

# Ab initio symmetry-adapted no-core shell-model results for intermediate- and medium-mass nuclei

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... LSU Team ...

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

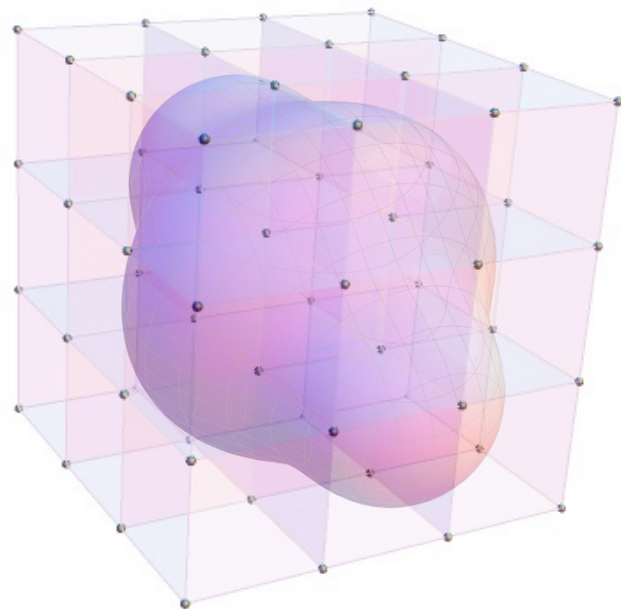
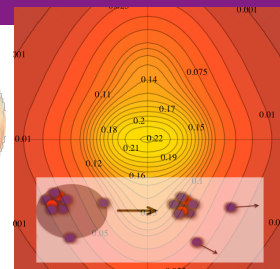
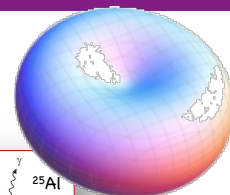
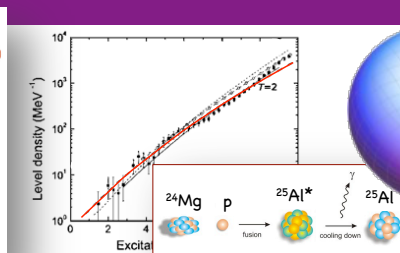
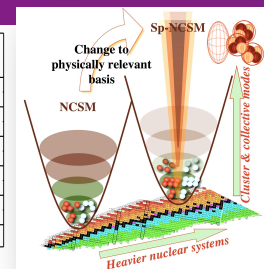
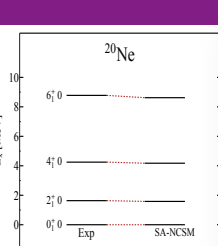
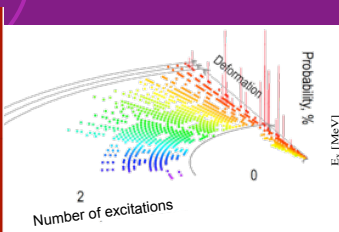
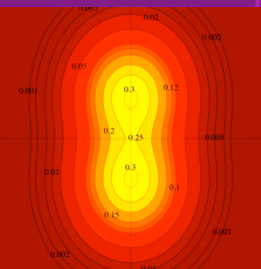
Supported by NSF & DOE-EPSCoR



HPC Resources

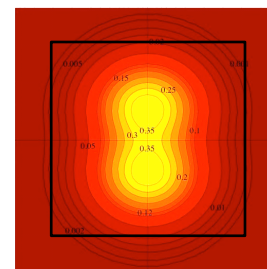
NSF/U. of Illinois ...BlueWaters

LSU...SuperMike-II



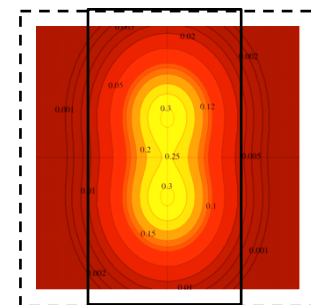
**NCSM**

Total HO quanta  
 $N_{\max}$



**SA-NCSM**

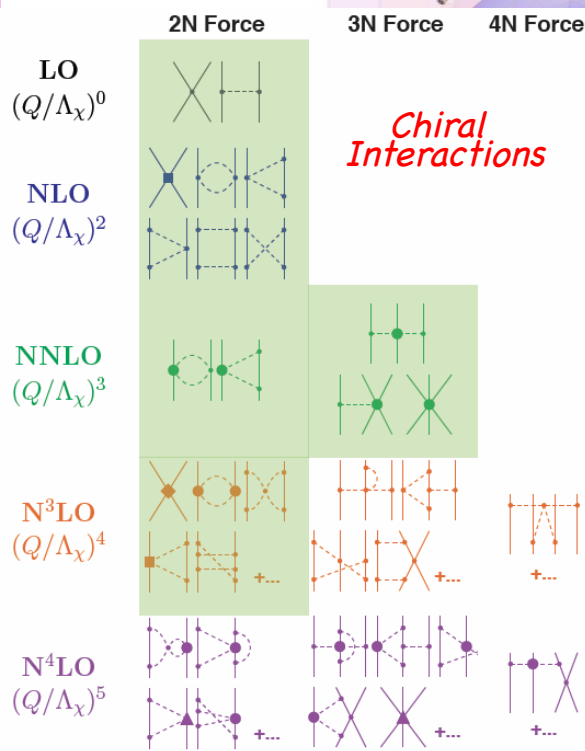
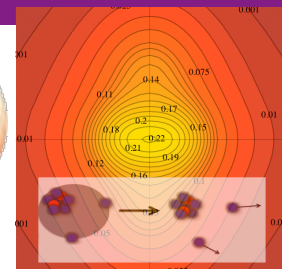
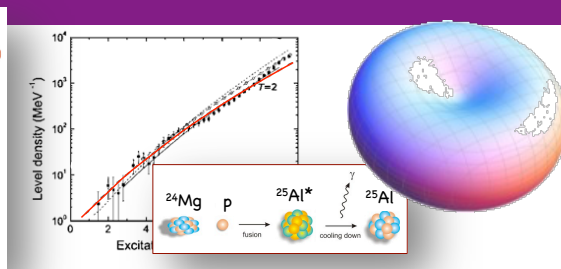
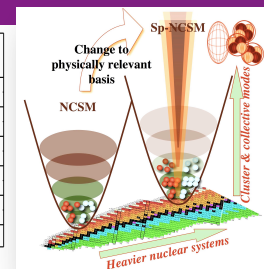
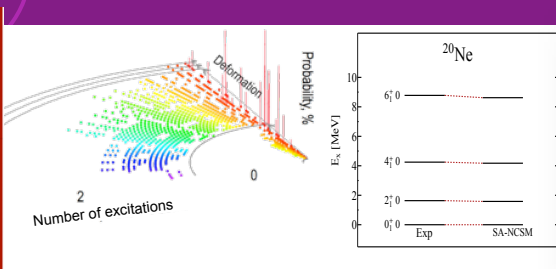
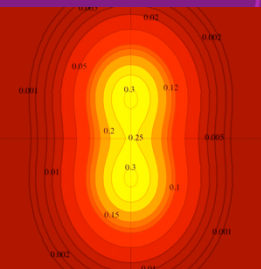
Total HO quanta  
 $N_{\max} + 1$   
Distribution:  
z, x, y



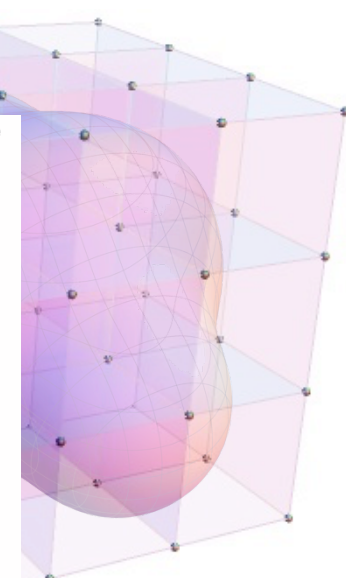
Dytrych et al., Phys. Rev. Lett. 111 (2013) 252501

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

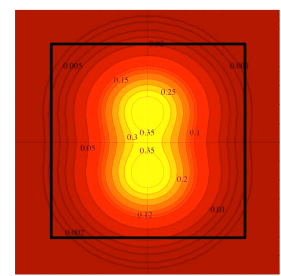
*Ab initio* SA-NCSM results for intermediate- and medium-mass nuclei -- K. Launey



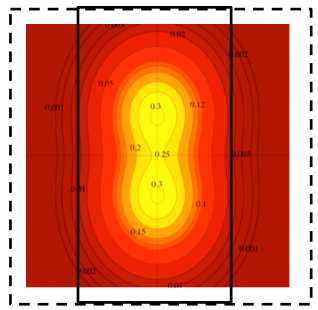
*Chiral Interactions*



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



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

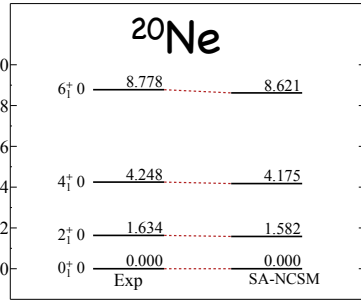
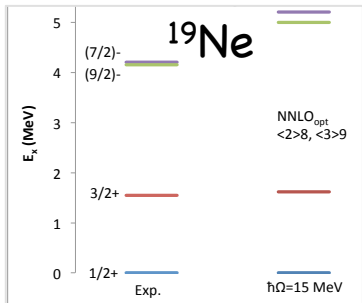
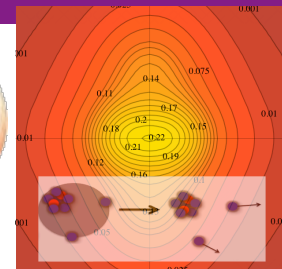
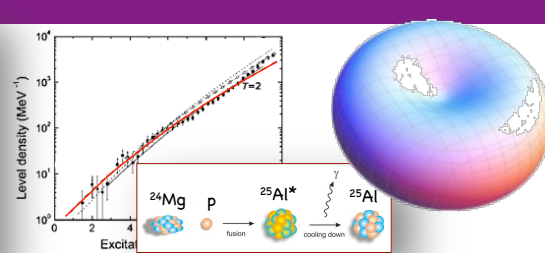
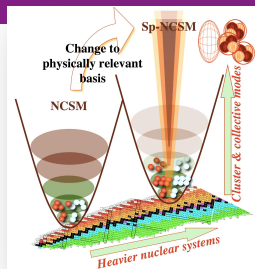
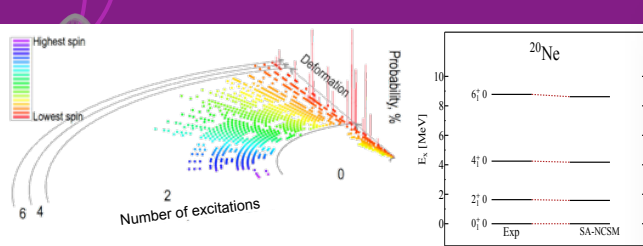


Weinberg, van Kolck, Machleidt, Entem, Meissner, Epelbaum, Krebs, Bernard,... (from A. Calci)

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

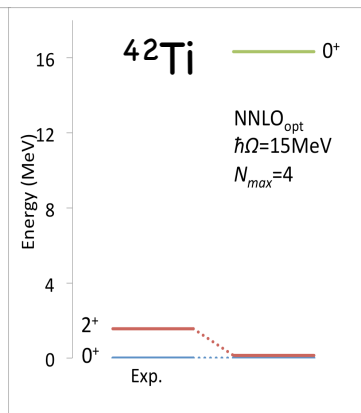
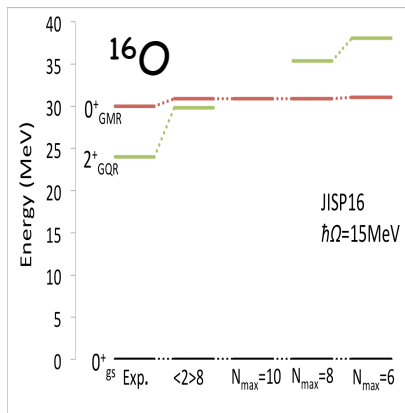
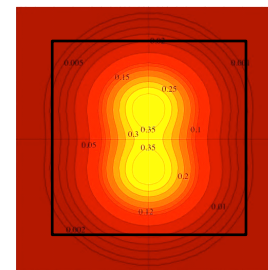






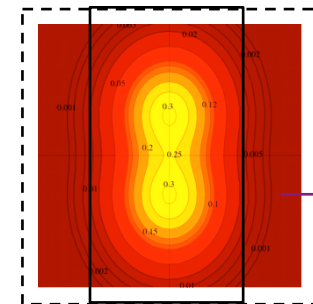
SU(3) basis

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



Symplectic  
Sp(3,R) basis

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

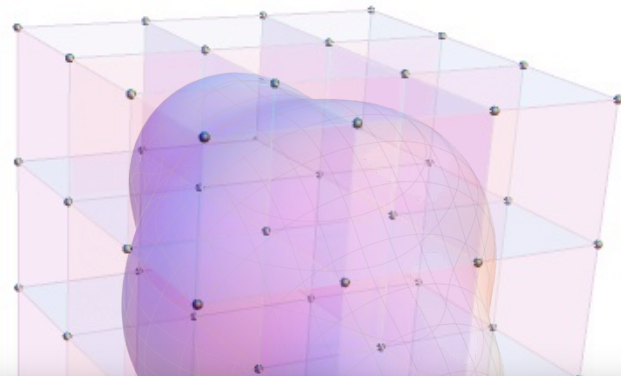
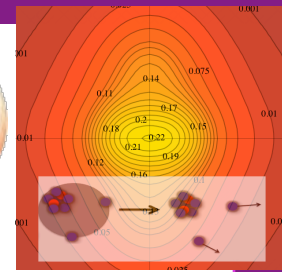
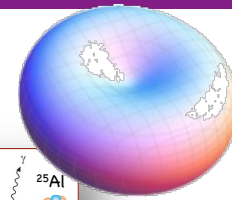
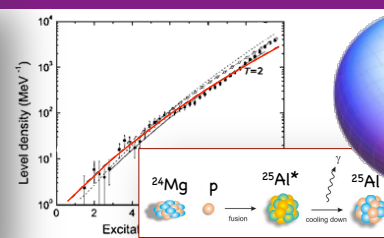
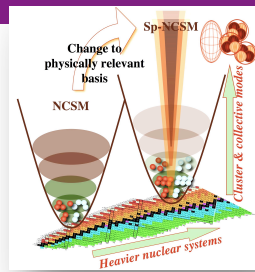
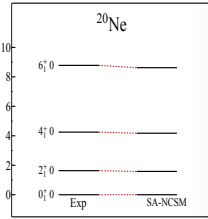
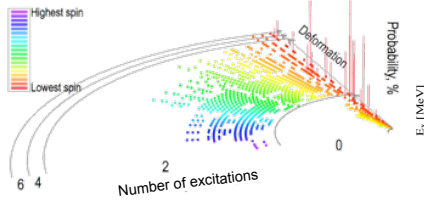


Describes deformation ← Symmetry-adapted: SU(3), Sp(3,R) → Guided by Symplectic symmetry

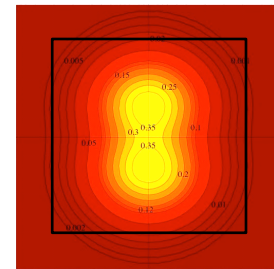
LSU code (LSU3shell): [sourceforge.net/projects/lsu3shell](https://sourceforge.net/projects/lsu3shell)  
Dytrych et al., Phys. Rev. Lett. 111 (2013) 252501  
Launey et al., Prog. Part. Nucl. Phys. 89 (2016) 101



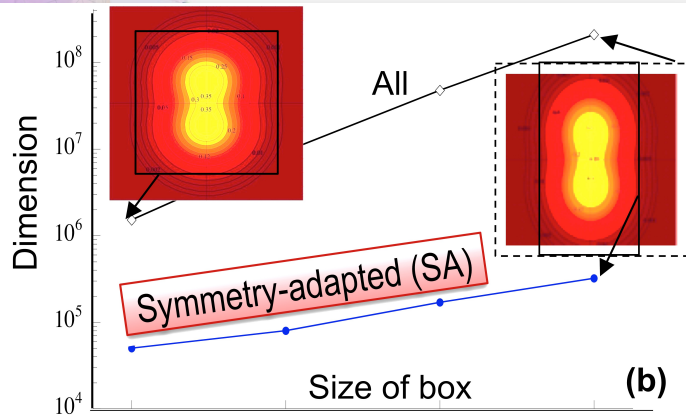
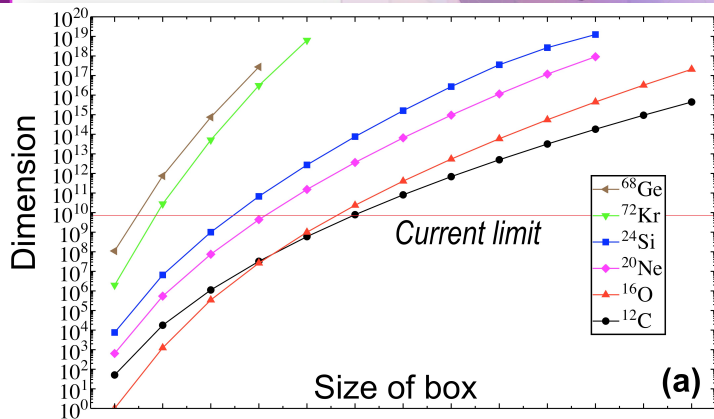
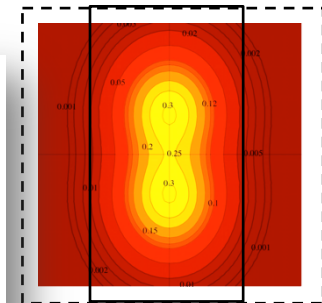




**NCSM**  
Total HO quanta  
 $N_{\text{max}}$



**SA-NCSM**

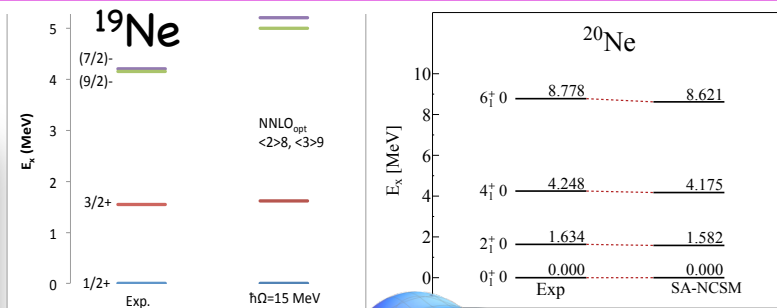
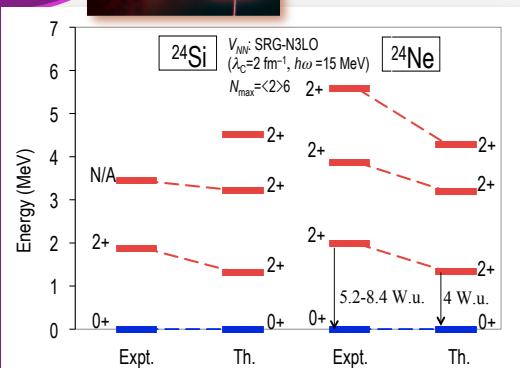


Dytrych et al., Phys. Rev. Lett. 111 (2013) 252501

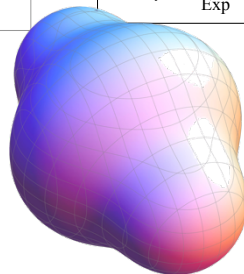
Launey et al., Prog. Part. Nucl. Phys. 89 (2016) 101

*Ab initio* SA-NCSM results for intermediate- and medium-mass nuclei -- K. Launey

# Deformed (in intrinsic frame)...

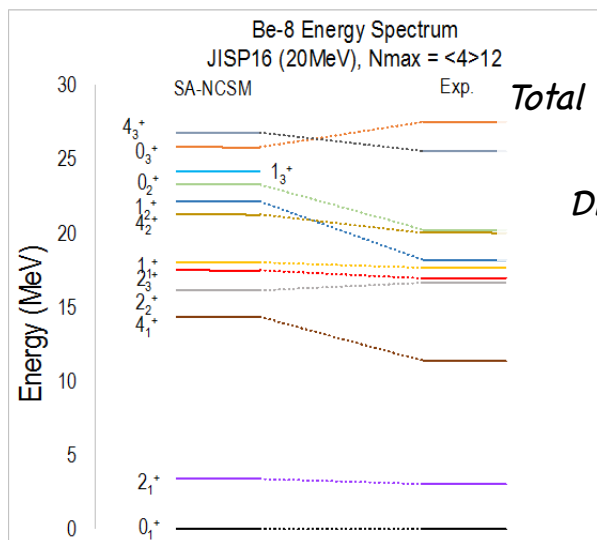
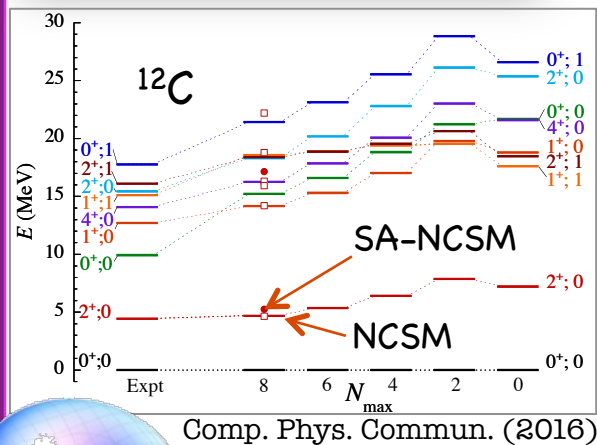
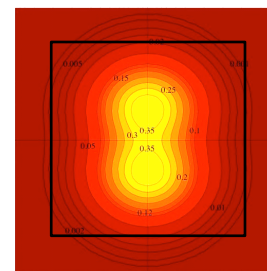


Robert Baker, LSU



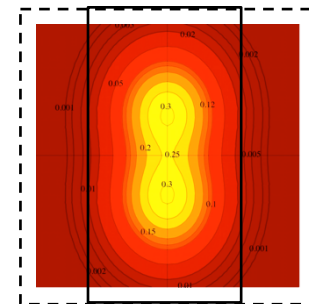
NCSM

Total HO quanta  $N_{\max}$



SA-NCSM

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

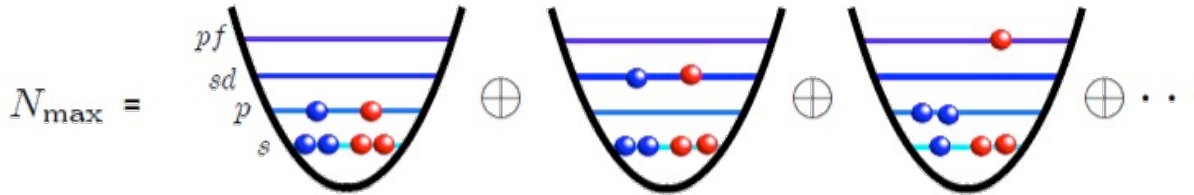


Deformation/collectivity:  
important in nuclear  
wave functions

Harvey Shows, LSU

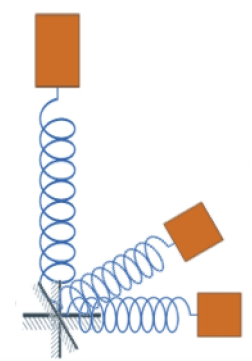
# Symmetry-adapted NCSM (SA-NCSM) ... Basis

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



**SU(3)** is the exact symmetry of 3-D HO

- HO excitations in  $z, x, y$ :  $n_z n_x n_y$
- $(\lambda \mu)$  label an SU(3) configuration - related to *spatial deformation*

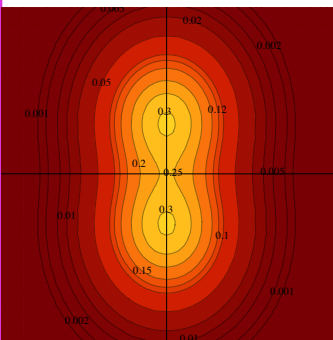
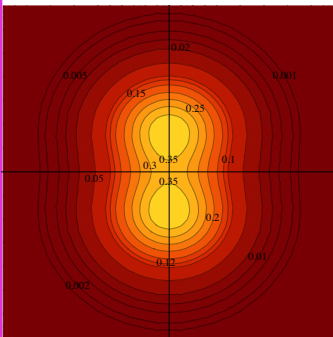


$$\lambda = n_z - n_x; \quad \mu = n_x - n_y$$

E.g.: **Be-8**  $0p-0h(4 0)$  -  $n_z=8, n_x=4, n_y=4$

$0p-0h(4 0)$ ,  
 $N_{\max}=0$

N3LO,  
 $\hbar\Omega=25\text{MeV}$ ,  
 $N_{\max}=8$



A particles in 3-D space:

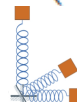
complete basis for the shell model (all linear canonical transformations of the  $3A$ -particle phase space +spin/isospin)

$$\text{Sp}(3(A-1), \mathbb{R}) \quad \times \quad \text{U}(4)$$

$$\cup \quad \cup$$

$$\boxed{\text{Sp}(3, \mathbb{R})} \times \text{O}(A-1) \quad \text{SU}(2)_S \times \text{SU}(2)_T$$

$$\text{Sp}(3, \mathbb{R}) \supset \text{U}(3) \supset \text{SO}(3) \supset \text{SO}(2)$$

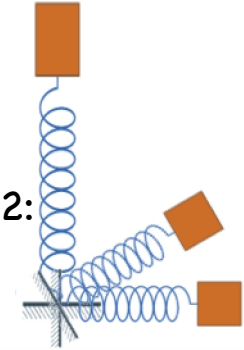
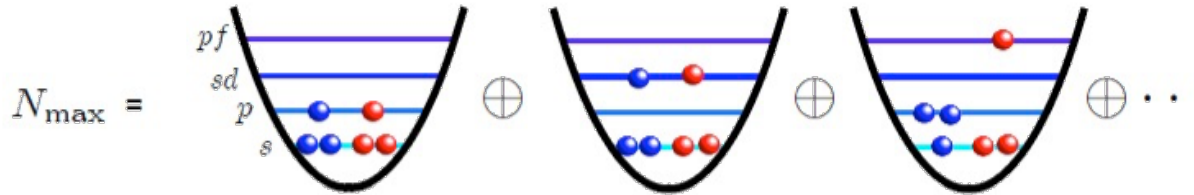
Body-fixed frame 

Lab frame 



# Symmetry-adapted NCSM (SA-NCSM) ... Basis

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



**SU(3) basis states** (unitary transformation from  $m$ -scheme), e.g.  $A=2$ :

$$\frac{1}{N} \left[ a_{(n_1 0)st}^\dagger \times a_{(n_2 0)st}^\dagger \right]^{(\lambda\mu)\kappa(LS)JM;TT_0} |0\rangle \quad [\dots \text{not used}]$$

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

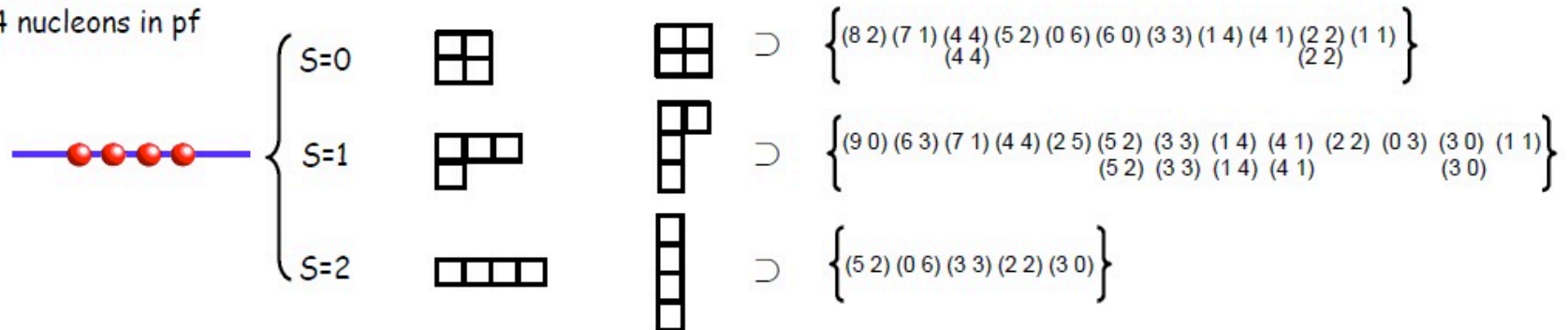
**Fast basis construction!** ... based on Gel'fand patterns

$$\text{quantum labels: } U(2) \otimes U(10) \supset SU(3)$$

$S \quad [f] \quad \alpha \quad (\lambda \mu)$

• Example:

4 nucleons in pf



... followed by multi-shell coupling of SU(3) configurations

Using SU(3) coupling/recoupling coefficients ... analogous to SU(2), but outer/inner multiplicities!

# SA-NCSM ... NN Interaction

**SU(3)** tensors of NN interaction  $\langle (\chi\omega ST)_f \| V^{\omega_0 S_0 T_0=0} \| (\chi\omega ST)_i \rangle_{\rho_0}$

$$= (-)^{S_f+S_0} \Pi_{T S_0} \frac{\dim \omega_0}{\dim \omega_f} \sum_{J(\kappa L)_{if}} \begin{Bmatrix} L_f & S_f & J \\ S_i & L_i & S_0 \end{Bmatrix} \langle \omega_i \kappa_i L_i; \omega_0 \kappa_0 L_0 \| \omega_f \kappa_f L_f \rangle_{\rho_0} \times$$

$n_r \downarrow n_s \downarrow (\lambda \downarrow \mu)$

$$(-)^{L_i+J} \Pi_{J^2 L_f} \Pi_{L_i L_f S_i S_f} \sum_{\substack{l_r, l_s, l_t, l_u \\ j_r, j_s, j_t, j_u}} \sqrt{\frac{(1+\delta_{rs})(1+\delta_{tu})}{(1+\delta_{\eta_r \eta_s})(1+\delta_{\eta_t \eta_u})}} \langle (\eta_r 0) l_r; (\eta_s 0) l_s \| (\omega \kappa L)_f \rangle \times$$

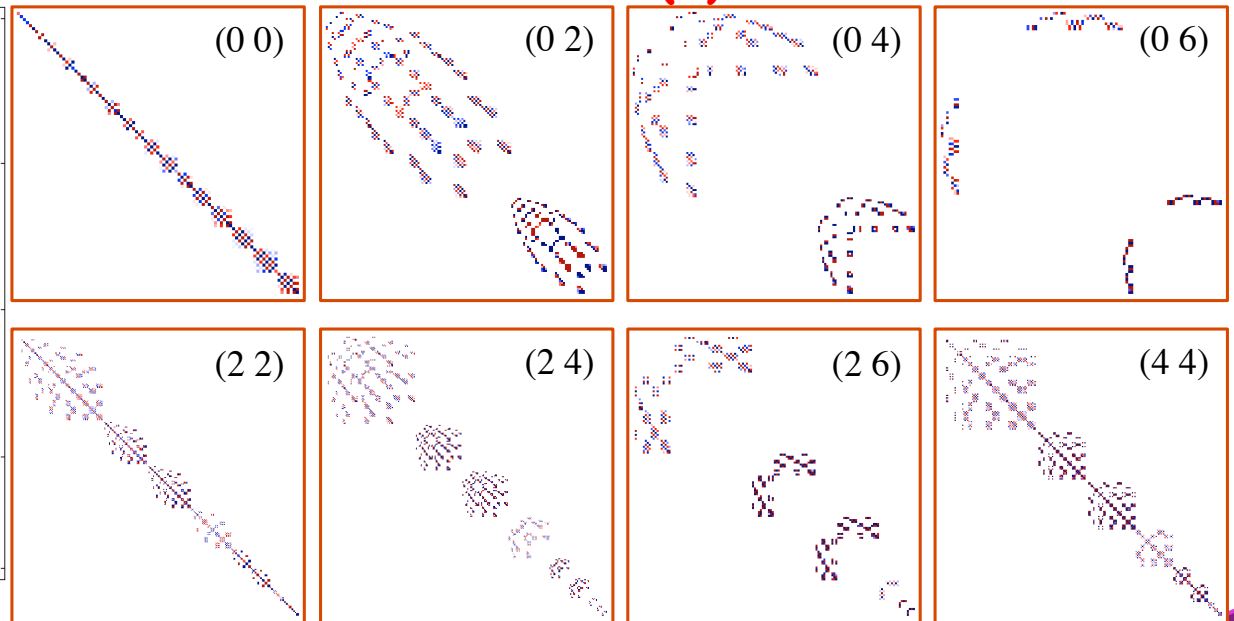
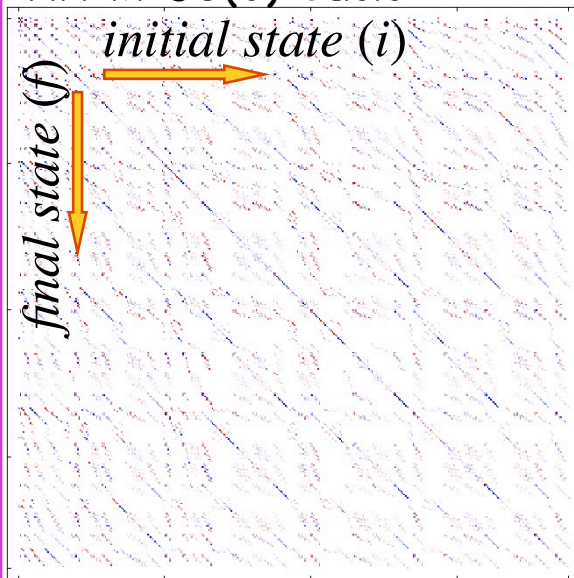
$$\Pi_{j_r j_s j_t j_u} \langle (\eta_t 0) l_t; (\eta_u 0) l_u \| (\omega \kappa L)_i \rangle \begin{Bmatrix} l_r & \frac{1}{2} & j_r \\ l_s & \frac{1}{2} & j_s \\ L_f & S_f & J \end{Bmatrix} \begin{Bmatrix} l_t & \frac{1}{2} & j_t \\ l_u & \frac{1}{2} & j_u \\ L_i & S_i & J \end{Bmatrix} V_{rstu}^\Gamma$$

$\rightarrow$  *jj-coupled NN*

**NN SU(3) Tensors**

N3LO ( $N_{\max}=6$ )  
 $\hbar\Omega = 11$  MeV

NN in SU(3) basis

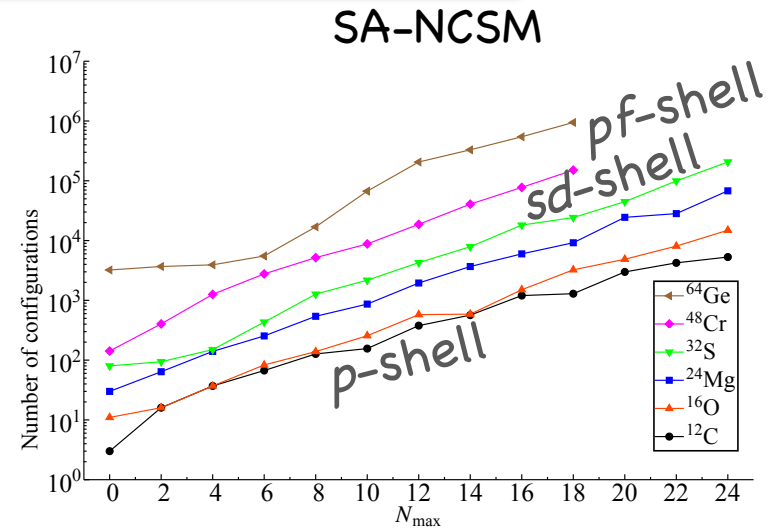
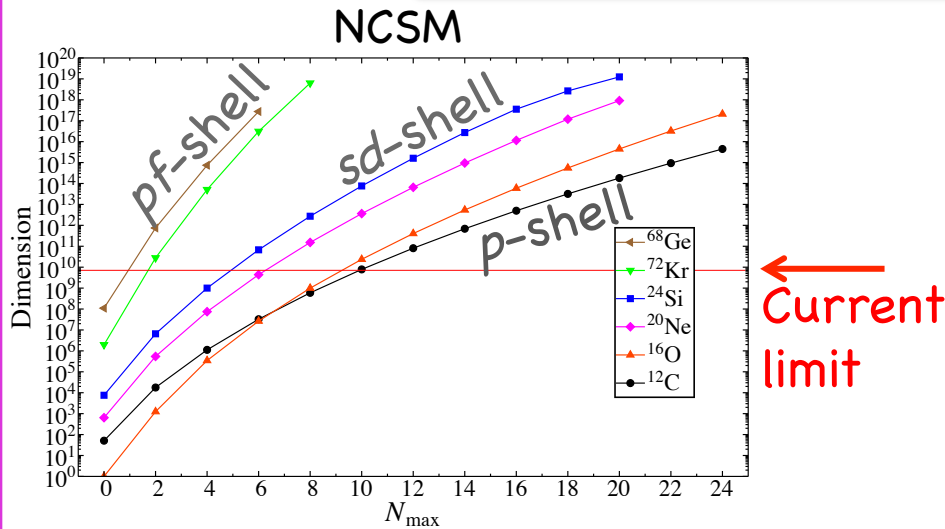


# SA-NCSM ... Hamiltonian

## SA-NCSM:

- **SU(3)-coupled basis** – fast construction (Gel'fand patterns)
- **NN interaction SU(3) tensors** – generated once per interaction
- **Hamiltonian** –
  - Wigner-Eckart theorem ... reduced matrix elements (rme's)
  - Decoupling to single-shell tensors  $T_{n_1 n_2 n_1 n_1} \rightarrow T_{n_2} \times T_{n_1 n_1 n_1}$
  - Important pieces of information ... single-shell rme's

Important pieces of information (memory requirement)



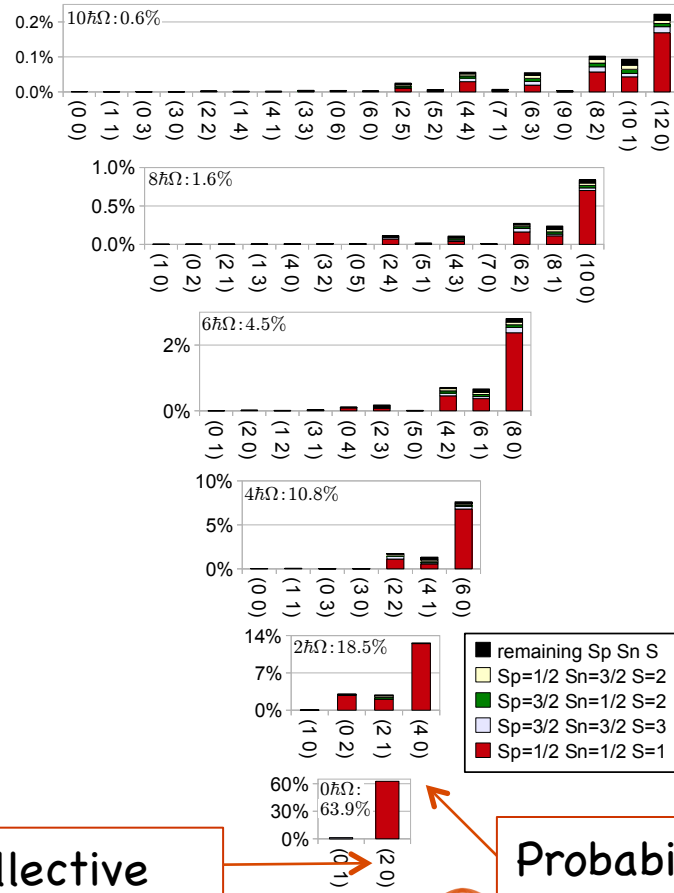
**INFORMATION REDUCTION**



# Preference of Nature

**<sup>6</sup>LI** JISP16,  
complete model space

From first principles:  
**light/intermediate-mass nuclei,**  
low-lying states

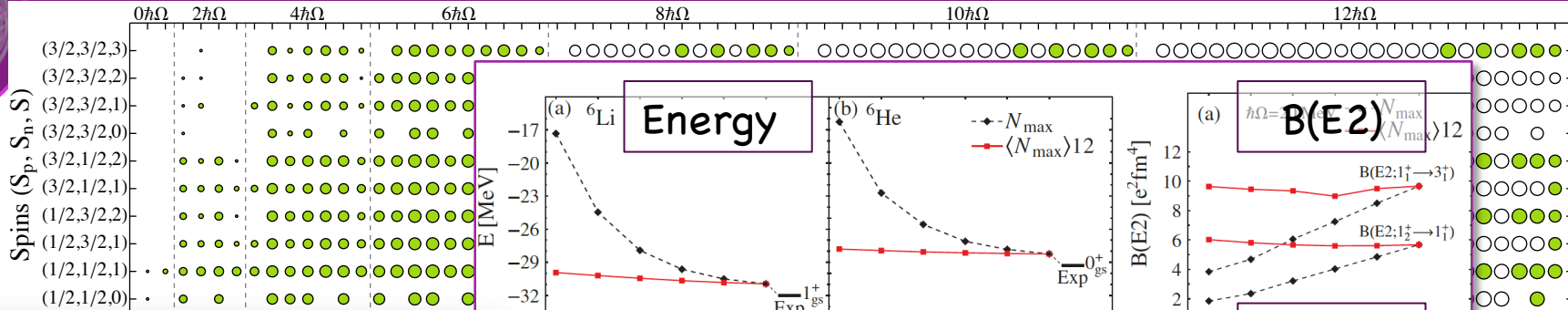


Collective modes

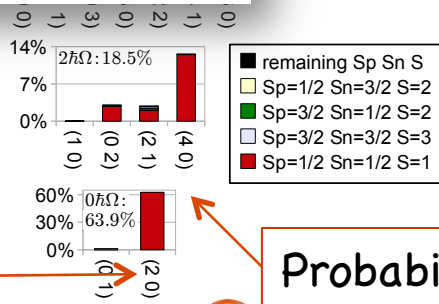
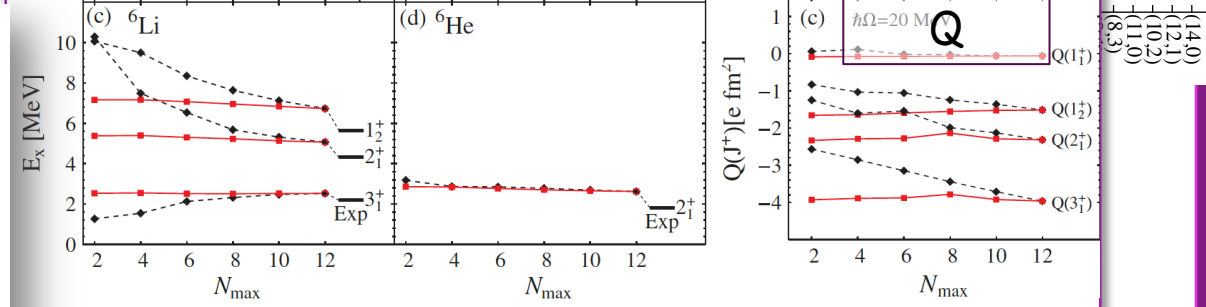
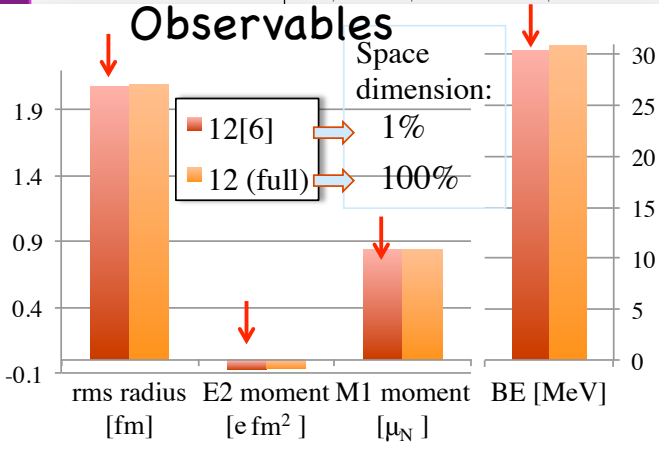
Probability (%)



# Preference of Nature

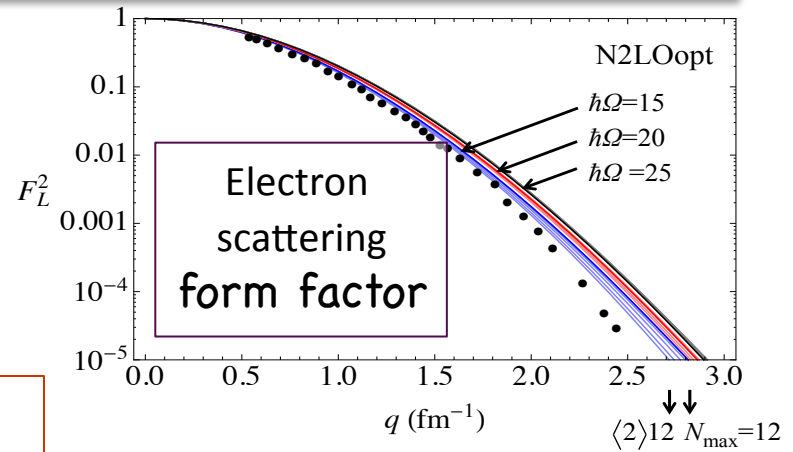


## Observables



Collective modes

Probability (%)



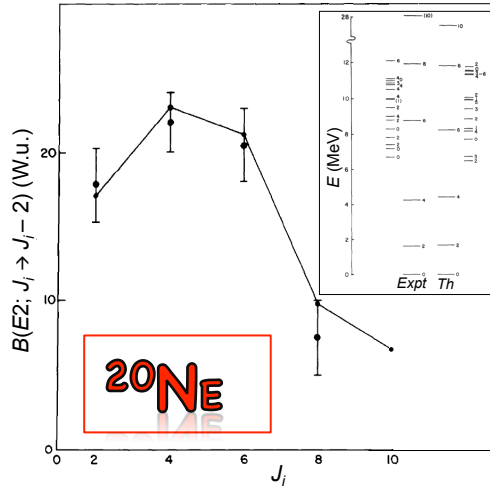
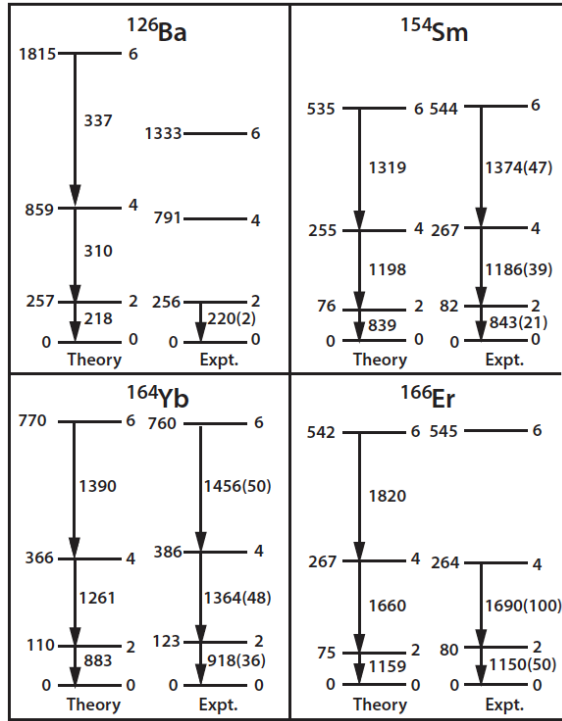
Launey et al., Prog. Part. Nucl. Phys. 89 (2016) 101;  
Dytrych et al., Phys. Rev. C 91 (2015) 024326

Ab initio SA-NCSM results for intermediate- and medium-mass nuclei -- K. Launey



# 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,  $Sp(3,R)$**

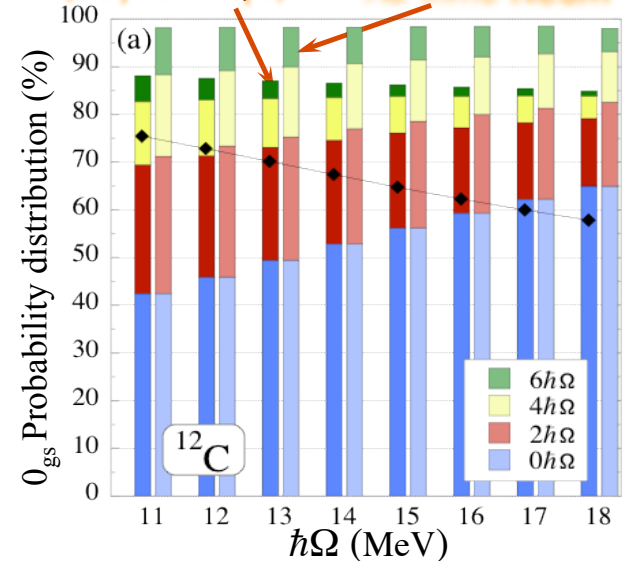
Rowe, Rosensteel, Draayer, Hecht, Suzuki, Escher, Bahri, ...

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

Symplectic basis

(only 2 irreps)

*Ab initio* NCSM

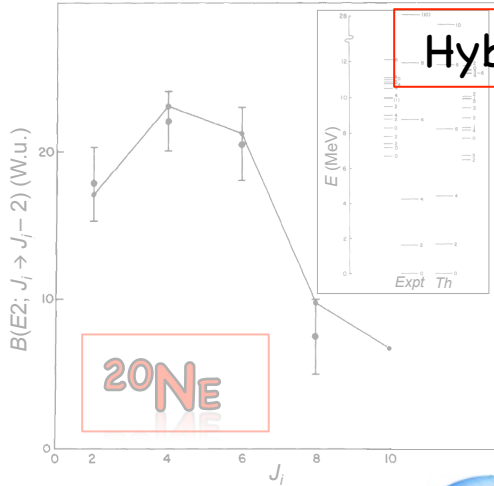
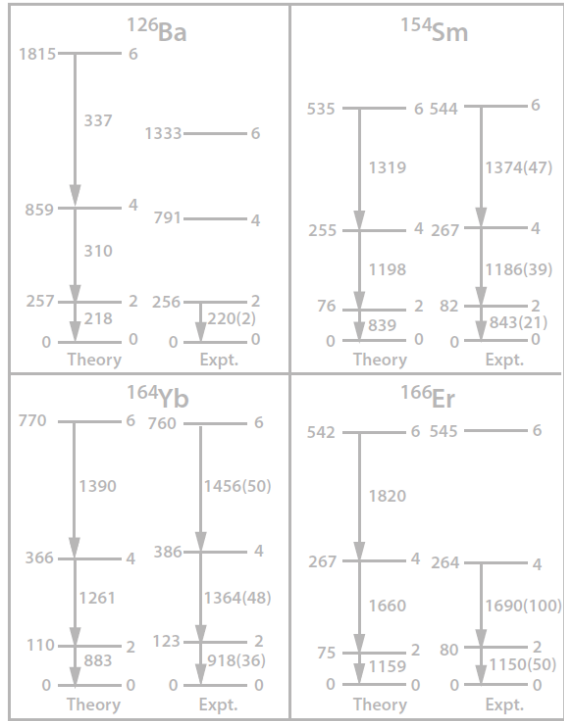


Dytrych, Launey, Bahri, Draayer, Vary,  
Phys. Rev. Lett. 98 (2007) 162503



# Earlier studies ... algebraic models

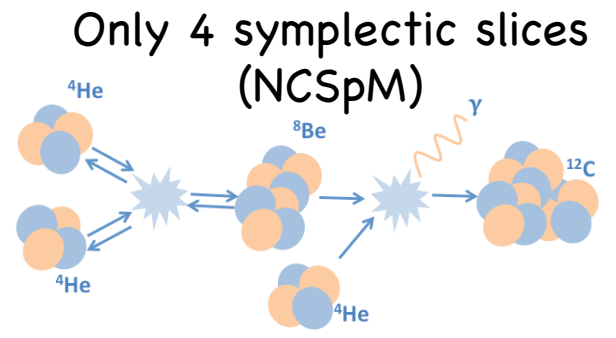
Quite successful, but symmetries are assumed *a priori*:  
Typically 1 (a few) irrep(s) + symmetry-preserving interaction



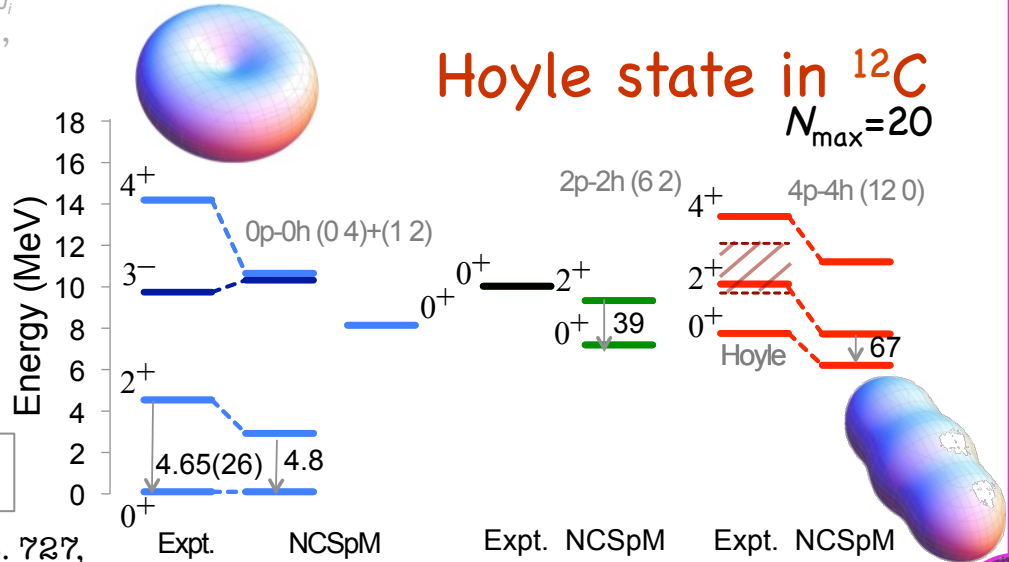
J. Draayer, et al.,  
Nucl. Phys. A4.  
(1984)

No effect

Hybrid: JISP16 (NM) + schematic (mM)



Hoyle state in <sup>12</sup>C  
 $N_{max}=20$



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

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

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

Dreyfuss et al., Phys. Lett. B. 727,  
511 (2013)

*Ab initio* SA-NCSM results for intermediate-  
and medium-mass nuclei -- K. Launey



# What can we learn from *ab initio* modeling?

SA-NCSM

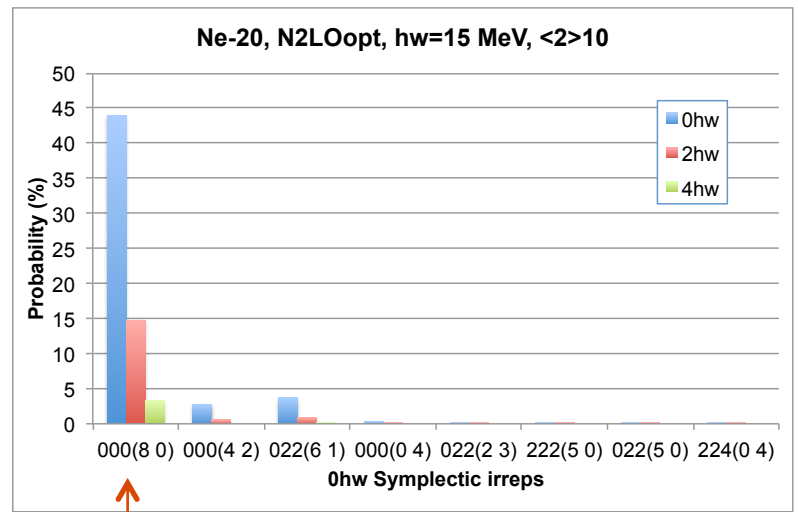
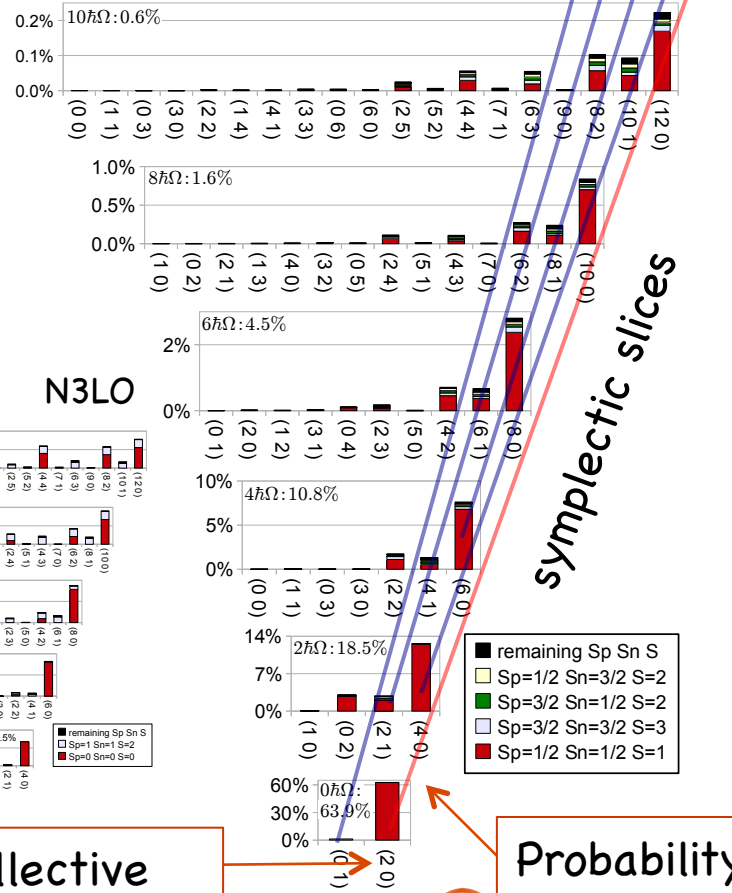
<sup>6</sup>Li

N3LO  
1.4%  
1.2%  
2.0%  
2.9%  
79.4%

JISP16

From first principles:  
light/intermediate-mass nuclei,  
low-lying states

Approximate  
symplectic symmetry  
in nuclei



single dominant symplectic slice

Collective modes

Probability (%)



# What is Symplectic Symmetry?

## Formal definition

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

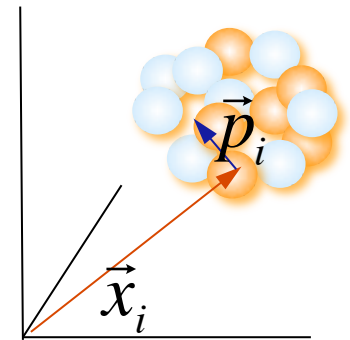
$$x_{i\alpha} \rightarrow \sum_{\beta=x,y,z} a_{\alpha\beta} x_{i\beta} + b_{\alpha\beta} p_{i\beta}$$

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

that **preserve the canonical commutation relation**

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

Nucleus with A nucleons



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)

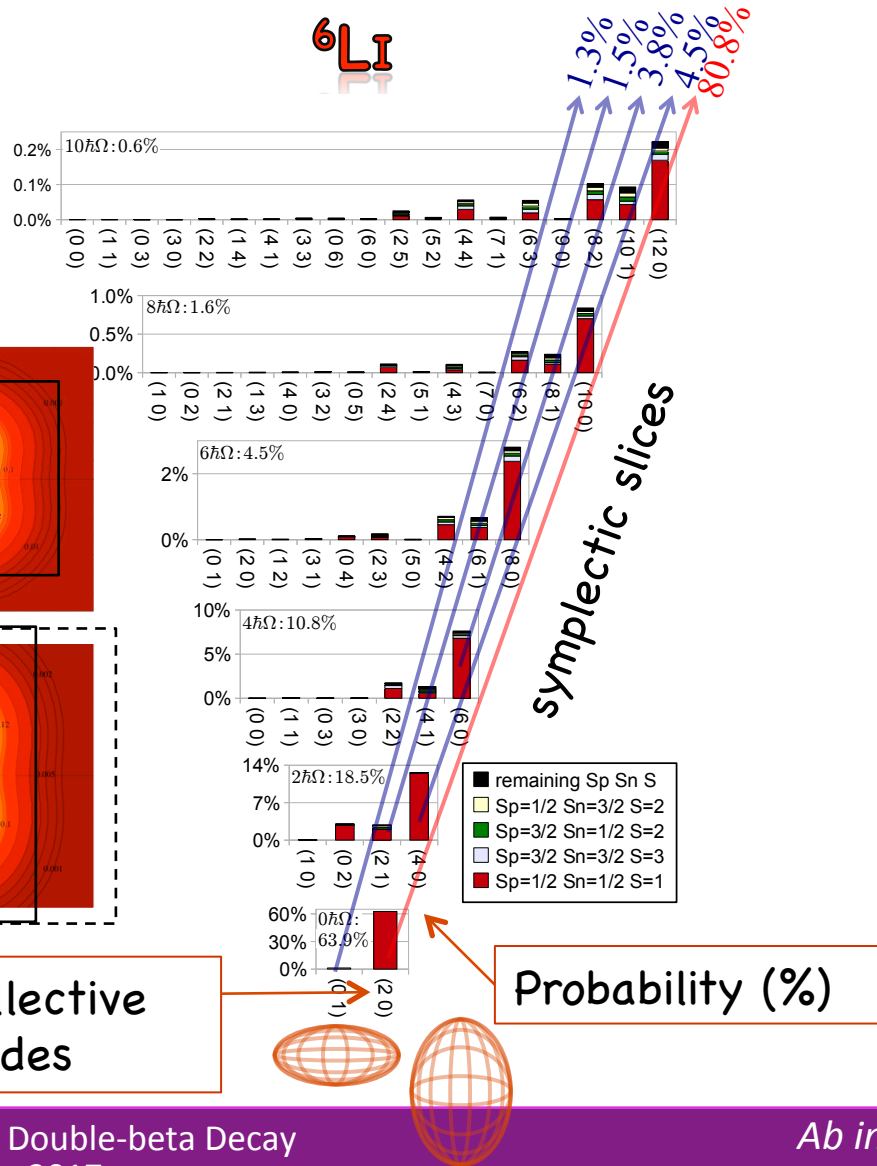
geometry

**Symplectic Model**

Rosensteel & Rowe,  
PRL 38 (1977) 10

kinematics

# What can we learn from symplectic symmetry?



Symplectic slice:

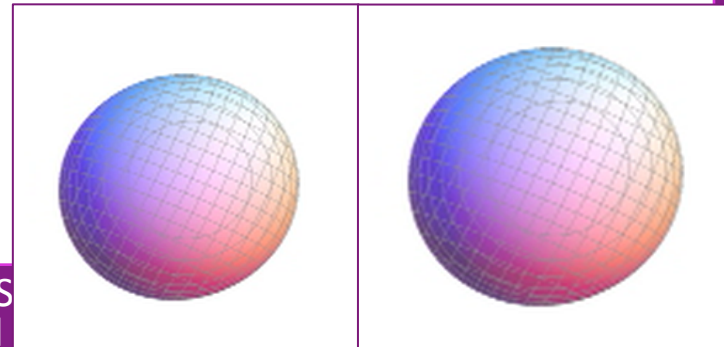
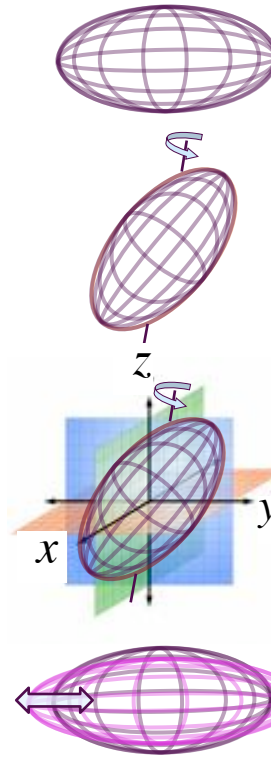
one equilibrium deformation ("shape")

rotations

space orientation

Vibrations

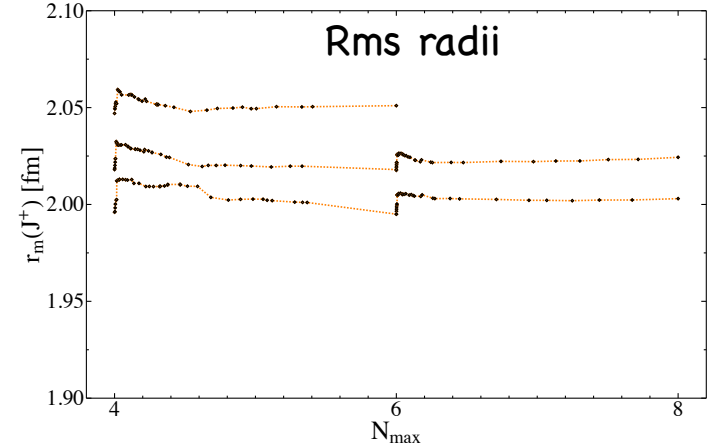
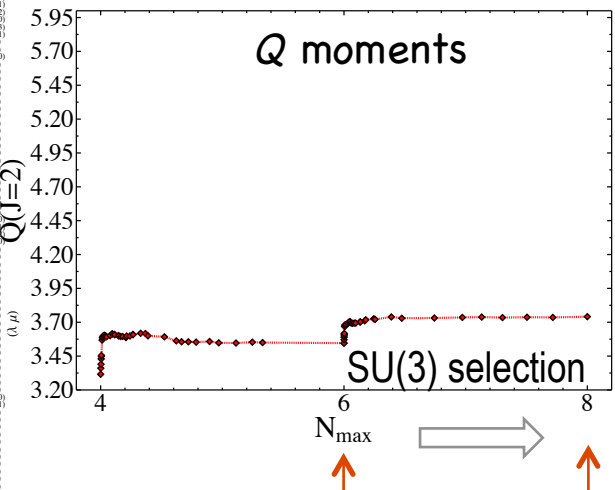
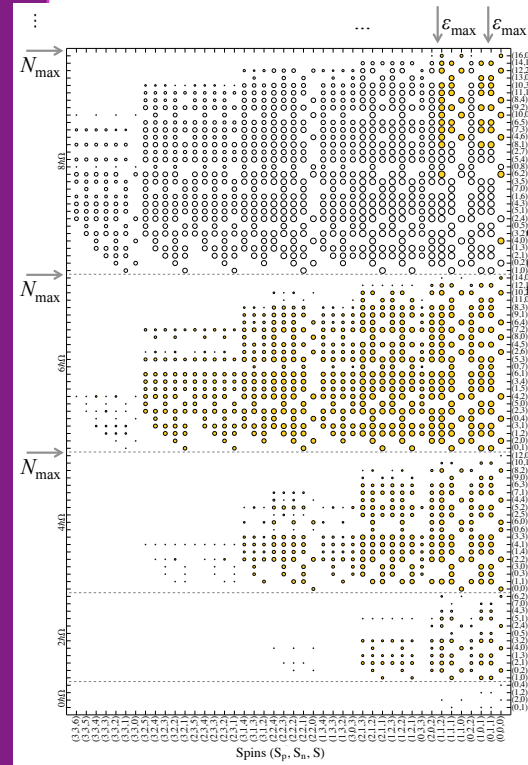
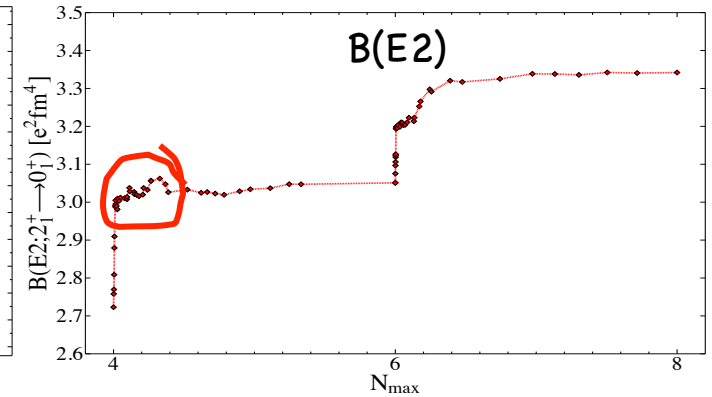
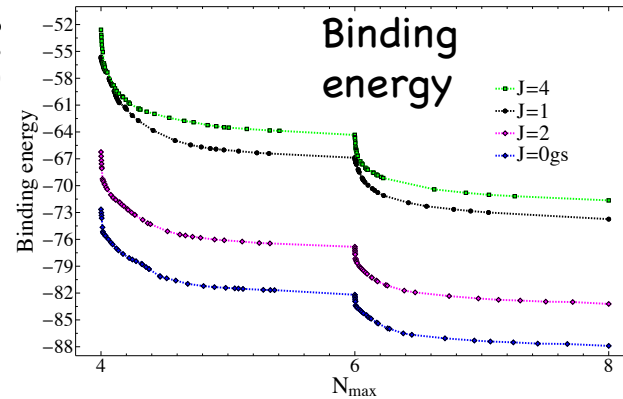
(of the giant resonance monopole ( $r^2$ )/ quadrupole (Q) type)





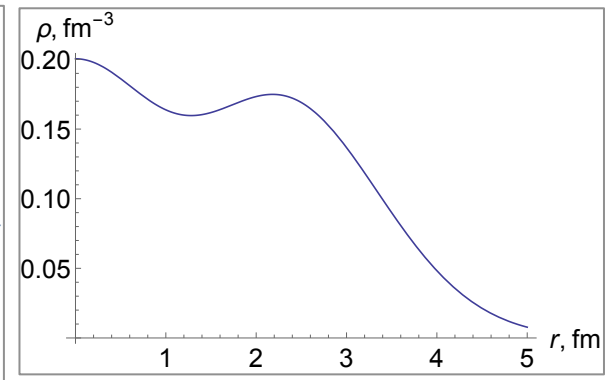
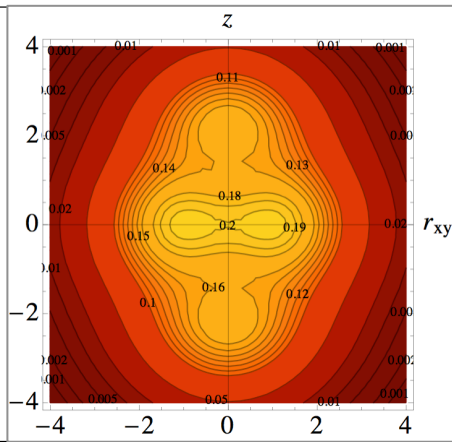
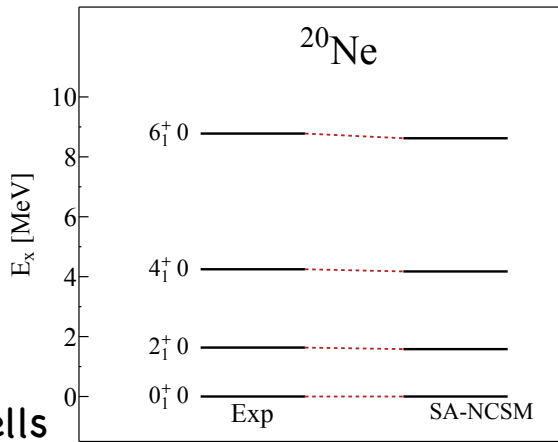
# Collectivity features

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



# Collectivity features

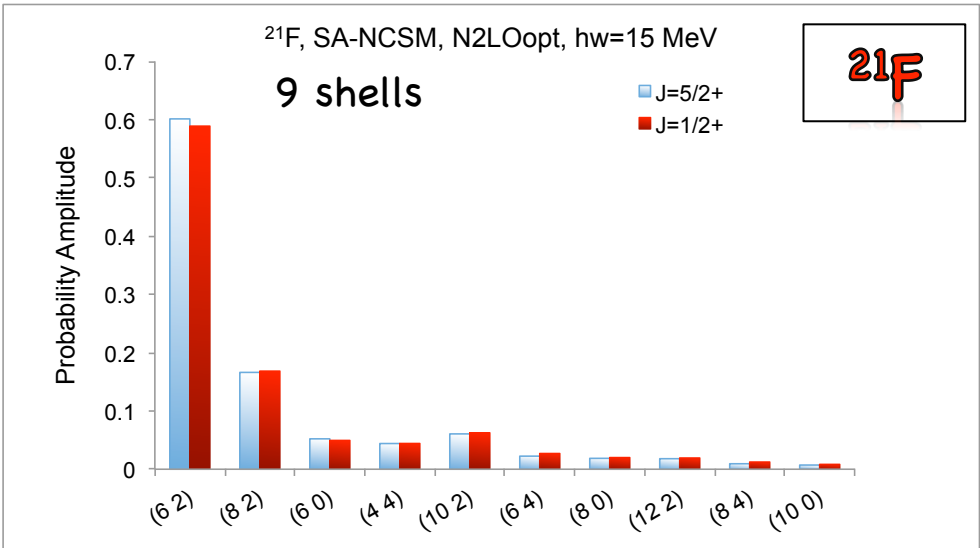
**20Ne**



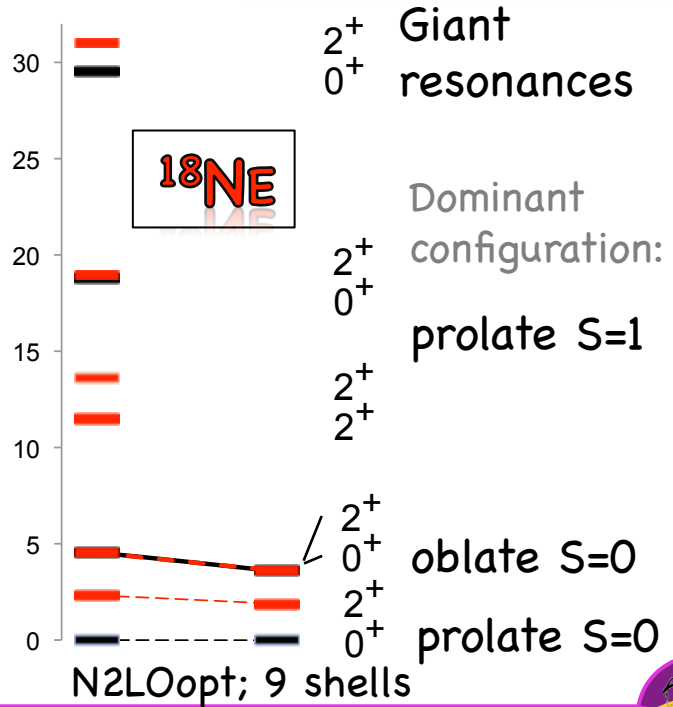
13 shells

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

**Ne & Mg isotopes**



Grigor Sargsyan, LSU

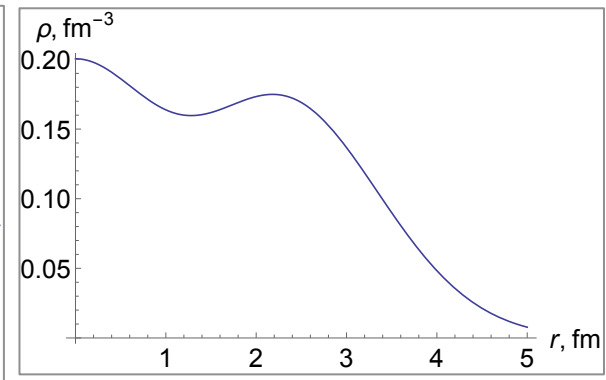
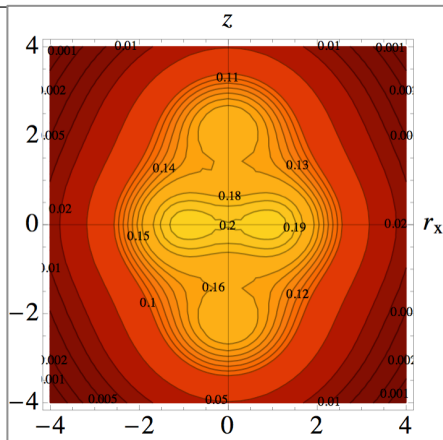
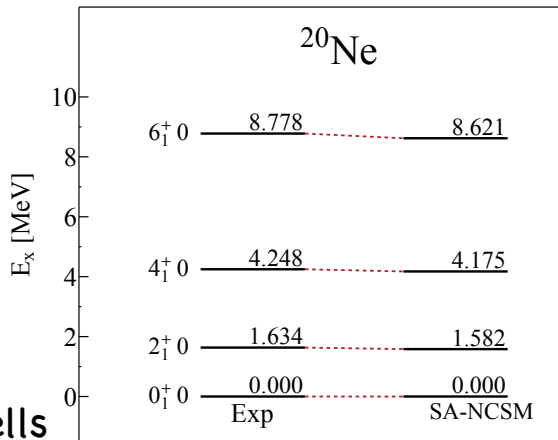


N2LOopt; 9 shells



# Collectivity features

**20Ne**



13 shells

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

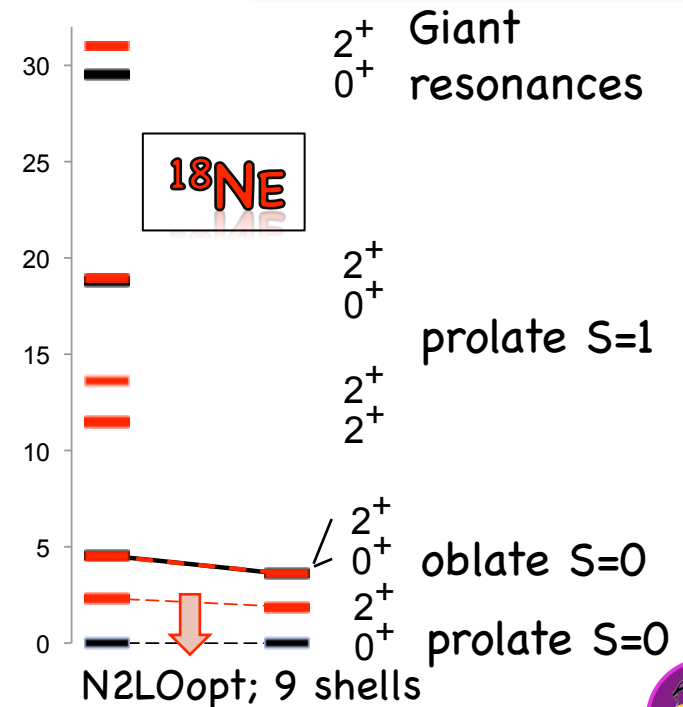
**Ne & Mg isotopes**

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

-----  
 Experiment..... 17.7(18) W.u.

9 shells ..... 1.13 W.u.

33 shells ..... 13.0(7) W.u.



Grigor Sargsyan, LSU

# Structure of Ca-48 and Ti-48

**48CA**

Neutrinoless double-beta decay  
... the "lightest" isotopes...

**48TI**

8 shells, N2LOopt  
0<sup>+</sup>

SA-NCSM (selected): .....966,152  
Complete model space: .....3,162,511,819

2<sup>+</sup>  
SA-NCSM (selected): .....3,055,554  
Complete model space: ...14,522,234,982

8 shells, N2LOopt  
0<sup>+</sup>

SA-NCSM (selected): .....602,493  
Complete model space: .....24,694,678,414

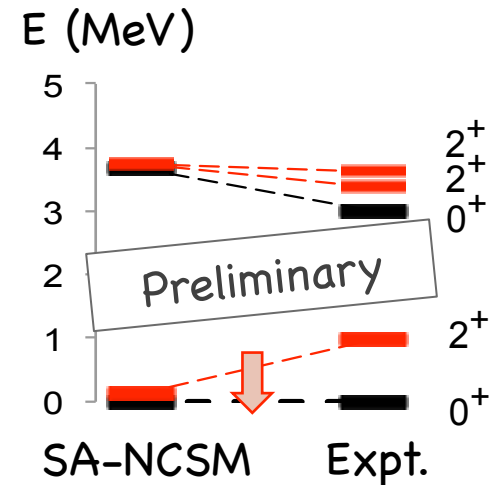
2<sup>+</sup>  
SA-NCSM (selected): .....1,178,834  
Complete model space: ...113,920,316,658

<sup>48</sup>Ti, B(E2: 2<sup>+</sup>→0<sup>+</sup>)

-----  
Experiment..... 14.7(4) W.u.

8 shells ..... 8.5 W.u.

34 shells ..... 13.6(6) W.u.

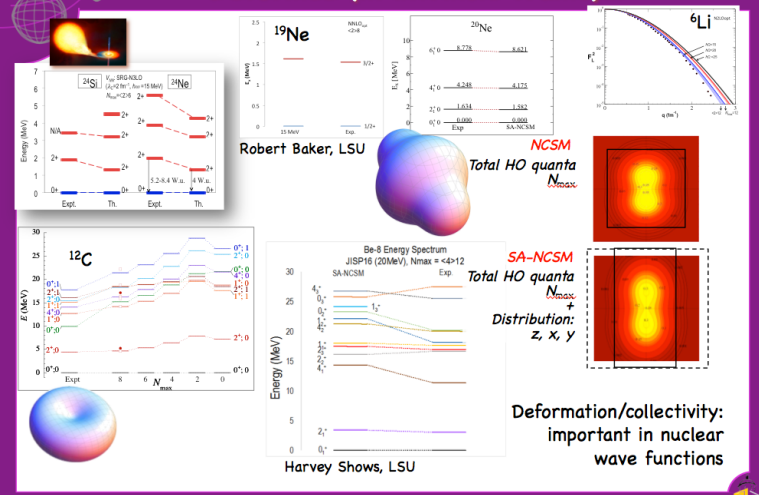


Grigor Sargsyan, LSU

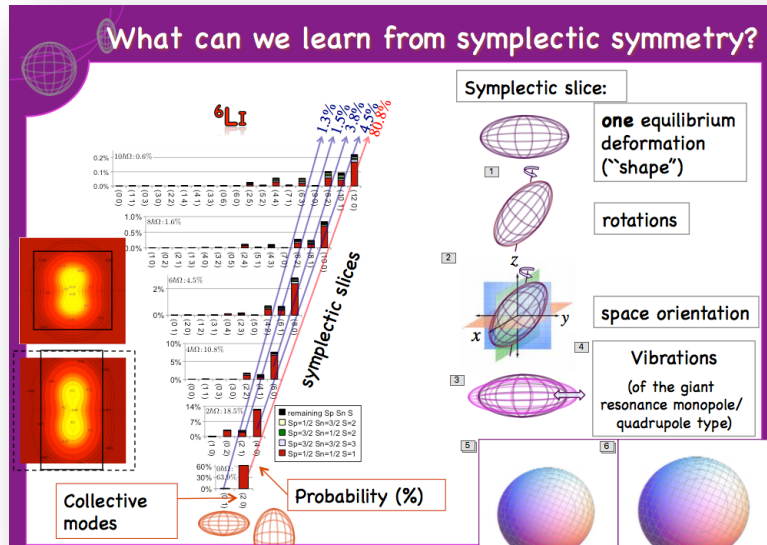
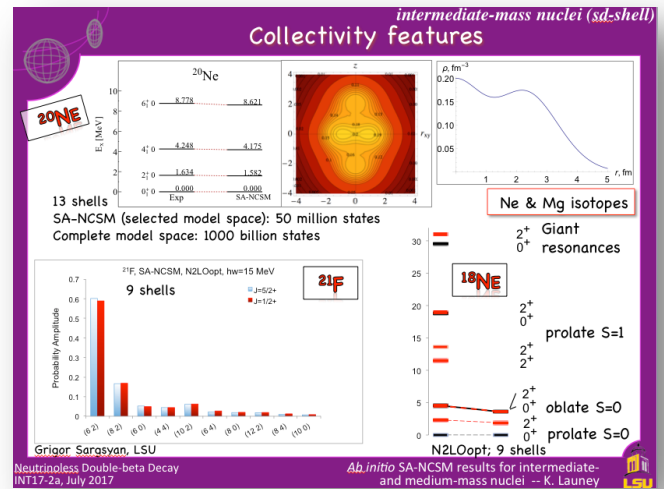


Deformed (in intrinsic frame)...

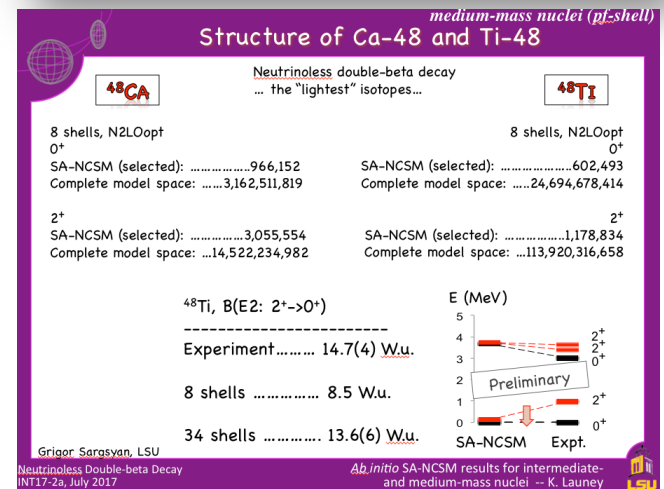
# Conclusions



Deformation/collectivity: important in nuclear wave functions



Simple physics: "shape" + vibrations + rotations



Collective features in intermediate- and medium-mass nuclei