

# Collectivity and clustering from the *ab initio* symmetry-adapted no-core shell model

Kristina Launey

... LSU Team ...

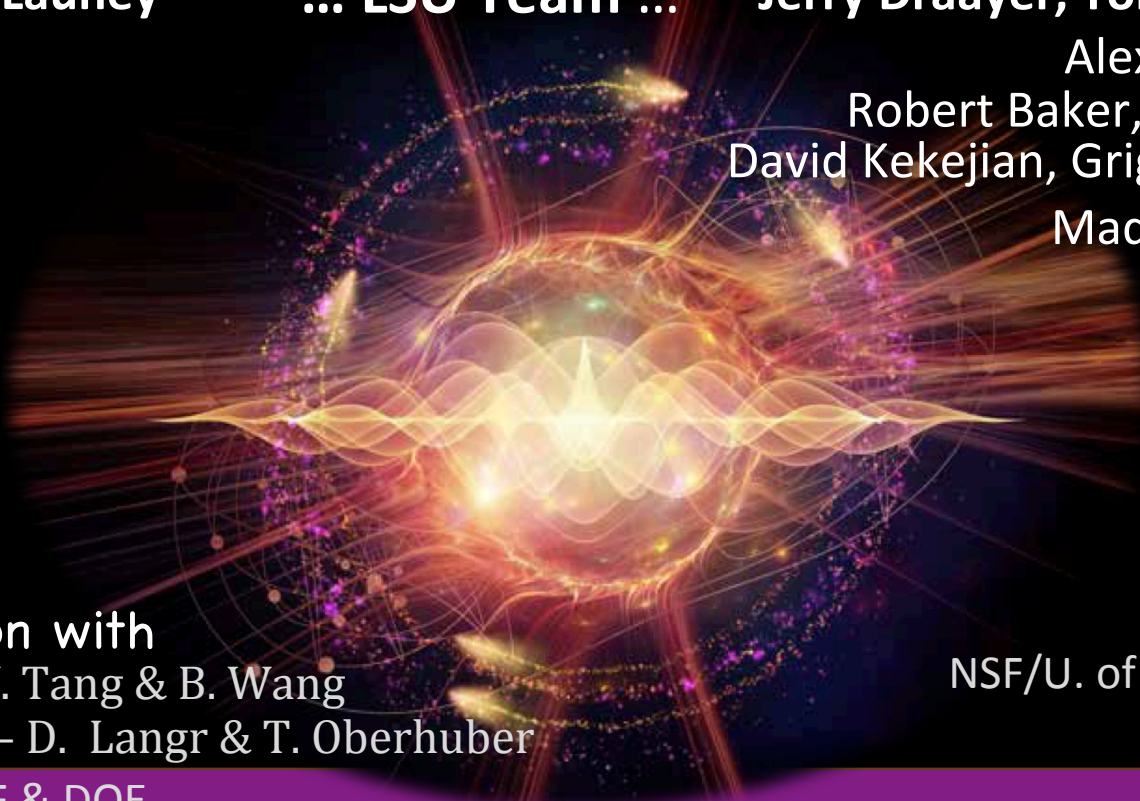
Jerry Draayer, Tomas Dytrych,

Alexis Mercenne

Robert Baker, Ali Dreyfuss,

David Kekejian, Grigor Sargsyan,

Madeleine Miora



In collaboration with  
Princeton U. – W. Tang & B. Wang  
Czech Republic – D. Langr & T. Oberhuber

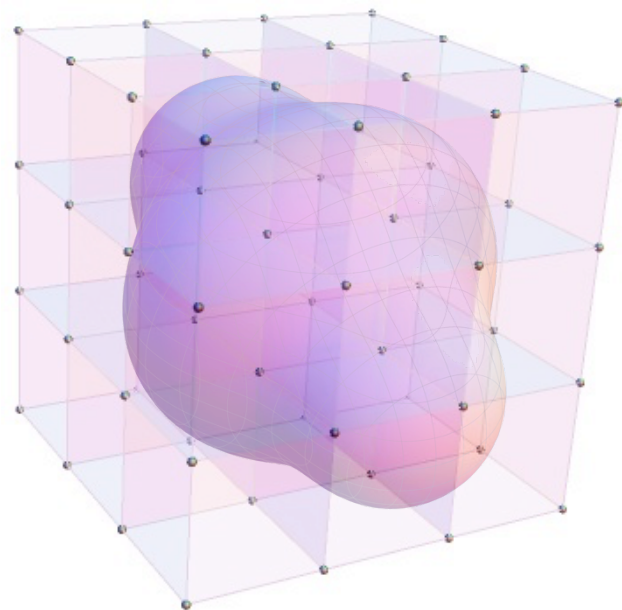
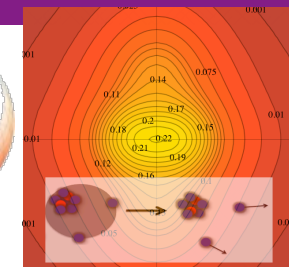
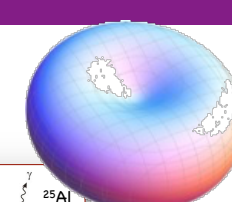
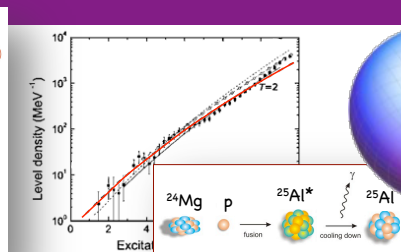
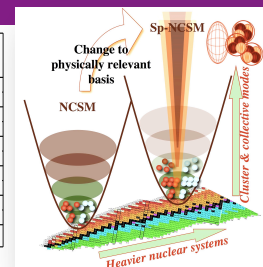
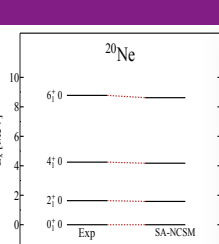
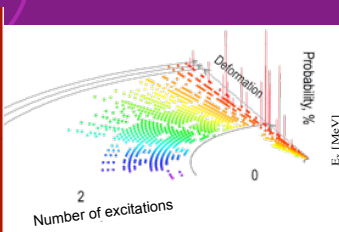
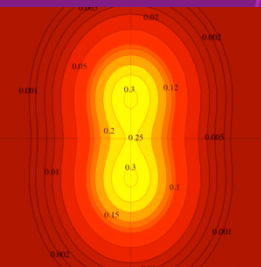
HPC Resources

NSF/U. of Illinois ...*BlueWaters*

LSU...*SuperMike-II*

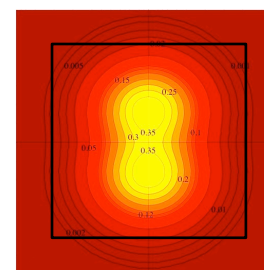
Supported by NSF & DOE





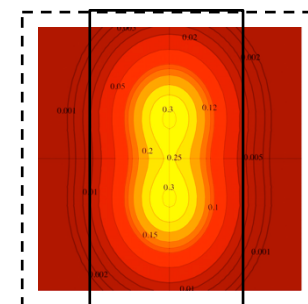
**NCSM**

Total HO quanta  
 $N_{\max}$



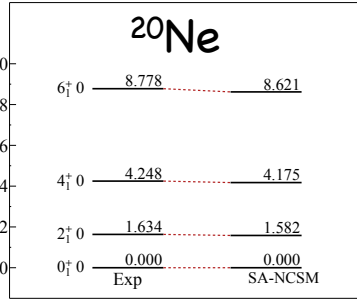
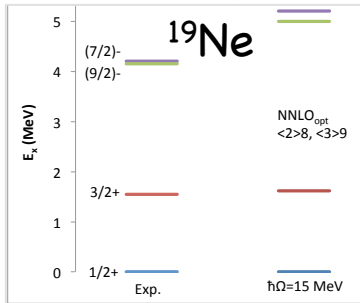
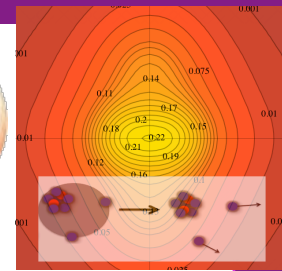
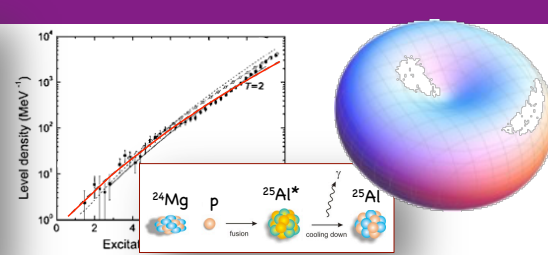
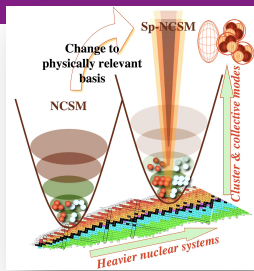
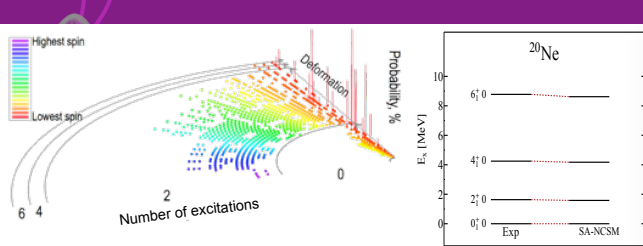
**SA-NCSM**

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



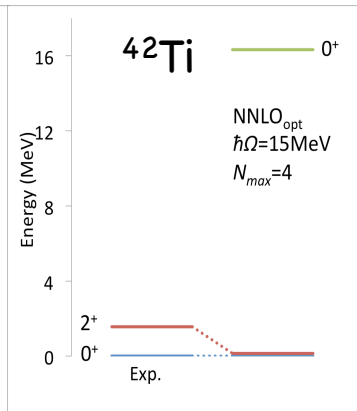
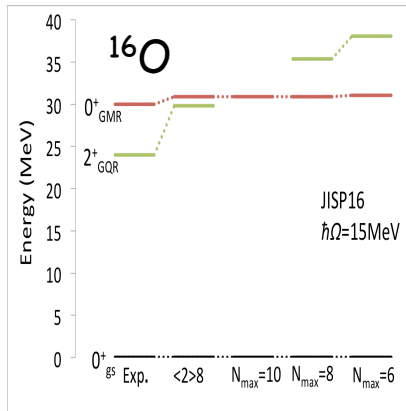
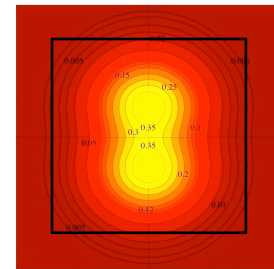
Dytrych et al., Phys. Rev. Lett. 111 (2013) 252501  
Launey et al., Prog. Part. Nucl. Phys. 89 (2016) 101





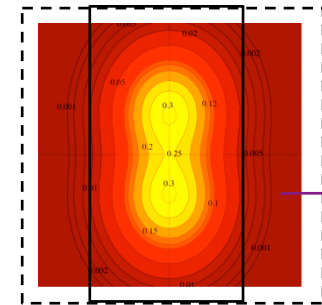
SU(3) basis

**NCSM**  
Total HO quanta  
 $N_{\text{max}}$



Symplectic  
Sp(3,R) basis

**SA-NCSM**  
Total HO quanta  
 $N_{\text{max}}$   
Distribution:  
 $z, x, y$



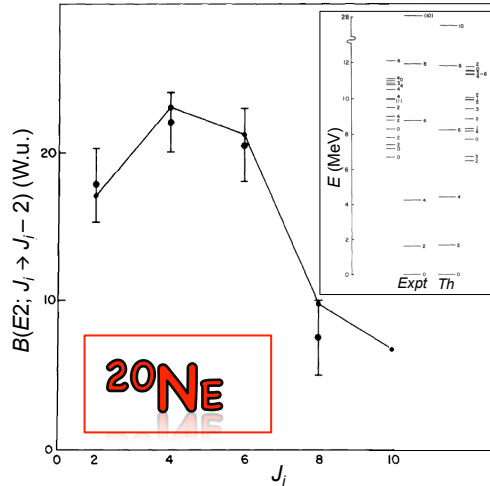
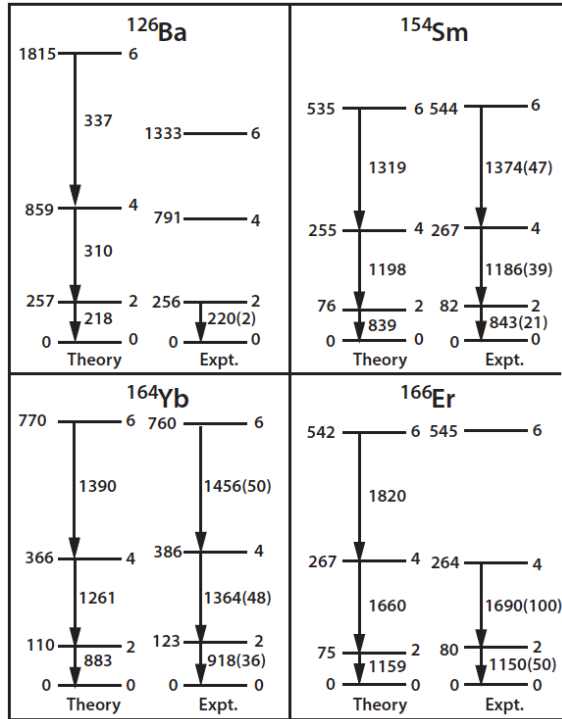
Deformation, rotations... & vibrations  
Symmetry-adapted: SU(3), Sp(3,R)  
Guided by Symplectic symmetry

LSU code (LSU3shell): [sourceforge.net/projects/lsu3shell](https://sourceforge.net/projects/lsu3shell)  
Dytrych et al., Phys. Rev. Lett. 111 (2013) 252501  
Launey et al., Prog. Part. Nucl. Phys. 89 (2016) 101



# Earlier studies ... algebraic models

Quite successful, but symmetries are assumed *a priori*:  
Typically 1 (a few) irrep(s) + symmetry-preserving interaction



J. Draayer, et al.,  
Nucl. Phys. A419, 1  
(1984)

No effective charges!

P. Park et al., Nucl. Phys. A. 414, 93 (1984)

D. J. Rowe, Rep. Prog. Phys. 48, 1419 (1985)

## SYMPLECTIC SYMMETRY, $Sp(3,R)$

Rosensteel & Rowe, PRL 38 (1977) 10

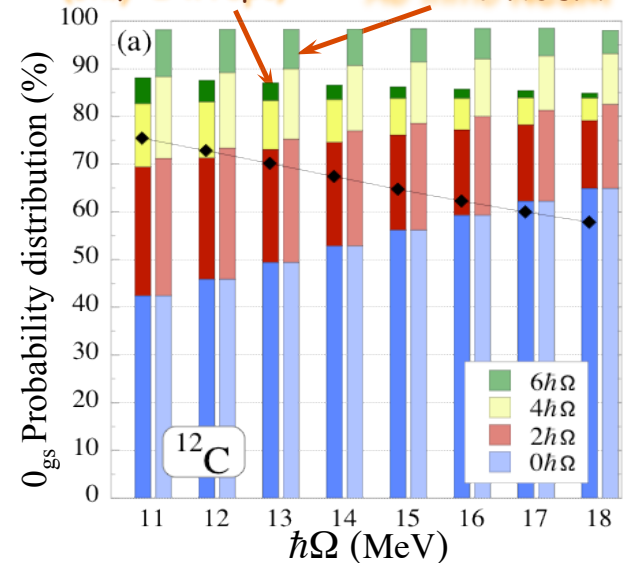
Rowe, Rosensteel, Draayer, Hecht, Suzuki, Escher, Bahri, ...

*Ab initio* results:  
No *a priori* symmetry assumptions  
(JISP16 NN)

Symplectic basis

(only 2 irreps)

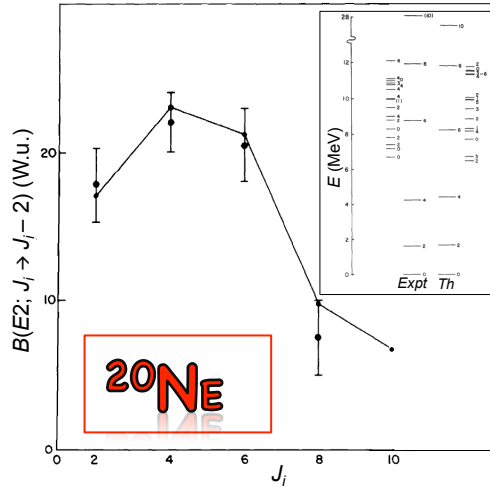
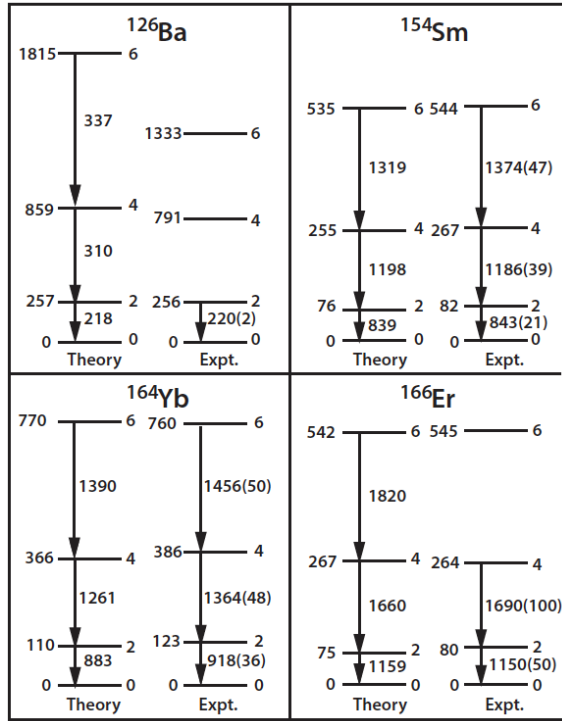
*Ab initio* NCSM



Dytrych, Launey, Bahri, Draayer, Vary,  
Phys. Rev. Lett. 98 (2007) 162503

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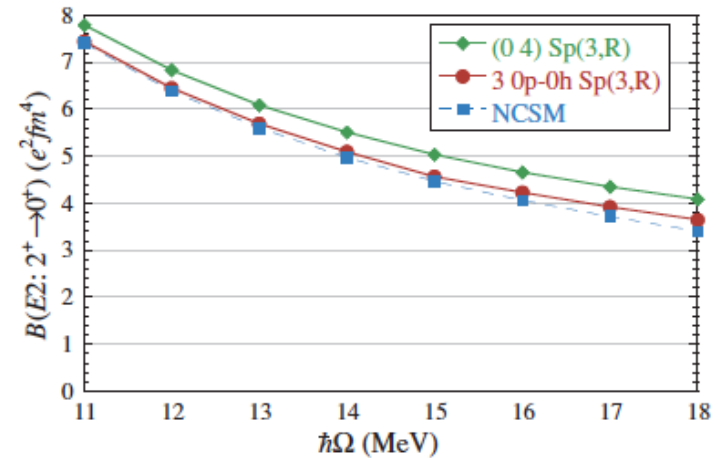
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## SYMPLECTIC SYMMETRY, $Sp(3,R)$

Rosensteel & Rowe, PRL 38 (1977) 10

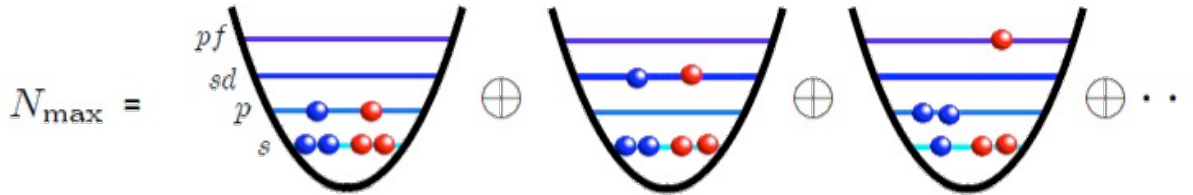
Rowe, Rosensteel, Draayer, Hecht, Suzuki, Escher, Bahri, ...

P. Park et al., Nucl. Phys. A. 414, 93 (1984)

D. J. Rowe, Rep. Prog. Phys. 48, 1419 (1985)

# Ab initio symmetry-adapted theory

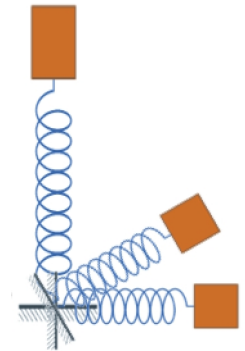
Distributions of nucleon over HO shells ( $0\hbar\Omega$ ,  $2\hbar\Omega$ , ...;  $0p-0h$ ,  $2p-2h$ , ...)



**SU(3) basis states/Sp(3,R) basis states: reorganization of model space**  
(unitary transformation from  $m$ -scheme), e.g. for  $A=2$ :

$$\lambda = n_z - n_x; \quad \mu = n_x - n_y$$

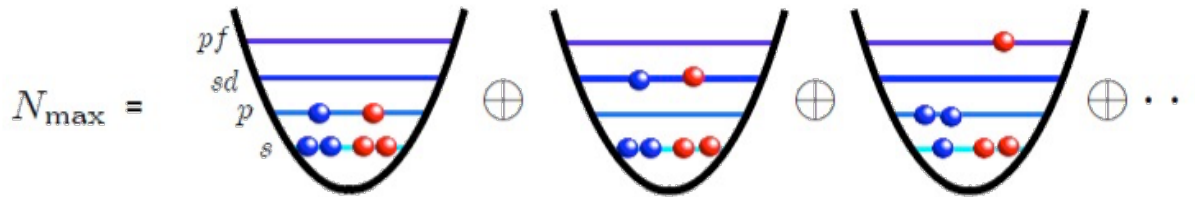
Model space scheme	Two-particle basis state
$L$ - $S$ scheme	$\{a_{\eta l \underline{st}_z}^\dagger \times a_{\eta' l' \underline{s't'_z}}^\dagger\}^{(LS)JM}  0\rangle$
$M$ scheme	$a_{\eta l j m t_z}^\dagger a_{\eta' l' j' m' t'_z}^\dagger  0\rangle$ , with $m + m' = M$
$J$ scheme	$\{a_{\eta l \underline{j}t_z}^\dagger \times a_{\eta' l' \underline{j't'_z}}^\dagger\}^{JM}  0\rangle$
SU(3) scheme	$\{a_{(\eta 0) \underline{st}_z}^\dagger \times a_{(\eta' 0) \underline{s't'_z}}^\dagger\}^{(\lambda \mu) \kappa (LS) JM}  0\rangle$
Sp(3, $\mathbb{R}$ ) scheme*	$\{\{\hat{A}^{(20)} \times \hat{A}^{(20)} \dots \times \hat{A}^{(20)}\}^{(\lambda_n \mu_n)} \times$ $\underbrace{\left[ a_{(\eta_1 0)}^\dagger \times a_{(\eta_2 0)}^\dagger \right]}_{A=2 \text{ bandhead}} \frac{(\lambda \sigma \mu \sigma)}{\kappa L M L} \rho^{(\lambda \omega \mu \omega)}\}_{\kappa L M L}  0\rangle$



J. P. Draayer, T. Dytrych and K. D. Launey, in  
"Emergent Phenomena in Atomic Nuclei ...", World Scientific Co. (2017)

# Ab initio symmetry-adapted theory

Distributions of nucleon over HO shells ( $0\hbar\Omega$ ,  $2\hbar\Omega$ , ...;  $0p-0h$ ,  $2p-2h$ , ...)



## SU(3) package for SU(3) coupling/recoupling coefficients

... analogous to SU(2), but outer/inner multiplicities!

Draayer & Akiyama, JMP 14 (1973) 1904

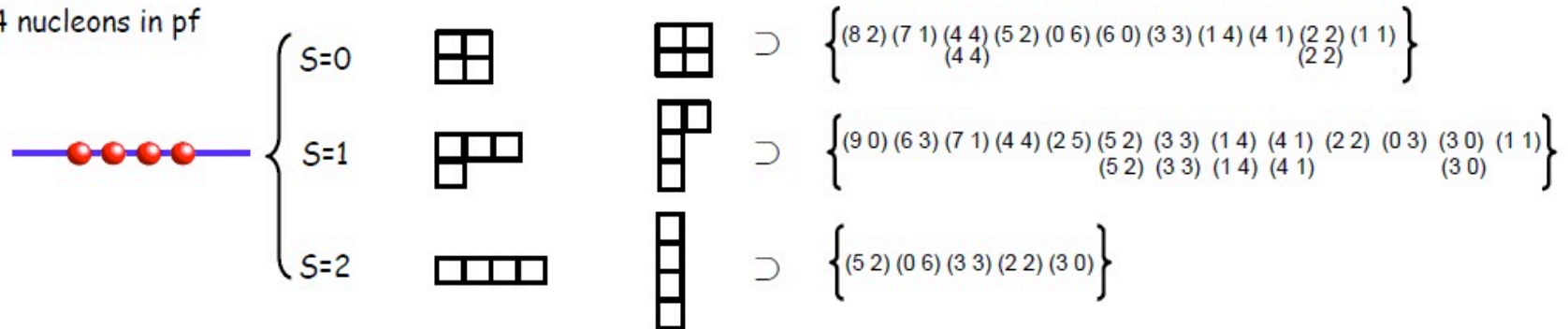
Akiyama & Draayer, Comp. Phys. Commun. 5(1973)405

## SU(3) basis construction ... based on Gel'fand patterns (fast and efficient!)

$$\text{quantum labels: } \begin{matrix} U(2) & \otimes & U(10) & \supset & SU(3) \\ S & & [f] & \alpha & (\lambda \mu) \end{matrix}$$

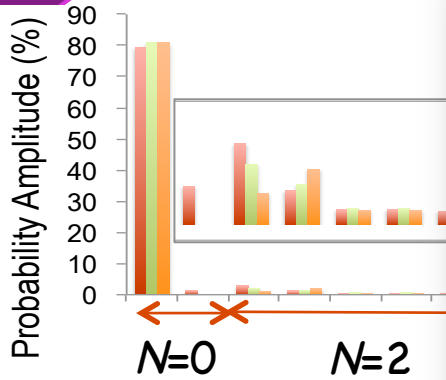
### Example:

4 nucleons in pf

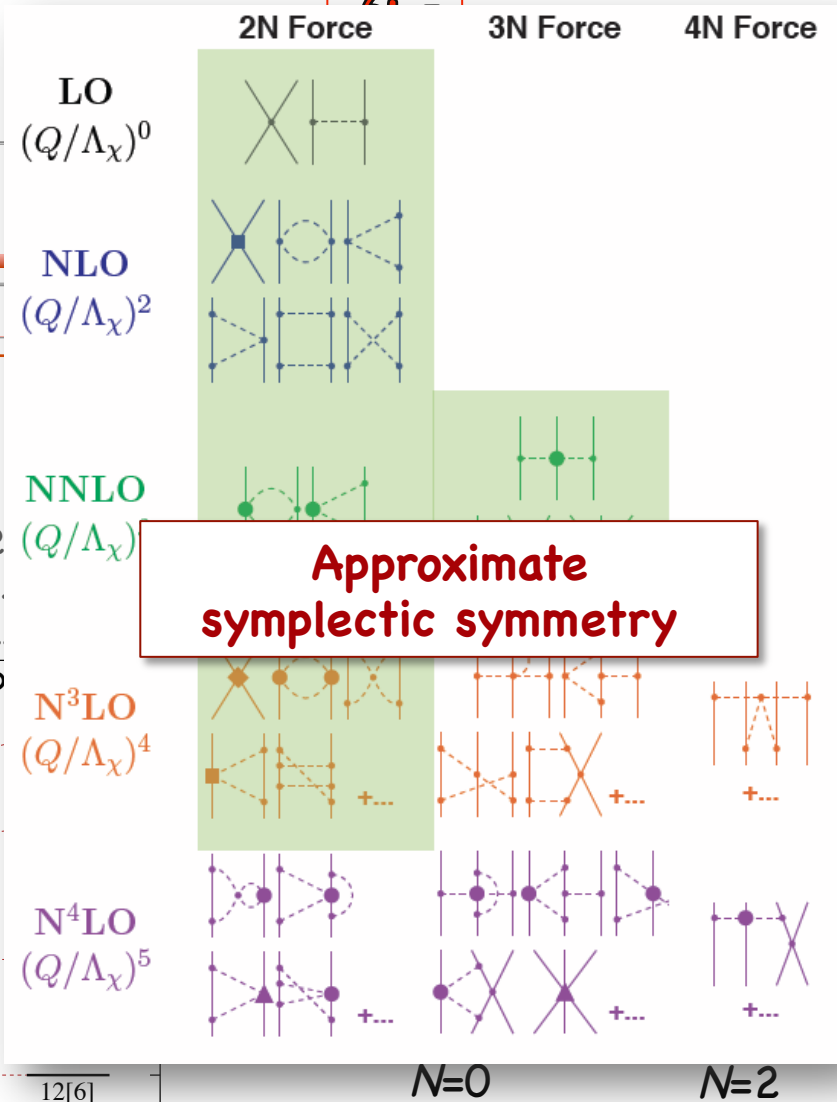
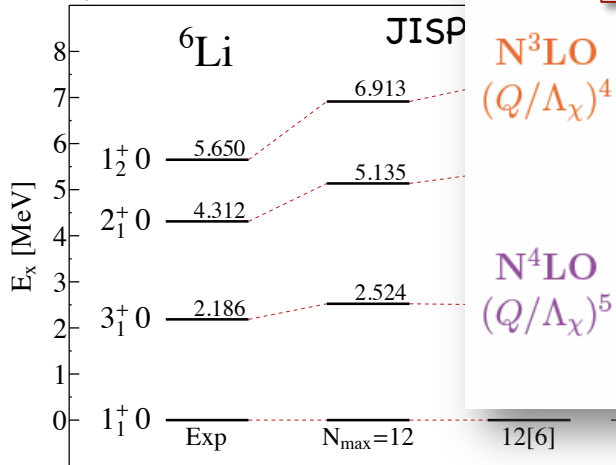


Draayer et al., "Representations of  $U(3)$  in  $U(N)$ ", Comp. Phys. Commun. 56 (1989) 279

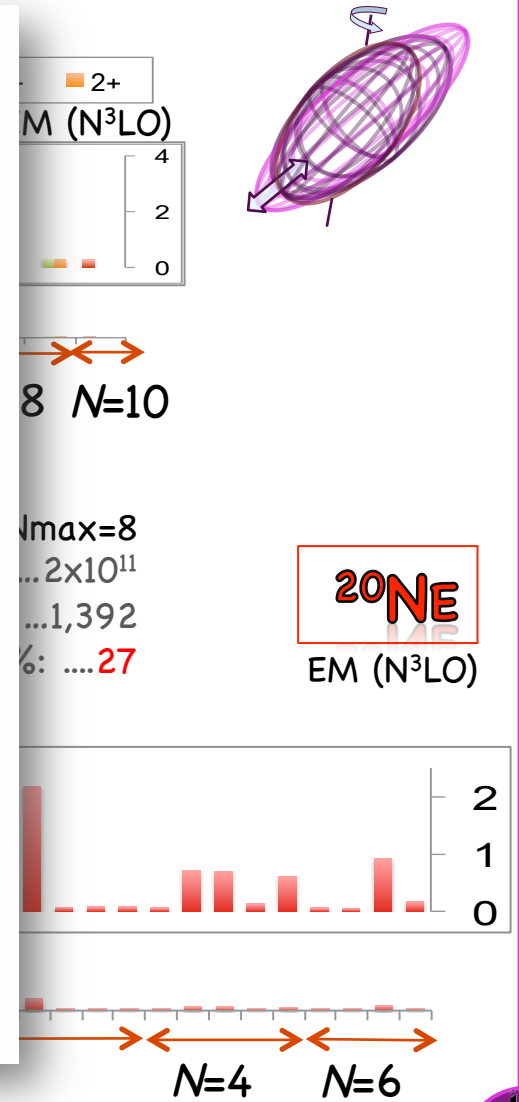
# What physics can we learn?



${}^6\text{Li}$ ,  $N_{\text{max}}=12$   
 #  $J=1,2,3$  states.....2  
 #  $\text{Sp}(3,\text{R})$  irreps.....  
 #  $\text{Sp}(3,\text{R})$  with  $P>0.2\%$ .....



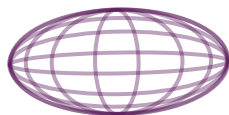
**Approximate symplectic symmetry**



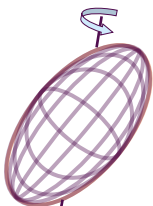


# What physics can we learn?

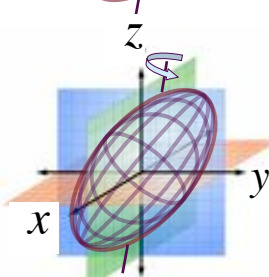
$Sp(3,R)$  (collective) basis configuration:



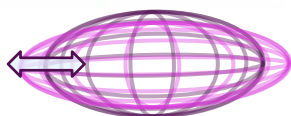
**one** equilibrium deformation ("shape")



rotations

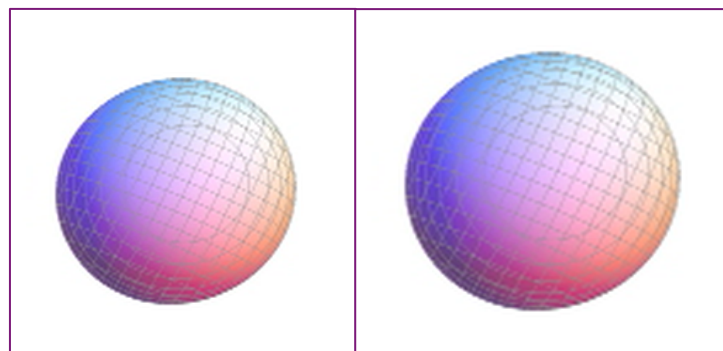


space orientation

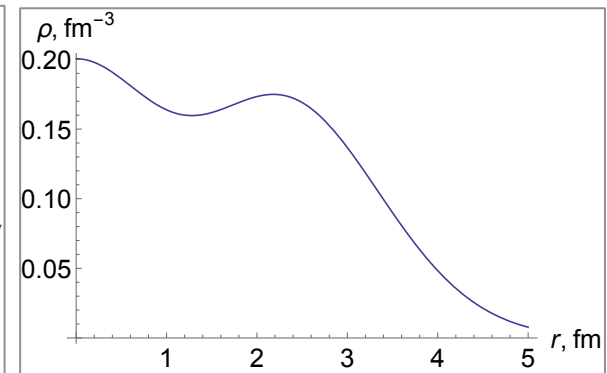
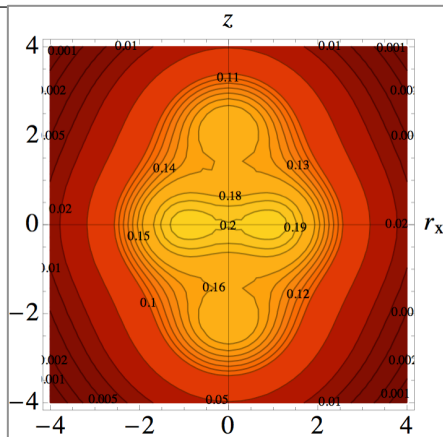
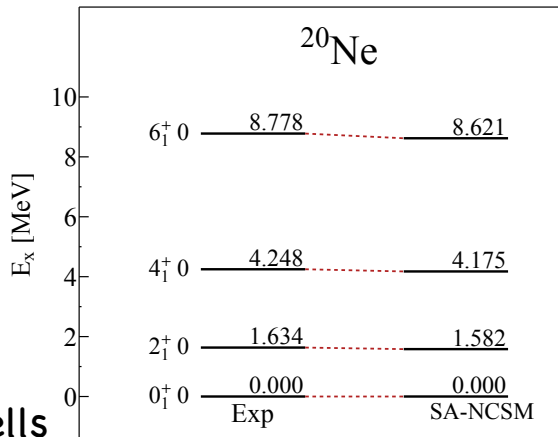


**Vibrations**  
(of the giant resonance monopole ( $r^2$ )/ quadrupole (Q) type)

**Symplectic symmetry:**  
All states preserve the equilibrium shape



# Collectivity features

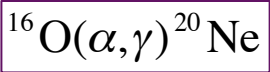
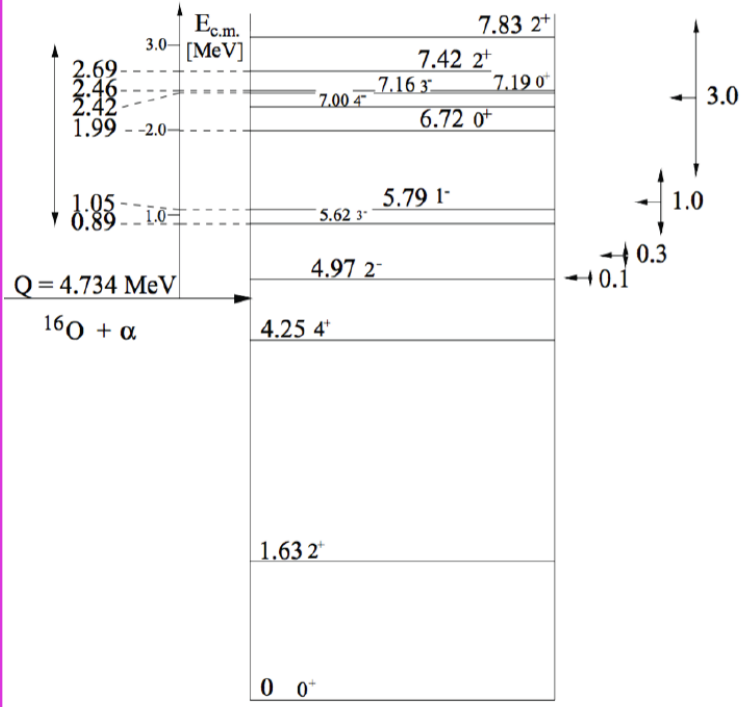


20NE

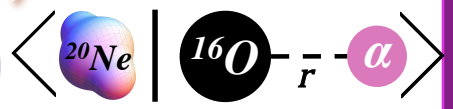
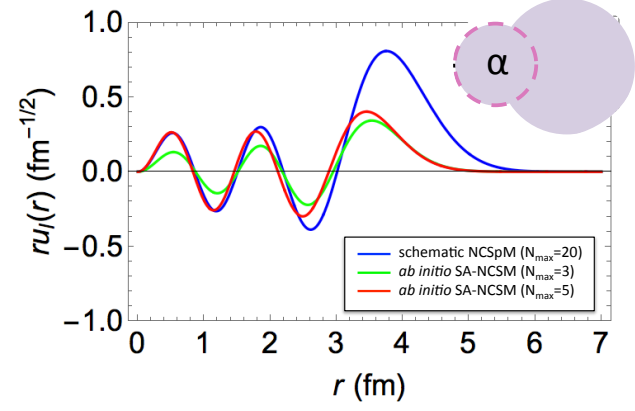
SA-NCSM (selected model space): 50 million SU(3) states  
Complete model space: 1000 billion states



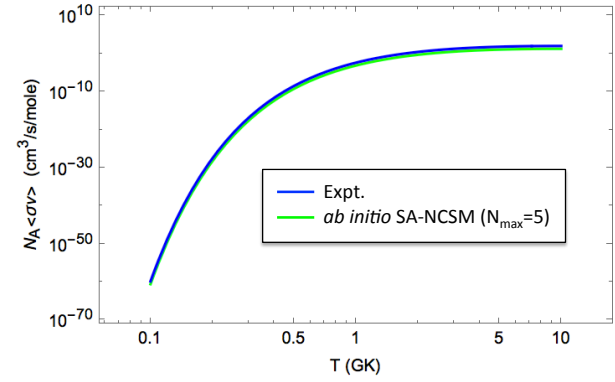
# Alpha clustering and effect on X-ray burst nucleosynthesis



Ali Dreyfuss, PhD student, LSU



Wave functions from *ab initio* SA-NCSM



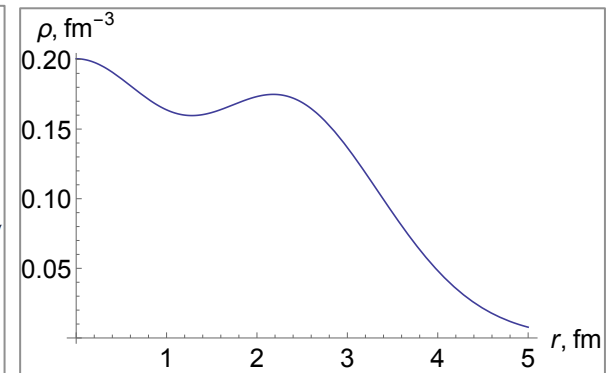
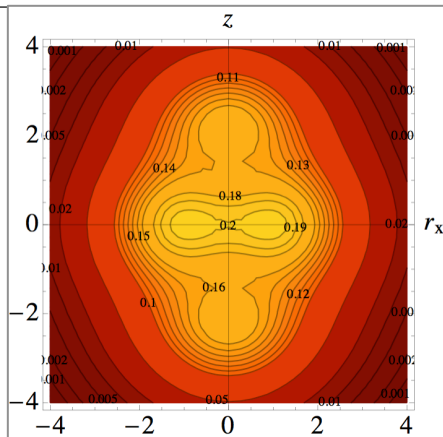
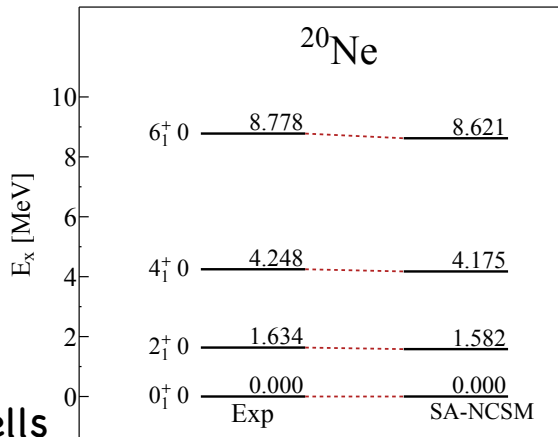
Reaction rates

Nucleosynthesis simulations:  
XRB abundance pattern



# Collectivity features

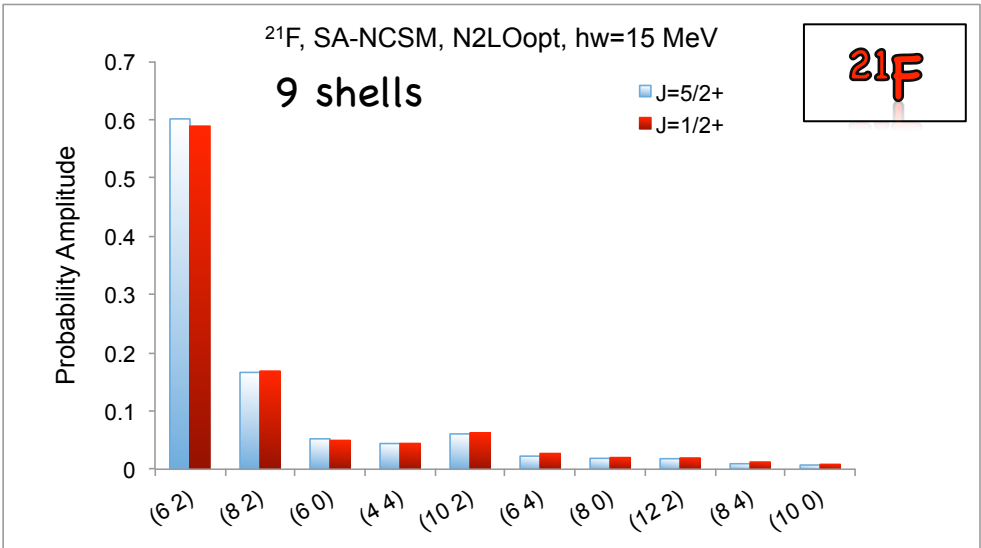
**20Ne**



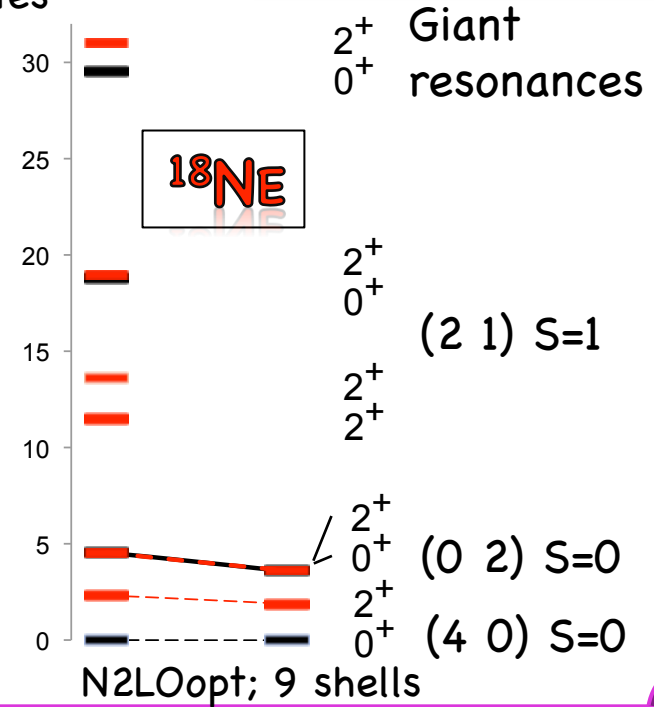
13 shells

SA-NCSM (selected model space): 50 million SU(3) states  
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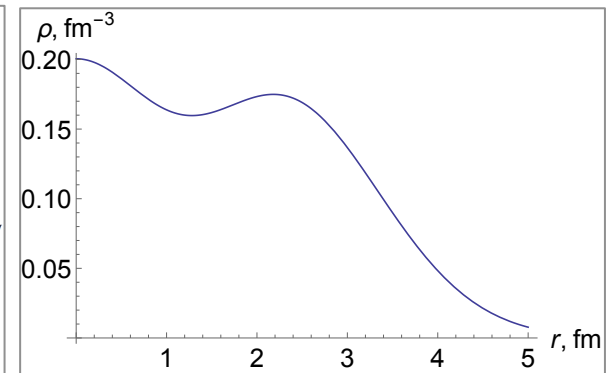
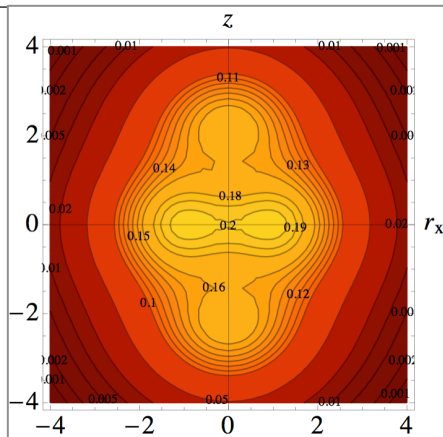
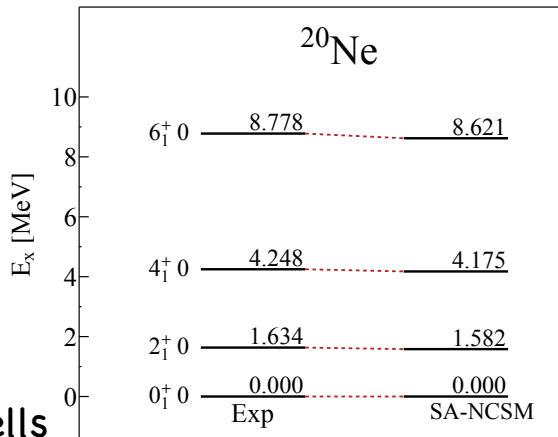
**Ne & Mg isotopes**



Grigor Sargsyan, PhD student, LSU



# Collectivity features



**20NE**

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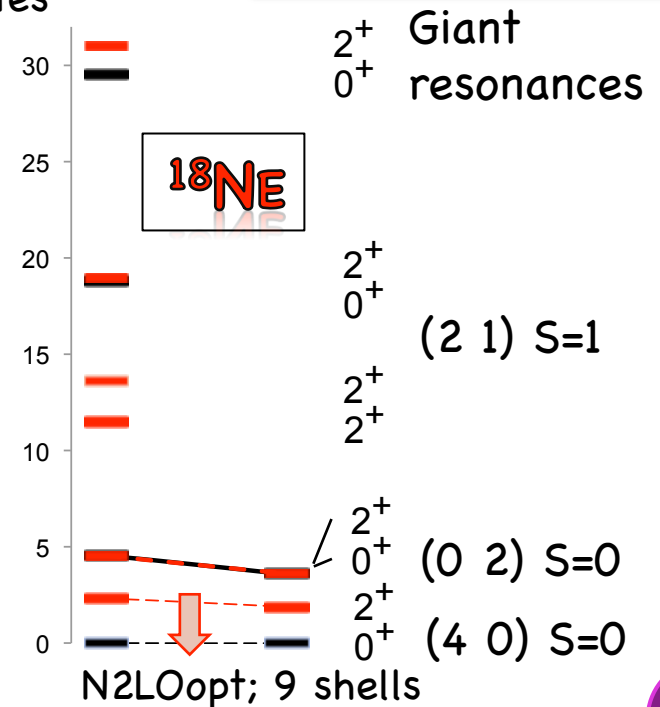
**Ne & Mg isotopes**

<sup>18</sup>Ne, B(E2: 2<sup>+</sup>→0<sup>+</sup>)

-----  
 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

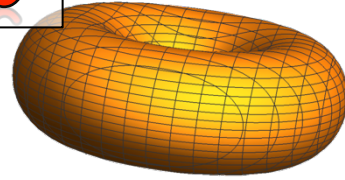
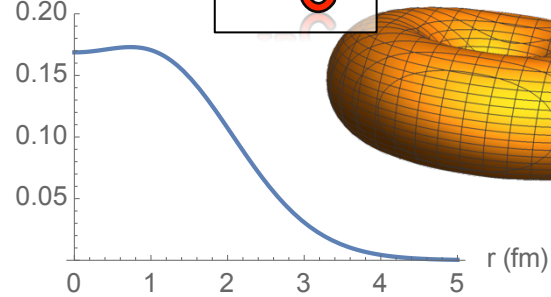


# Carbon isotopes

$\rho(r)$  (fm<sup>-3</sup>)

**<sup>12</sup>C**

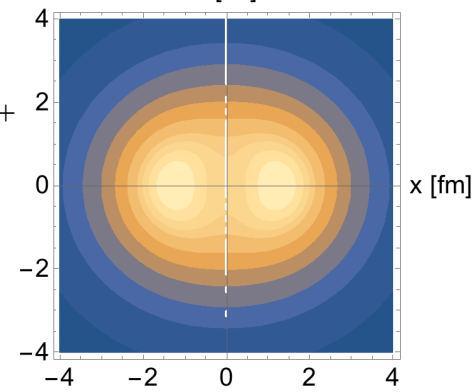
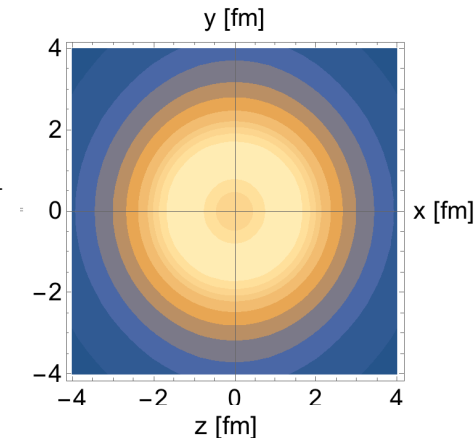
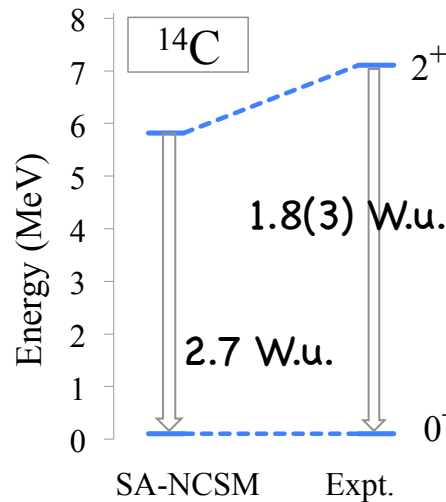
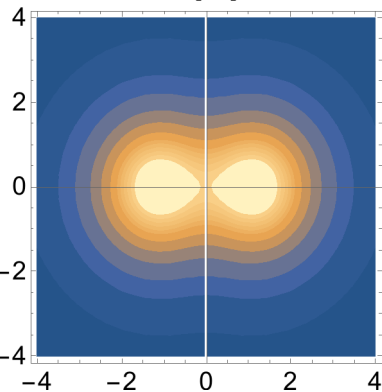
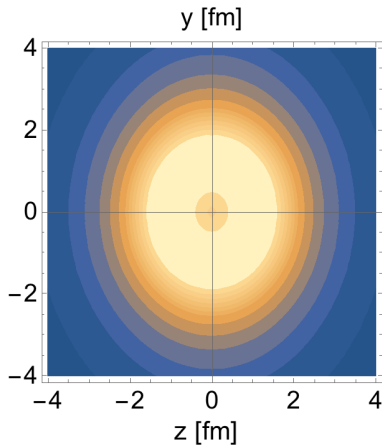
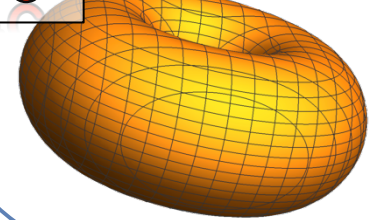
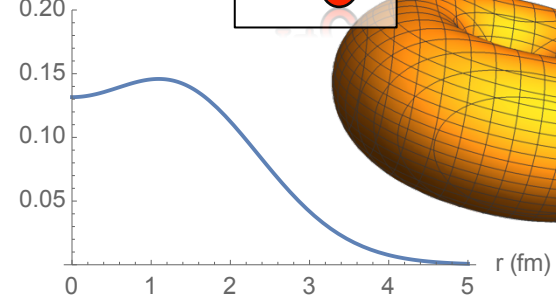
JISP16, hw = 18 MeV



$\rho(r)$  (fm<sup>-3</sup>)

**<sup>14</sup>C**

N2LOopt, hw = 15 MeV

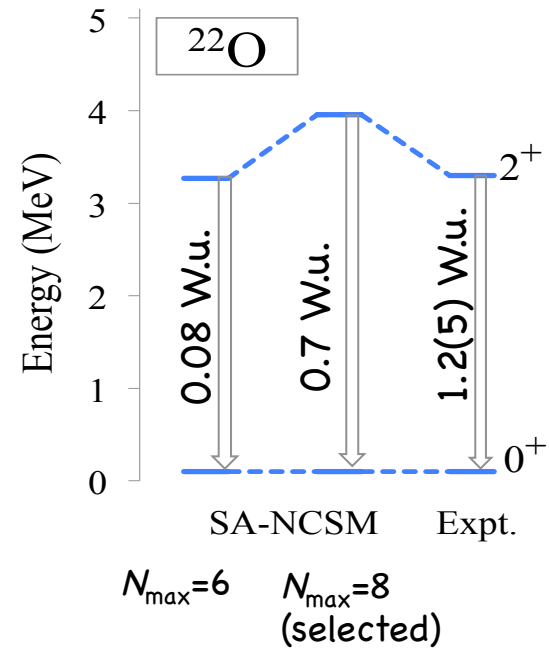
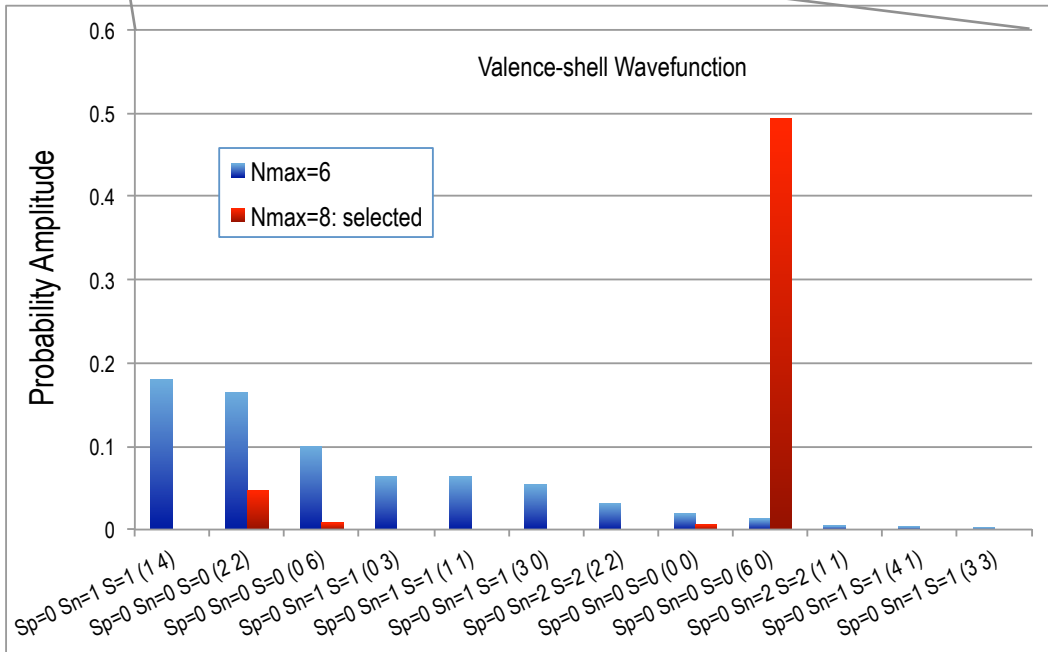
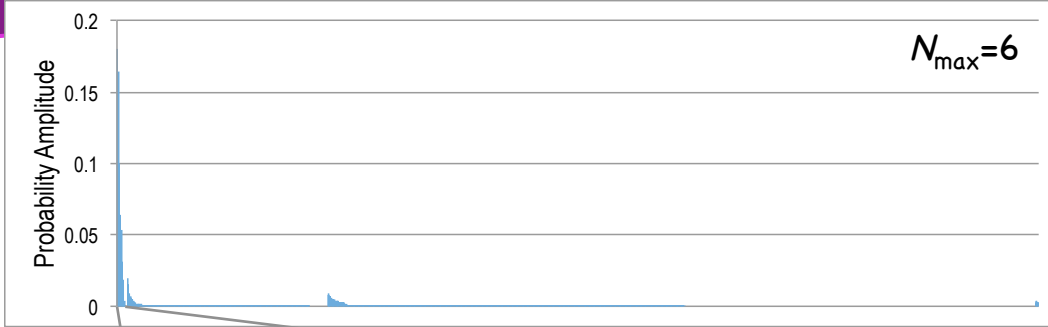
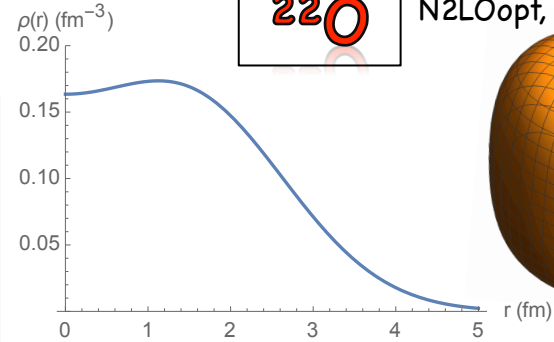


Grigor Sargsyan, PhD student, LSU

# Oxygen isotopes

**22O**

N2LO<sub>opt</sub>, hw = 15 MeV



Grigor Sargsyan, PhD student, LSU

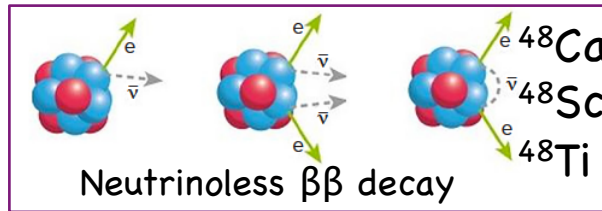
# Structure of Ca-48 and Ti-48

**$^{48}\text{Ca}$**

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



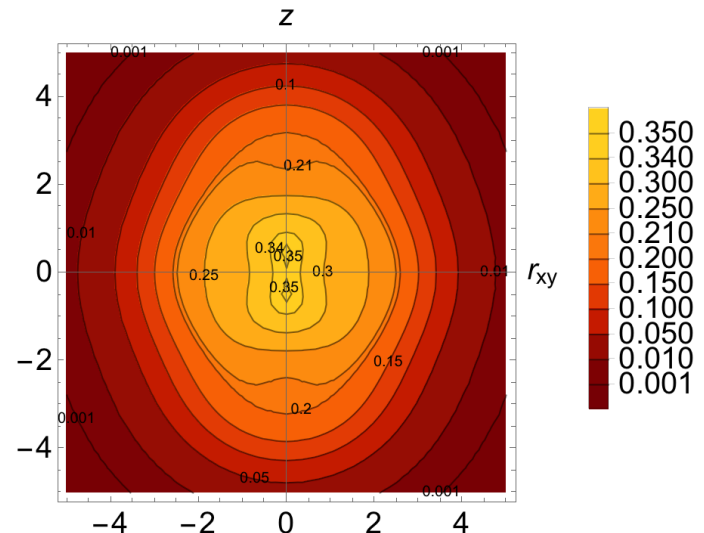
**$^{48}\text{Ti}$**

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

$^{48}\text{Ti}$ ,  $Q(2^+)$  [ $e \text{ fm}^2$ ]  
 -----  
 Experiment..... -17.7  
 8 shells ..... -19.3  
 (no effective charges)



Grigor Sargsyan, PhD student, LSU



# Spectral Distribution Theory: Particle-rank tensors

French ('66), Draayer, Hecht, Kota, ...

3-body interaction (scalar partitioning)

$$H(3) = \binom{A}{3} \mathcal{H}^{(3)}(0) + \binom{A-1}{2} \mathcal{H}^{(3)}(1) + (A-2) \mathcal{H}^{(3)}(2) + \mathcal{H}^{(3)}(3).$$

Depend on  $A$ ,  
model-space dimension

Centroids

$$\mathcal{H}^{(3)}(0) = \frac{1}{3!} \frac{1}{\binom{N}{3}} D^3 H(3) \equiv W_c^{(3)}, \quad \mathcal{H}^{(3)}(1) = \frac{1}{2!} \frac{1}{\binom{N-2}{2}} \left( D^2 H(3) - \frac{A}{N} D^3 H(3) \right),$$

$$\mathcal{H}^{(3)}(2) = \frac{1}{N-4} \left( DH(3) - \frac{A-1}{N-2} D^2 H(3) + \frac{1}{2} \frac{\binom{A}{2}}{\binom{N-1}{2}} D^3 H(3) \right),$$

$$\mathcal{H}^{(3)}(3) = H(3) - \frac{A-2}{N-4} DH(3) + \frac{1}{2} \frac{\binom{A-1}{2}}{\binom{N-3}{2}} D^2 H(3) - \frac{1}{3!} \frac{\binom{A}{3}}{\binom{N-2}{3}} D^3 H(3).$$

Particle-rank tensors  
(effective  
0-,1-,2-,3-body)

Depends on *interaction*:

$$D^3 H(3) = \left( \sum_{ijq} W_{ijqiq} \right), \quad D^2 H(3) = \sum_{ir} \left( \sum_{jq} W_{ijqrjq} \right) a_i^\dagger a_r, \quad DH(3) = \frac{1}{4} \sum_{ijrs} \left( \sum_q W_{ijqrsq} \right) a_i^\dagger a_j^\dagger a_s a_r.$$

For  $NNN$ : Launey et al., Phys. Rev. C 85 (2012) 044003

For  $NN$ : Launey et al., Comput. Phys. Commun. 185 (2014) 254

# Spectral Distribution Theory: Particle-rank tensors

3-body interaction (scalar partitioning)

$$H(3) = \binom{A}{3} \mathcal{H}^{(3)}(0) + \binom{A-1}{2} \mathcal{H}^{(3)}(1) + (A-2) \mathcal{H}^{(3)}(2) + \mathcal{H}^{(3)}(3).$$

For given  $T$   
(isoscalar partitioning)

$$H_{mon} \equiv \frac{W_{2,0} + 3W_{2,1}}{4} \binom{\hat{n}}{2} + \frac{W_{2,1} - W_{2,0}}{2} (\mathbf{T}^2 - \frac{3}{4}\hat{n}) \leftarrow NN$$

$$+ \frac{W_{3,\frac{1}{2}} + W_{3,\frac{3}{2}}}{2} \binom{\hat{n}}{3} + \frac{W_{3,\frac{3}{2}} - W_{3,\frac{1}{2}}}{3} (\hat{n} - 2) (\mathbf{T}^2 - \frac{3}{4}\hat{n}) \leftarrow NNN$$

For  $NNN$ : Launey et al., Phys. Rev. C 85 (2012) 044003

For  $NN$ : Launey et al., Comput. Phys. Commun. 185 (2014) 254

# Spectral Distribution Theory: Particle-rank tensors

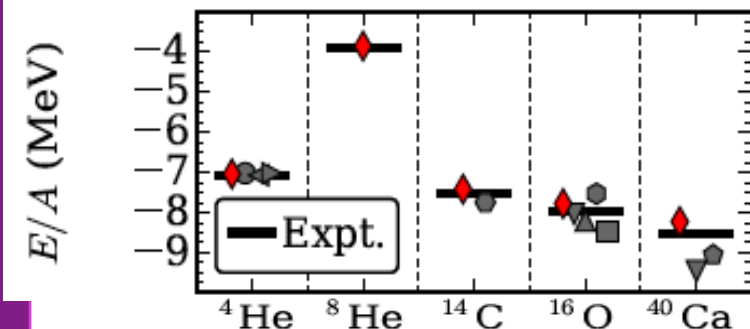
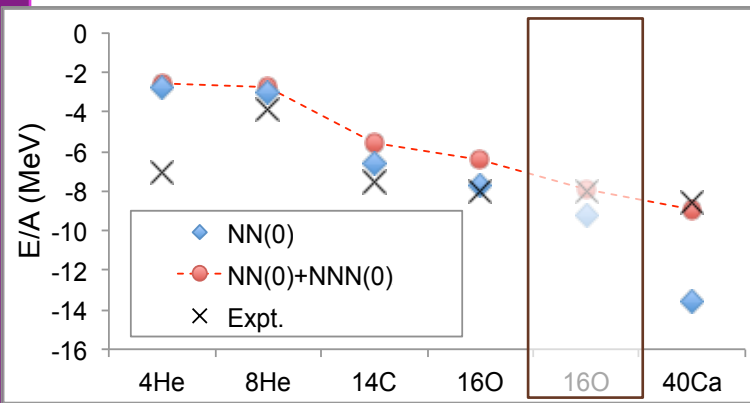
3-body interaction (scalar partitioning)

$$H(3) = \binom{A}{3} \mathcal{H}^{(3)}(0) + \binom{A-1}{2} \mathcal{H}^{(3)}(1) + (A-2) \mathcal{H}^{(3)}(2) + \mathcal{H}^{(3)}(3).$$

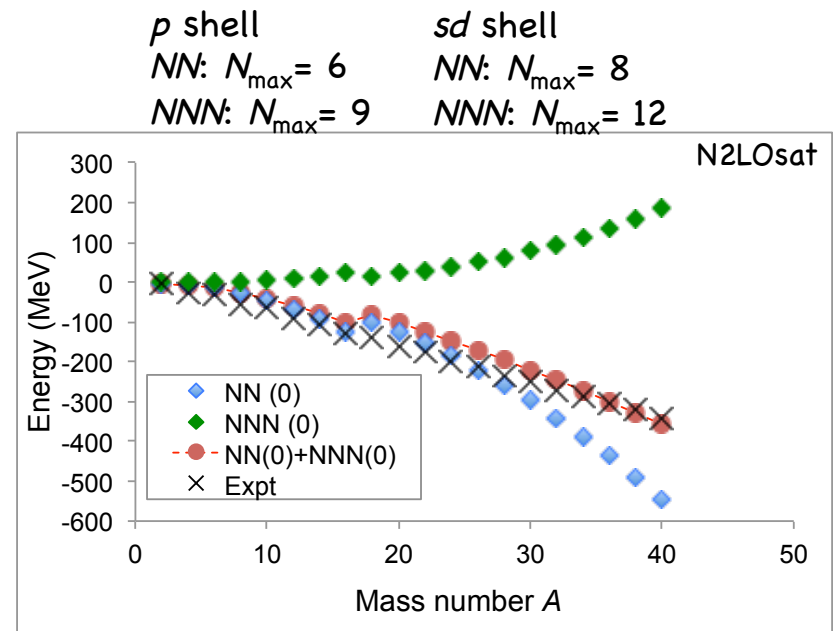
For given  $T$   
(isoscalar partitioning)

$$H_{mon} \equiv \frac{W_{2,0} + 3W_{2,1}}{4} \binom{\hat{n}}{2} + \frac{W_{2,1} - W_{2,0}}{2} (T^2 - \frac{3}{4}\hat{n}) \quad NN$$

$$+ \frac{W_{3,1/2} + W_{3,3/2}}{2} \binom{\hat{n}}{3} + \frac{W_{3,3/2} - W_{3,1/2}}{3} (\hat{n} - 2)(T^2 - \frac{3}{4}\hat{n}). \quad NNN$$



Ekström et al., Phys. Rev. C 91, 051301(R) (2015)



# Spectral Distribution Theory: Particle-rank tensors

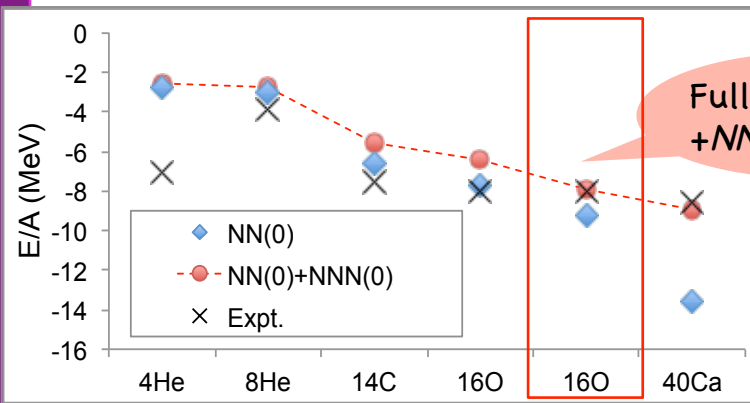
3-body interaction (scalar partitioning)

$$H(3) = \binom{A}{3} \mathcal{H}^{(3)}(0) + \binom{A-1}{2} \mathcal{H}^{(3)}(1) + (A-2) \mathcal{H}^{(3)}(2) + \mathcal{H}^{(3)}(3).$$

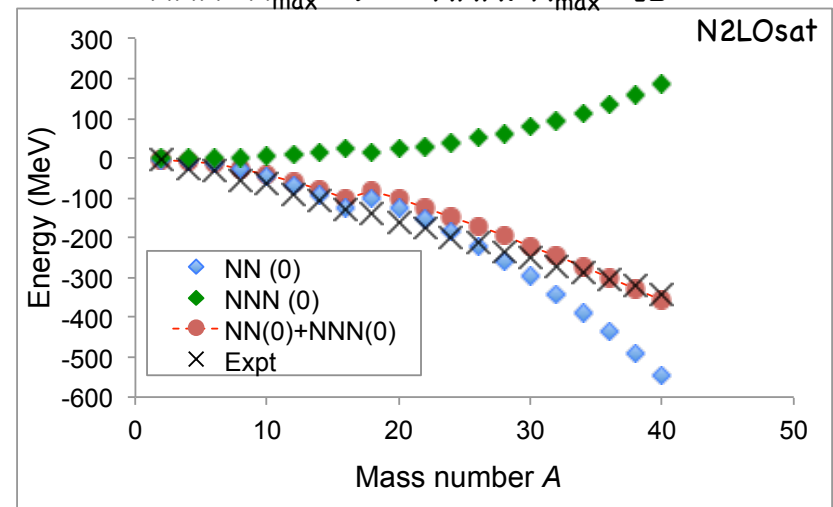
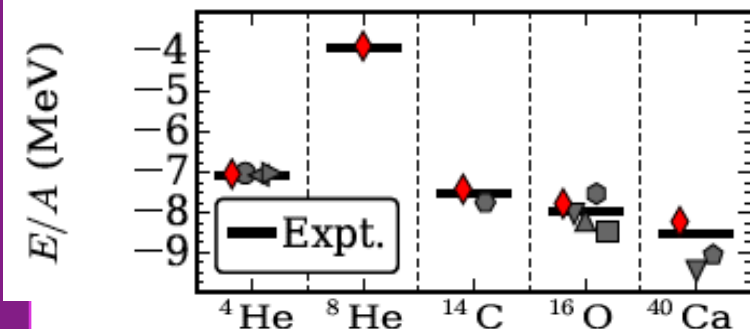
For given  $T$   
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$$H_{mon} \equiv \frac{W_{2,0} + 3W_{2,1}}{4} \binom{\hat{n}}{2} + \frac{W_{2,1} - W_{2,0}}{2} (T^2 - \frac{3}{4}\hat{n}) \quad NN$$

$$+ \frac{W_{3,1/2} + W_{3,3/2}}{2} \binom{\hat{n}}{3} + \frac{W_{3,3/2} - W_{3,1/2}}{3} (\hat{n} - 2)(T^2 - \frac{3}{4}\hat{n}). \quad NNN$$



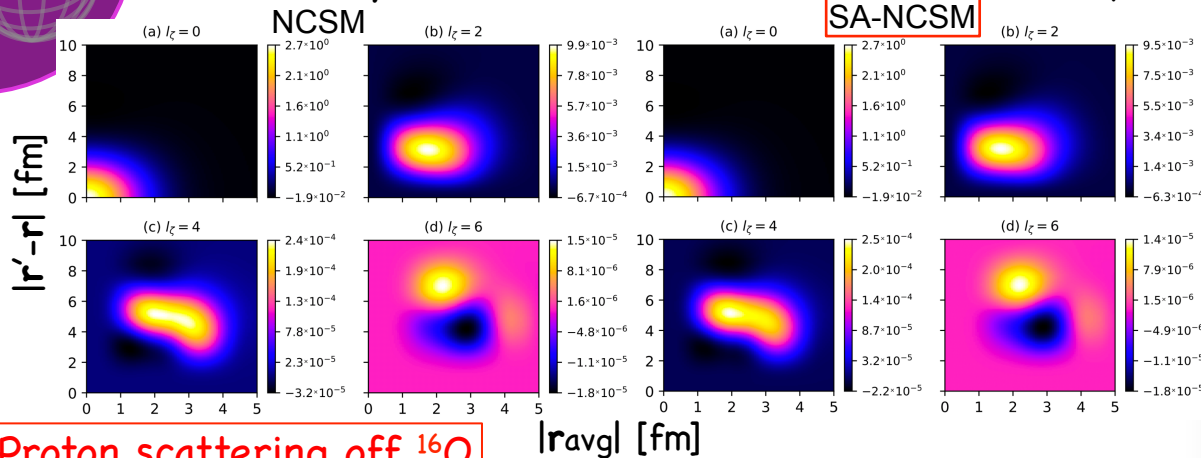
*p* shell      *sd* shell  
 NN:  $N_{max}=6$       NN:  $N_{max}=8$   
 NNN:  $N_{max}=9$       NNN:  $N_{max}=12$



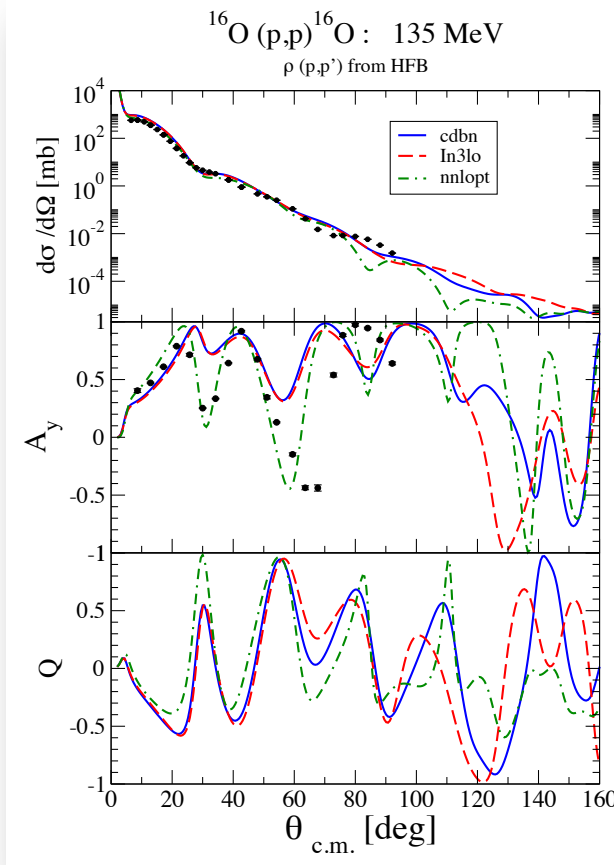
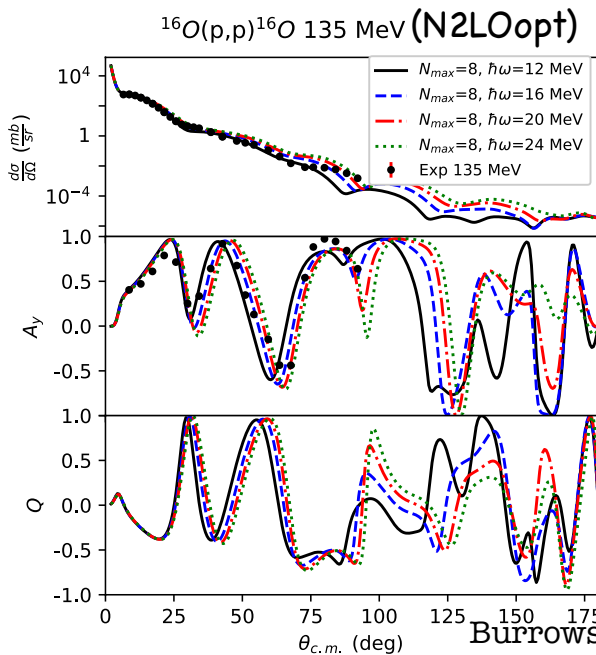
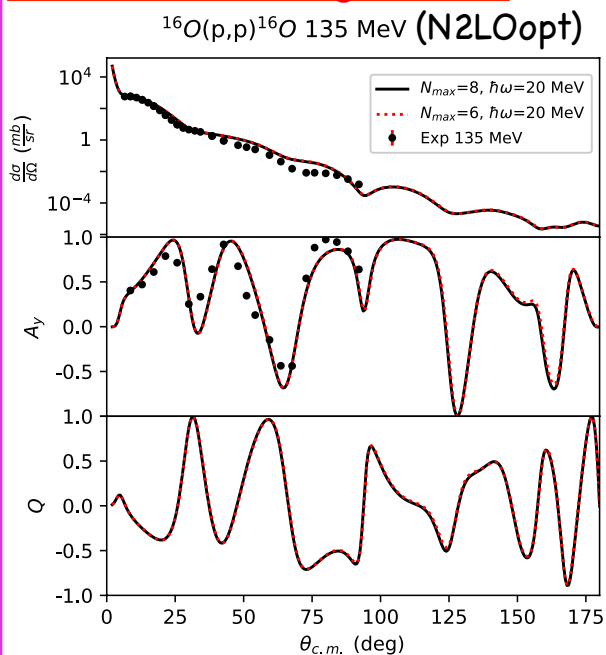
Ekström et al., Phys. Rev. C 91, 051301(R) (2015)

# Features of NN interactions

${}^6\text{Li}$ , Non-local densities N2LOopt



Proton scattering off  ${}^{16}\text{O}$



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

# Spectral Distribution Theory: Particle-rank tensors

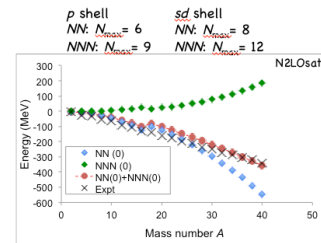
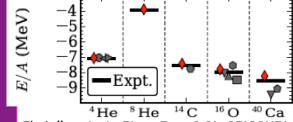
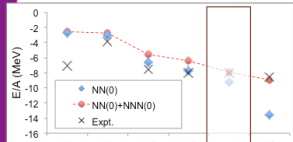
3-body interaction (scalar partitioning)

$$H(3) = \binom{A}{3} \mathcal{H}^{(3)}(0) + \binom{A-1}{2} \mathcal{H}^{(3)}(1) + (A-2) \mathcal{H}^{(3)}(2) + \mathcal{H}^{(3)}(3)$$

For given  $T$  (isoscalar partitioning)

$$H_{mon} \equiv \frac{W_{2,0} + 3W_{2,1} \binom{\tilde{n}}{2} + W_{2,1} - W_{2,0} (T^2 - \frac{3}{4} \tilde{n})}{4} \quad N\bar{N}$$

$$+ \frac{W_{3,3/2} + W_{3,3/2} \binom{\tilde{n}}{3} + W_{3,3/2} - W_{3,3/2} (\tilde{n} - 2)(T^2 - \frac{3}{4} \tilde{n})}{2} \quad N\bar{N}\bar{N}$$



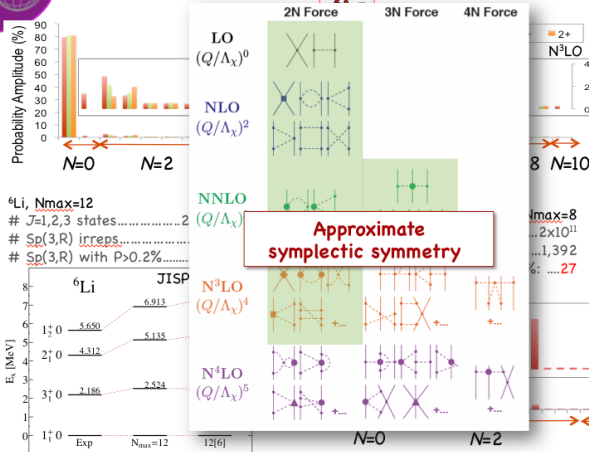
Ekström et al, Phys. Rev. C 91, 051301(R) (2015)

Progress in *Ab Initio* Techniques in Nuclear Physics TRIUMF, February 28, 2018

Collectivity and clustering from the SA-NCSM

## Binding energies with isospin-averaged 3-body interactions

### Preference of Nature



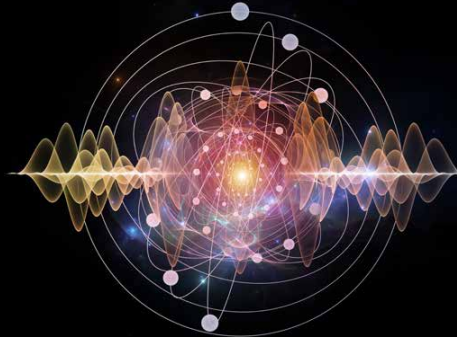
Approximate symplectic symmetry

Simple physics: "shape" + vibrations + rotations

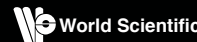
# Conclusions

## EMERGENT PHENOMENA IN ATOMIC NUCLEI FROM LARGE-SCALE MODELING

A Symmetry-Guided Perspective



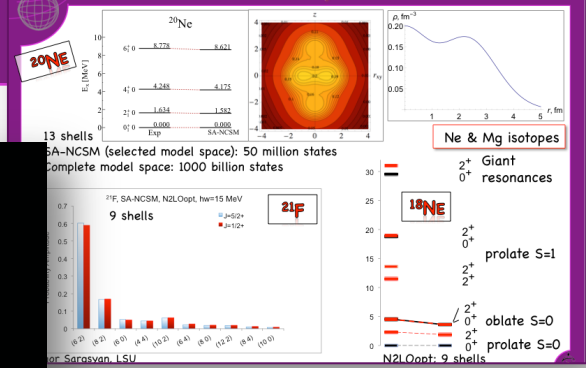
Kristina D Launey



- J. L. Wood
- C. W. Johnson
- D. J. Rowe
- J. E. Escher
- D. Lee
- Y. Alhassid

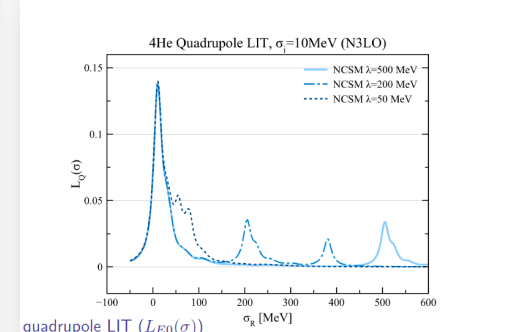
- T. Luu & A. Shindler
- Y. Suzuki & W. Horiuchi
- J. P. Draayer & T. Dytrych
- G. Rosensteel
- F. Pan & X. Guan

### intermediate-mass nuclei (sd-shell) Collectivity features



Collective and alpha clustering features in nuclei (see Ali Dreyfuss' poster)

Preliminary Results: <sup>4</sup>He



Sum rules : LSR+SA-NCSM (Nir Nevo Dinur 's talk)

