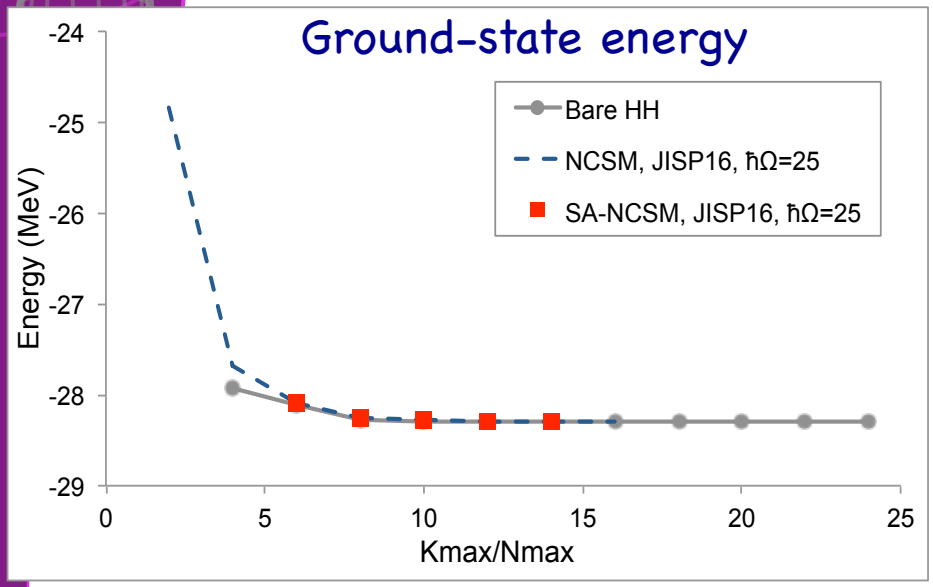
$$R(\omega) = \sum_f \left| \left\langle \psi_f \middle| \Theta \middle| \psi_0 \right\rangle \right|^2 \delta(E_f - E_0 - \omega)$$

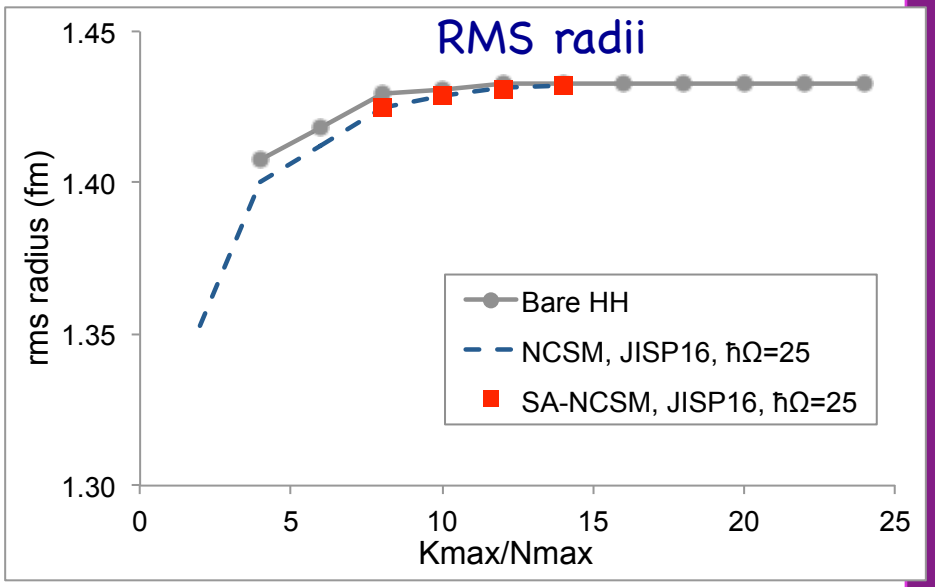
Sum rules

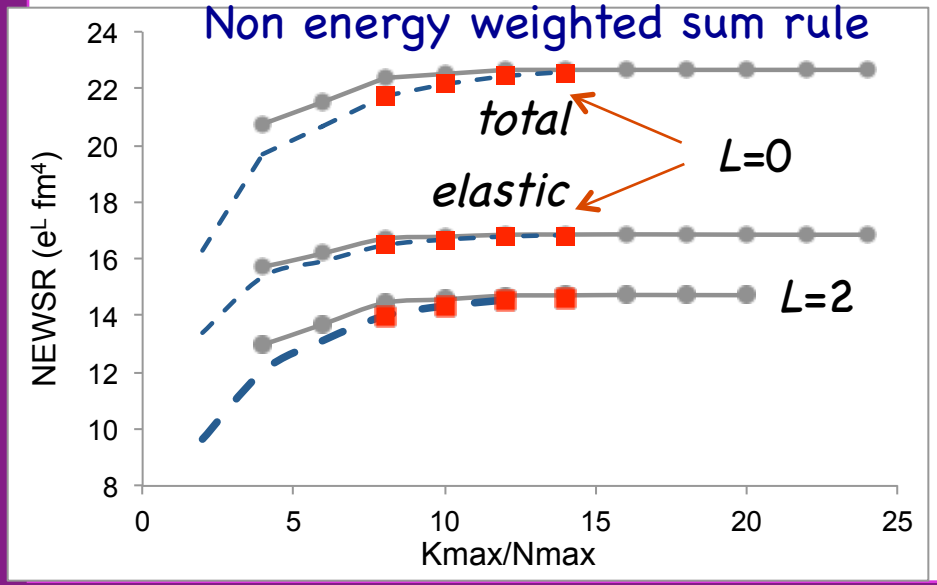
$$m_n = \int_0^\infty d\omega \; \omega^n R(\omega)$$

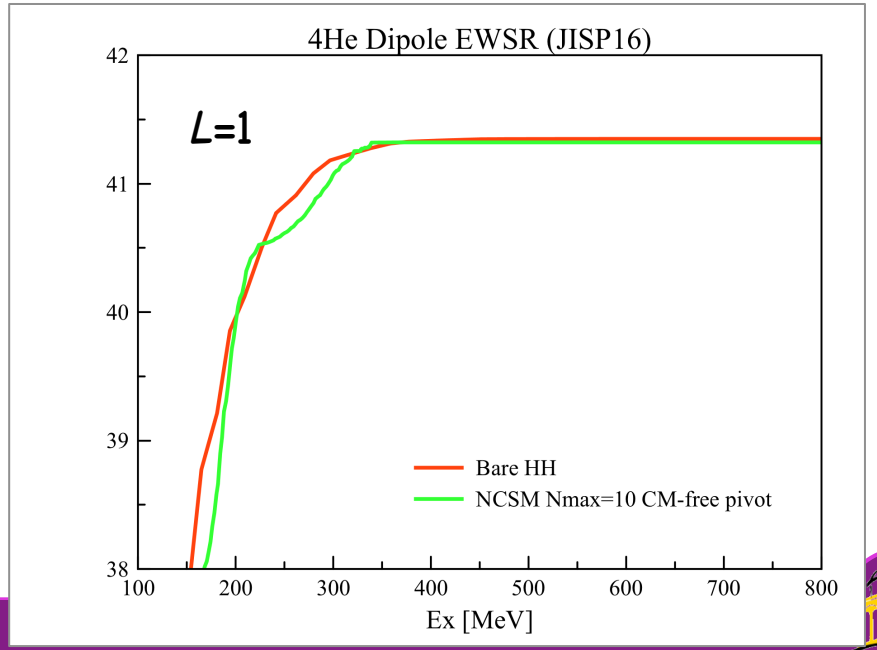
Baker et al., in preparation (2018)

Sum rules for ^{4}He: HH and SA-NCSM benchmark

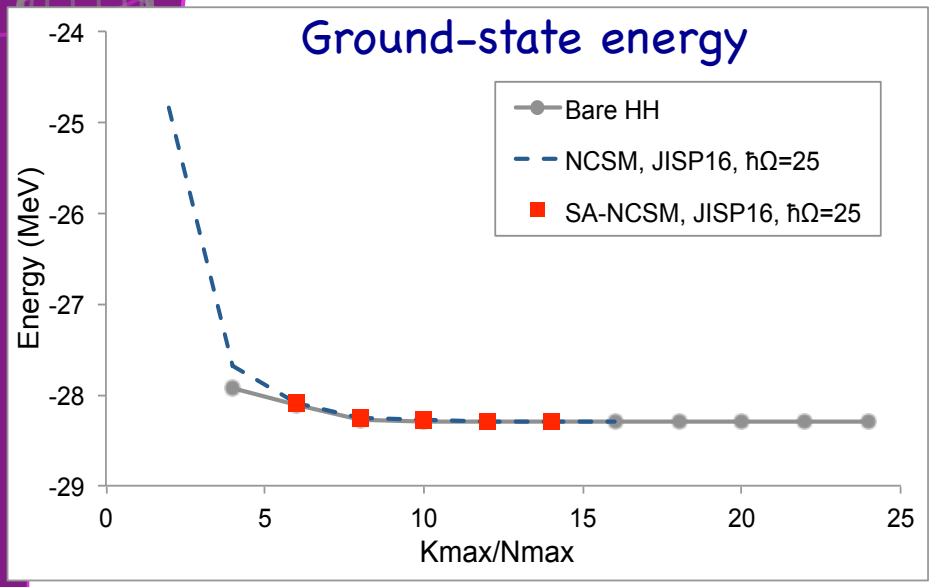


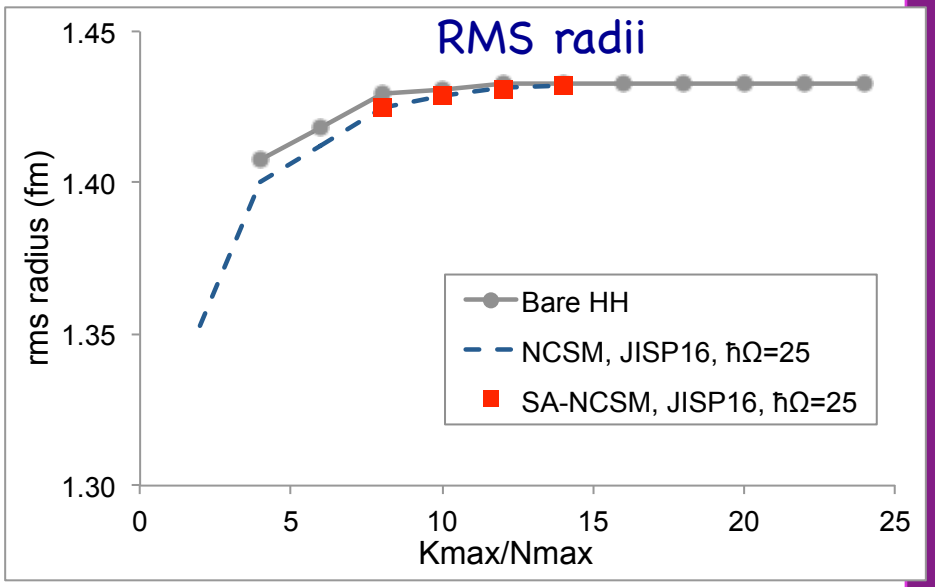


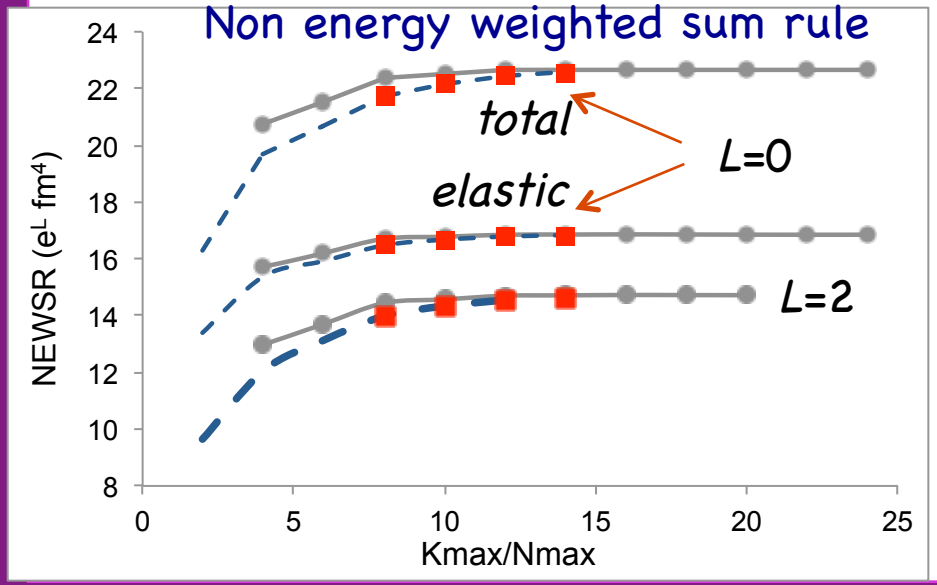


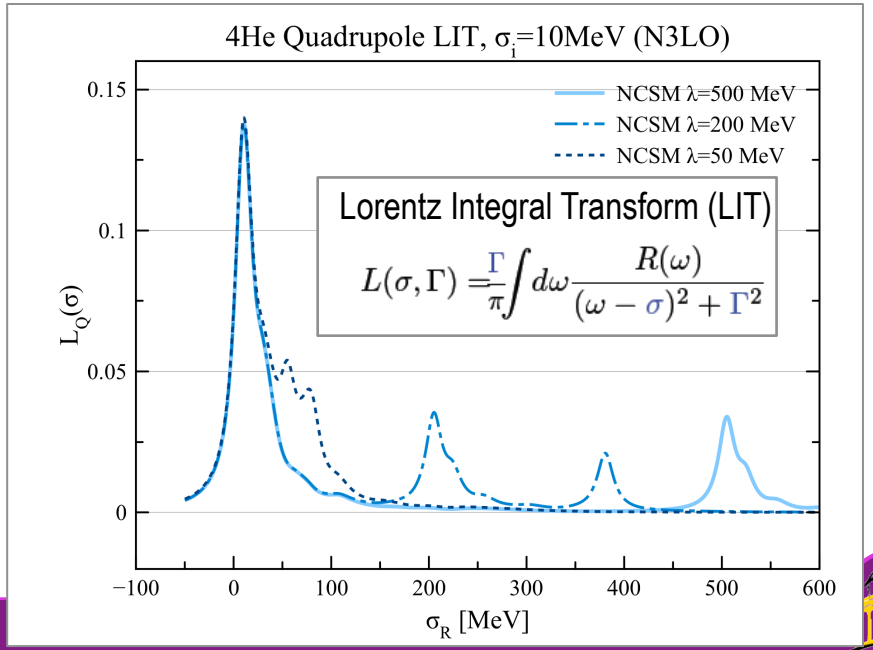


LIT: ^{4}He benchmark







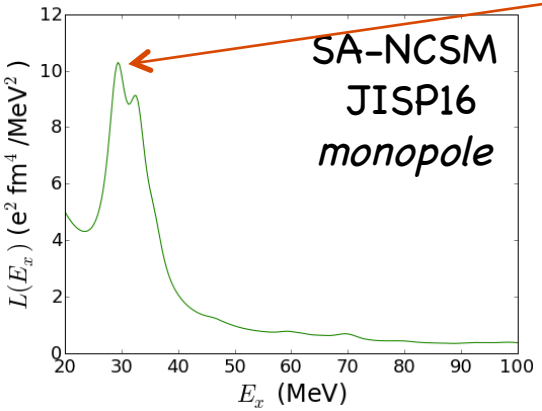


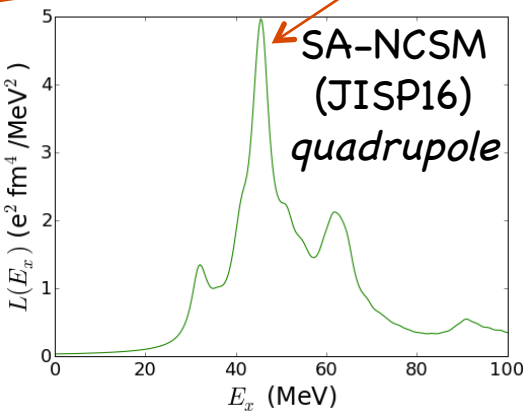
LIT: Heavier nuclei/giant resonances

^{16}O

Response functions

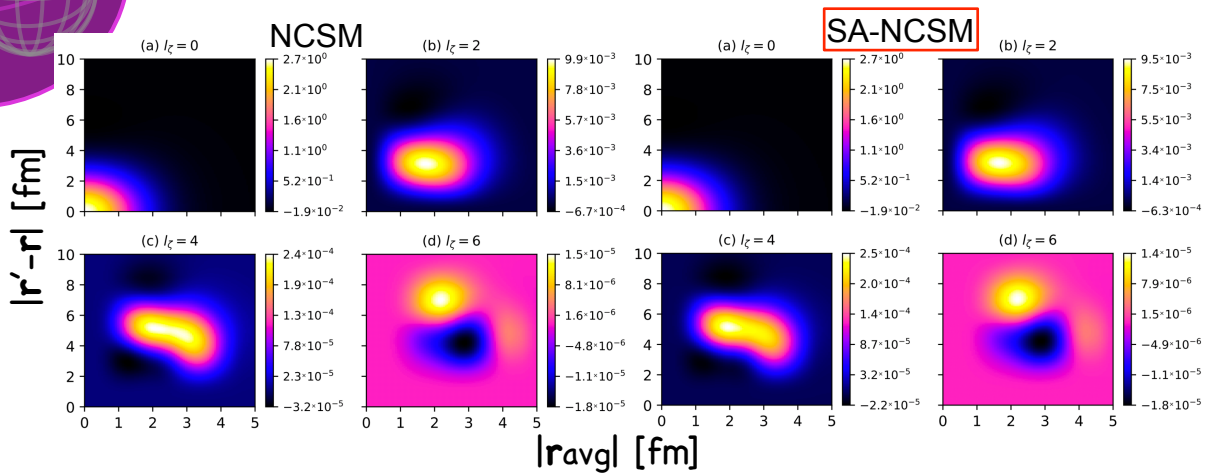
1p-1h excitations of ground-state shape





Baker et al., in preparation (2018)

Scattering observables from first principles



Burrows, Elster, Popa, Launey, Nogga, Maris, Phys. Rev. C 97 (2018) 024325

N2LOopt

^{6}Li, Non-local densities

Scattering observables from first principles

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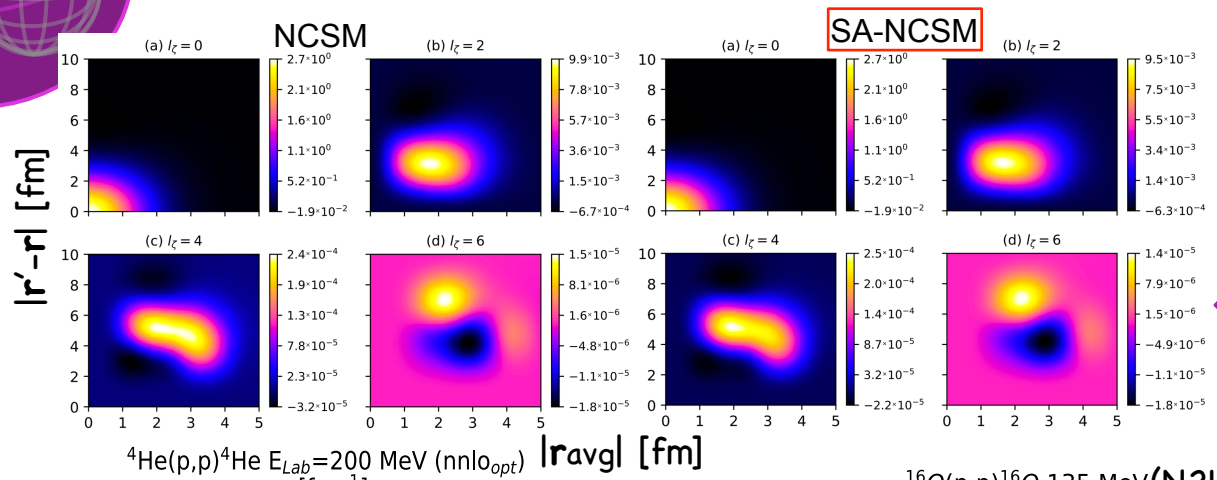
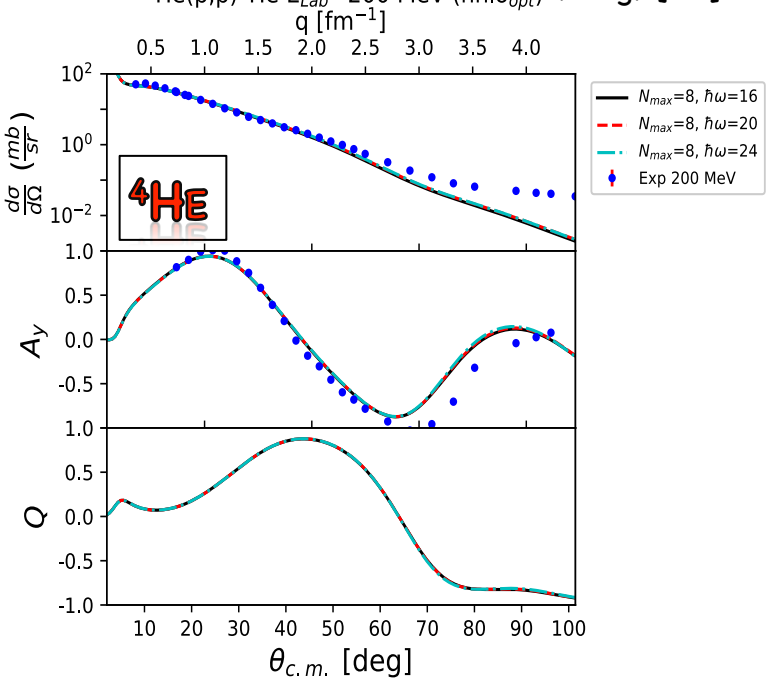
N2LOopt

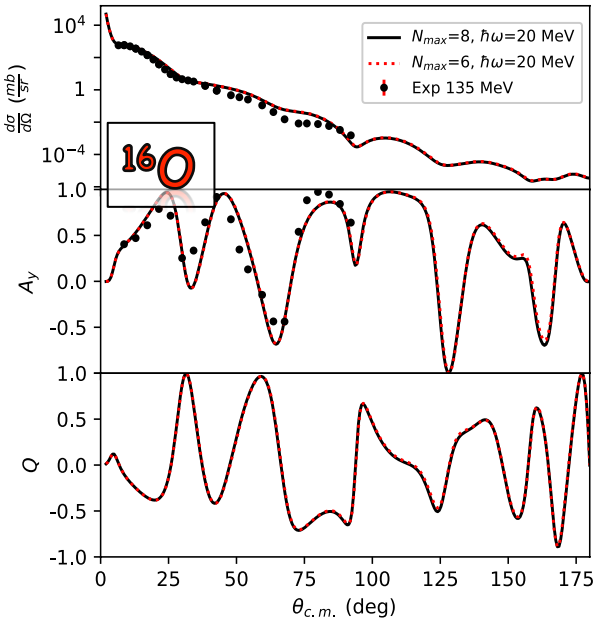
^{6}Li, Non-local densities

Elastic proton scattering

Consistent (*NN*, structure, *T*-matrix)





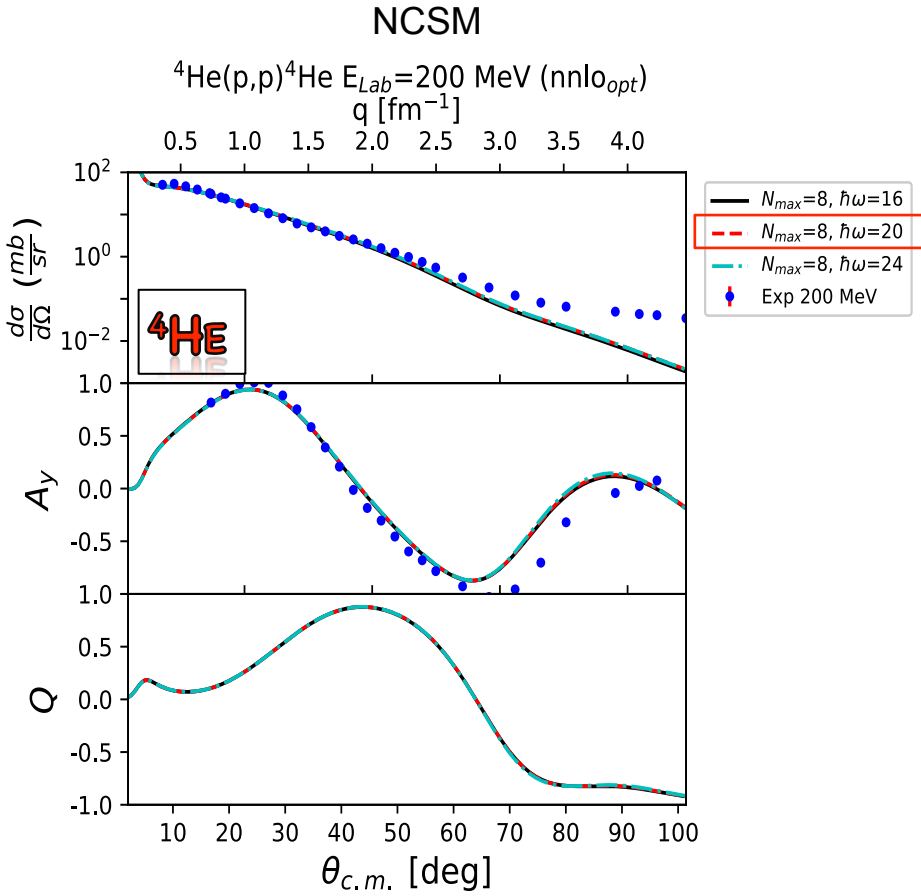


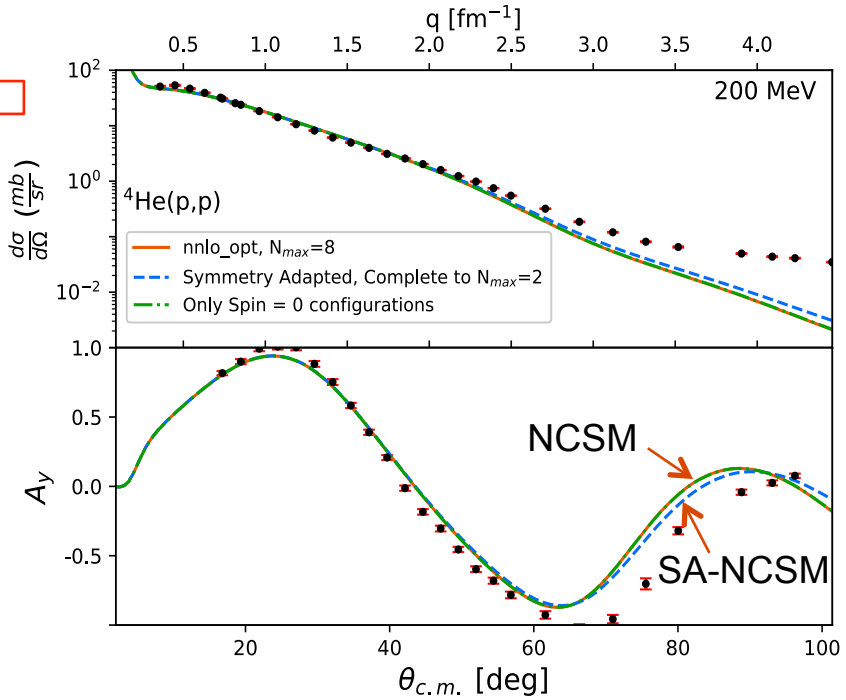
Burrows, Elster, et al., in preparation (2018)

Scattering observables from first principles

Elastic proton scattering

N2LOopt

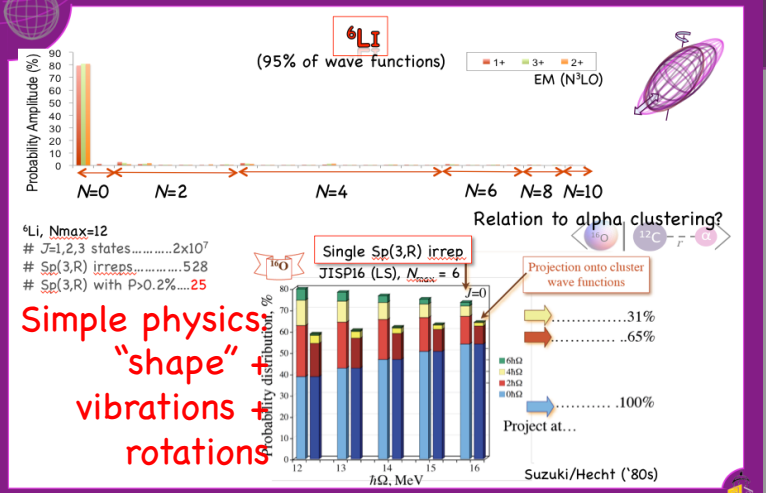




Burrows, Elster, et al., in preparation (2018)

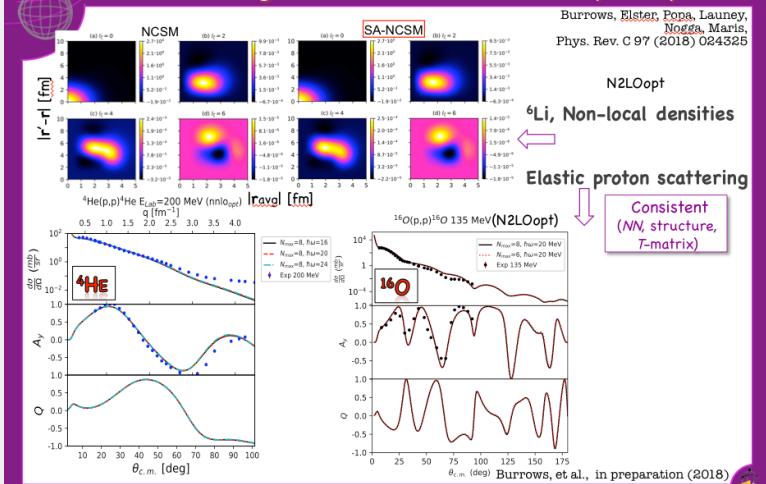
Conclusions

SA-NCSM with Sp(3,R) basis



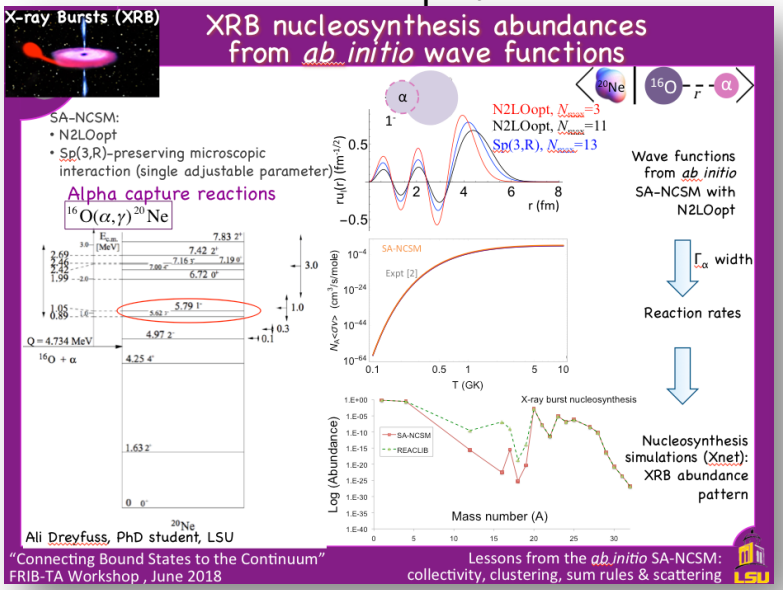
Collective/clustering features *from first principles* up to medium-mass nuclei

Scattering observables from first principles

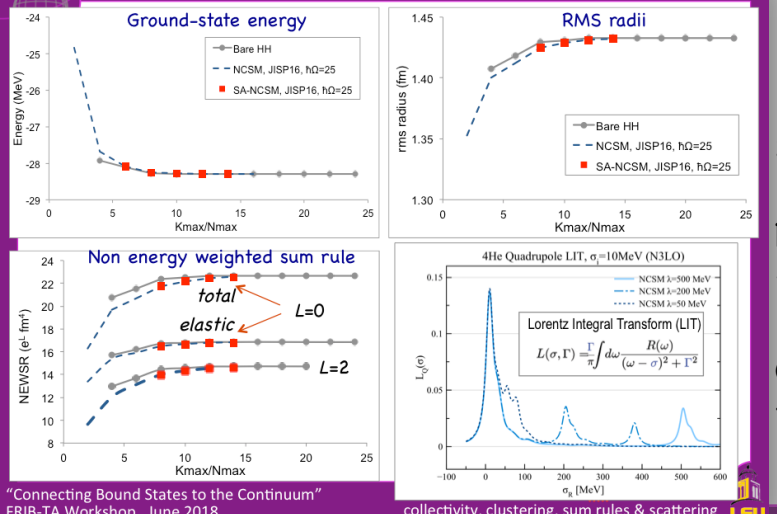


Scattering observables from *from first principles*

XRB nucleosynthesis abundances from *ab initio* wave functions



LIT: ^{4}He benchmark



Sum rules

Response functions

Giant resonances