Ab Initio SA-NCSM Modeling across the Intermediate-mass Region

LSU Team …

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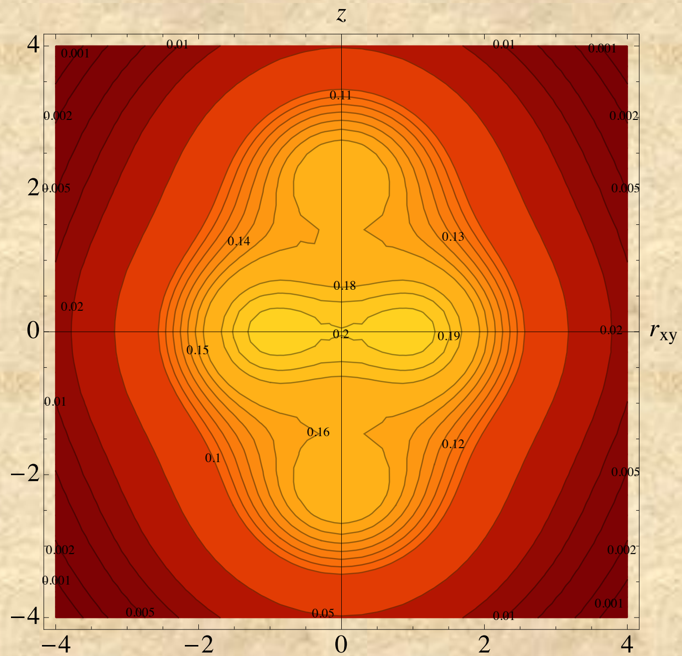


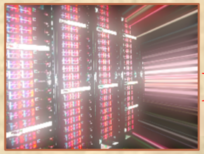
Ab initio description of Ne-20
(N2LOopt, $\hbar\Omega$=15 MeV, 13 HO shells)

PetaApps Collaboration …

J. Vary, P. Maris, M. Sosonkina (Iowa State U.)
U. Catalyurek, E. Saule
(The Ohio State U.)

A. Hayes (LANL)

D. Rowe (U. Toronto)
G. Rosensteel (Tulane U.)
D. Langr (Czech U.)

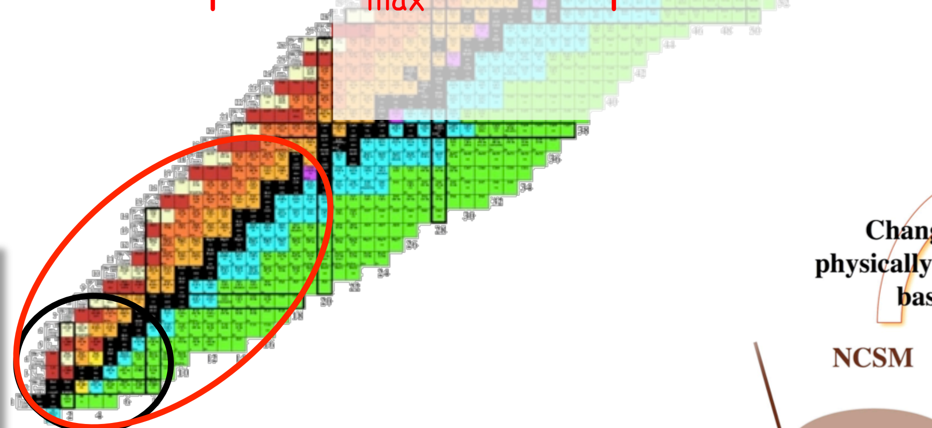


NERSC; Blue Waters;
LONI +CCT @ LSU

Kristina D. Launey (Louisiana State University)

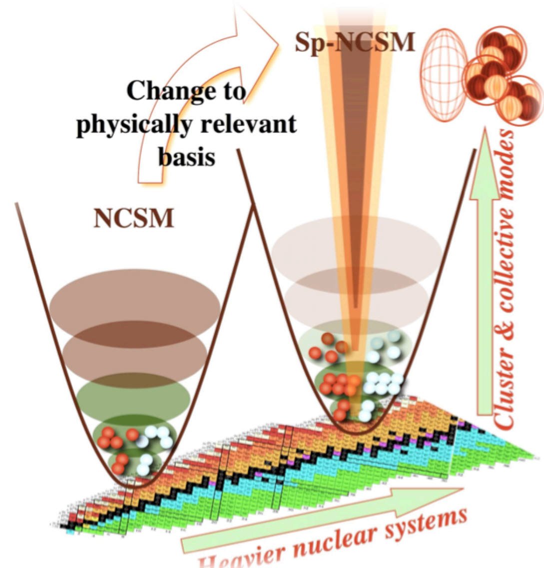
Symmetry-adapted no-core shell model (SA-NCSM): expanding the reach of *ab initio* models

SA-NCSM
- Fully *ab initio* (no restrictions on interactions …*NN, NNN,* non-local,…)
- NCSM with SU(3)-coupled basis states (reorganization of model space)
- Model space selection (truncation) -- physically relevant + *exact* center-of-mass (CM) factorization!
- Equal to NCSM in complete-N_{max} model space



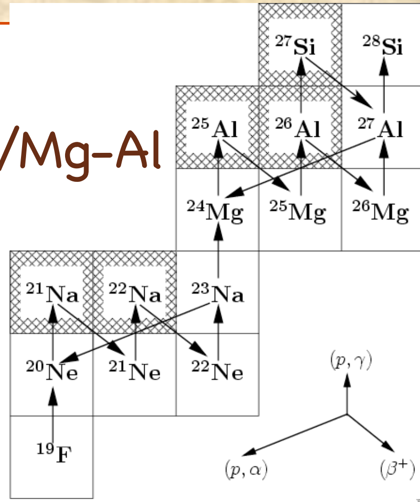
PetaApps Collaboration (First-principle Symmetry-guided Initiative)

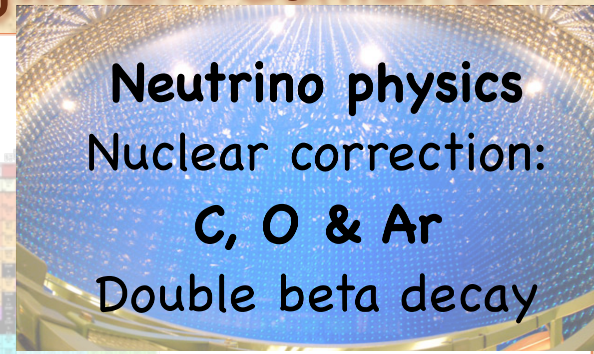
Current First-principle No-core Shell Model

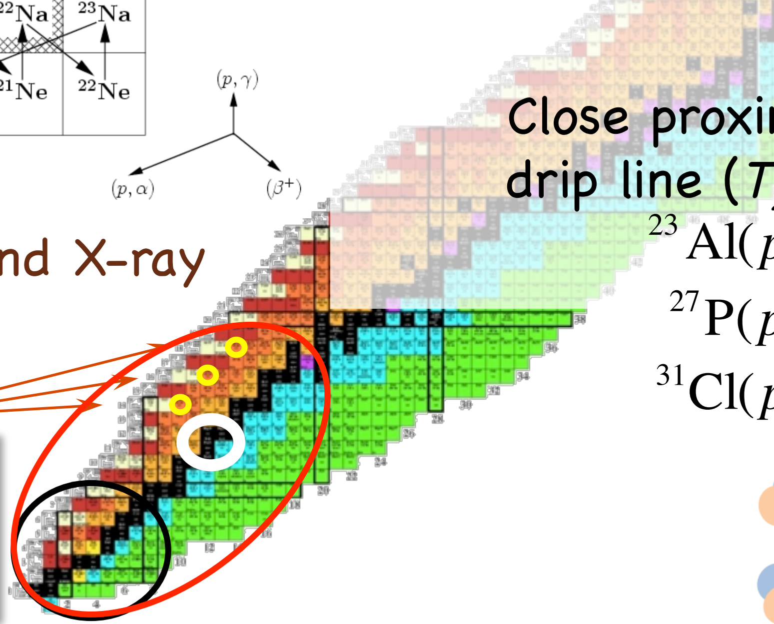


Ab initio SA-NCSM modeling…New domains

Ne-Na/Mg-Al chains





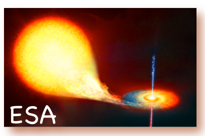


Close proximity of the proton drip line (T_z=+2 nuclei)

$^{23}\mathrm{Al}(p,\gamma)^{24}\mathrm{Si}$

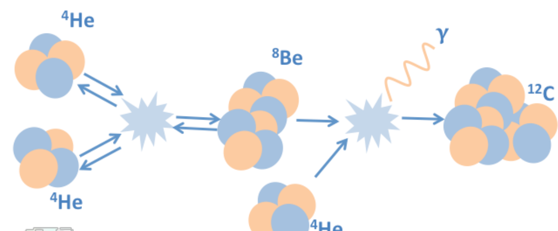
$^{27}\mathrm{P}(p,\gamma)^{28}\mathrm{S}$

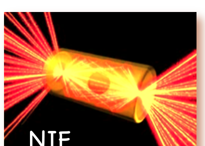
$^{31}\mathrm{Cl}(p,\gamma)^{32}\mathrm{Ar}$



Novae and X-ray bursts

PetaApps Collaboration (First-principle Symmetry-guided Initiative)





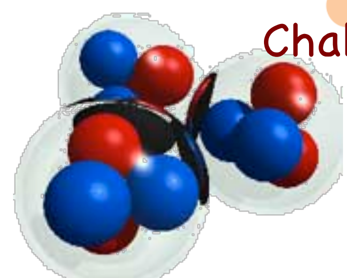
National Ignition Facility (NIF)

^{18}O, ^{20}F

A. Hayes et al. (LANL)

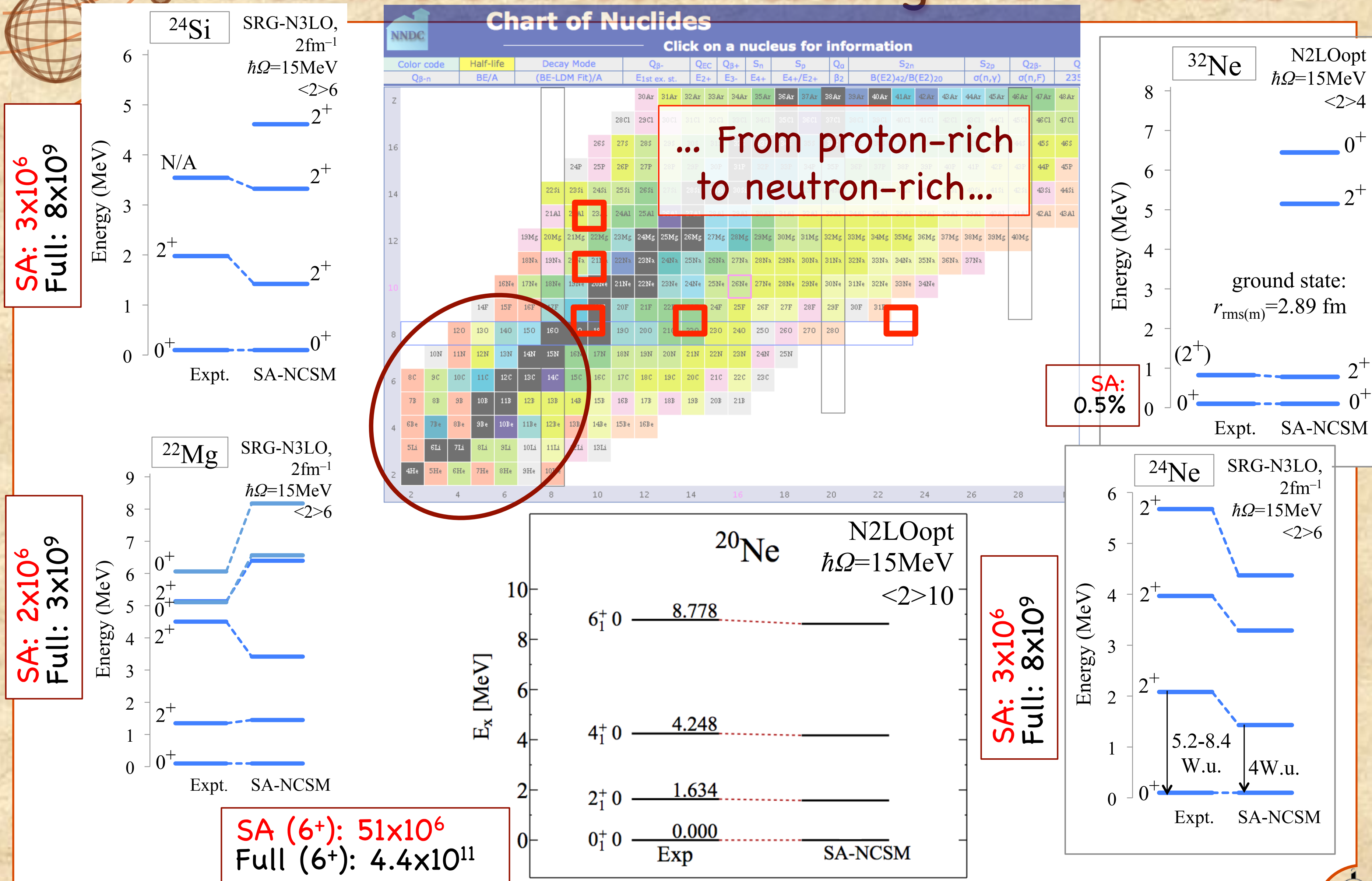
Reactions for successful fusion burn

Electron/Neutrino scattering



Challenging cluster structures:
Hoyle state

Ab initio SA-NCSM modeling…New domains



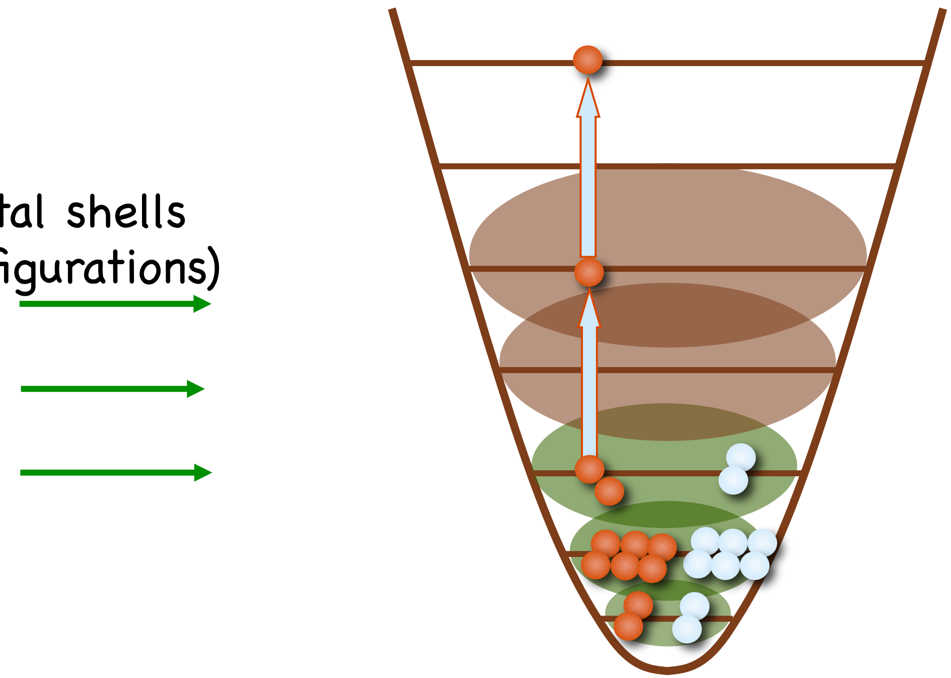
Ab initio No-Core Shell Model

No-Core Shell Model

(NCSM)

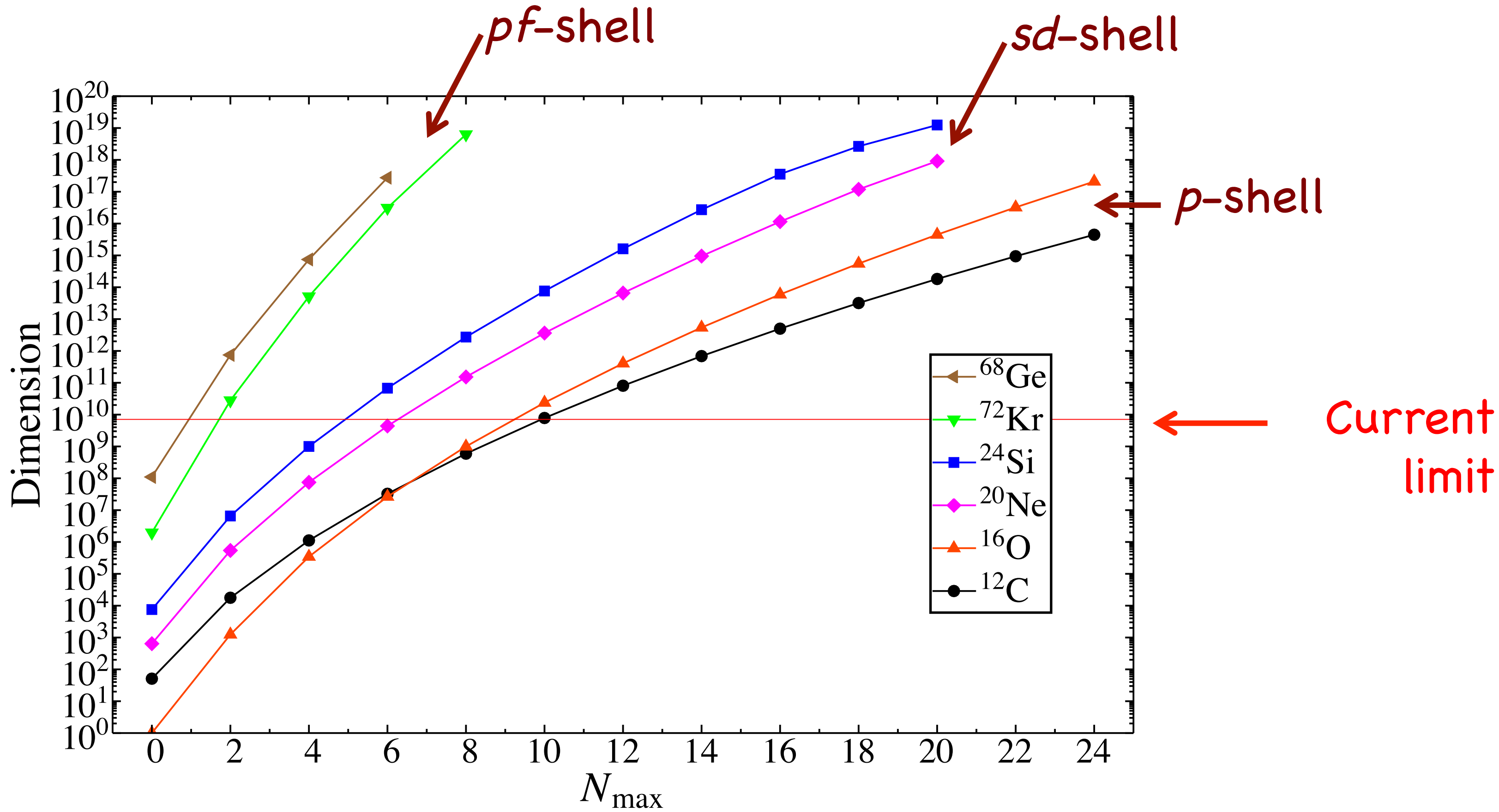
Navratil, Vary, & Barrett,
PRL 84 (2000) 5728

Horizontal shells
(all configurations)



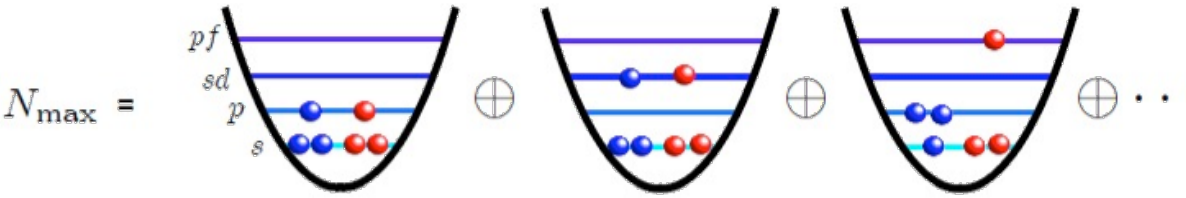
- No restrictions on interactions (*NN*, *NNN*, non-local,…)
- Model space – limited by N_{max}
- Successful descriptions up through ^{16}O

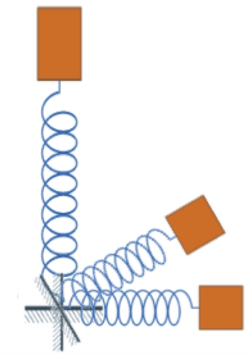
Model space for heavier nuclei



Symmetry-adapted NCSM (SA-NCSM) … Basis

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



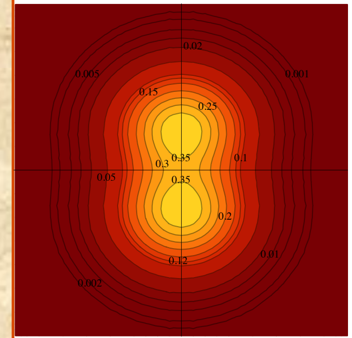


SU(3) is the exact symmetry of 3-D HO

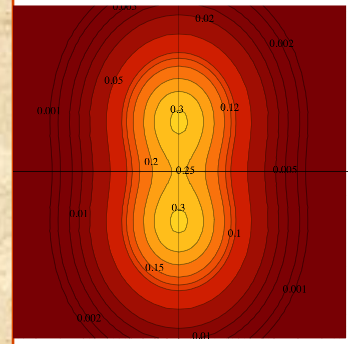
- HO excitations in *z, x, y*: $n_z\ n_x\ n_y$
- ($\lambda\ \mu$) label an SU(3) configuration – related to *spatial deformation*

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

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

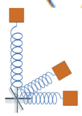
A particles in 3-D space:
complete basis for the shell model (all linear canonical transformations of the 3A-particle phase space +spin/isospin)

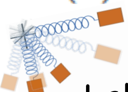
$$\mathrm{Sp}(3(A-1),\mathbb{R}) \times \mathrm{U}(4)$$

$$\cup \qquad \cup$$

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

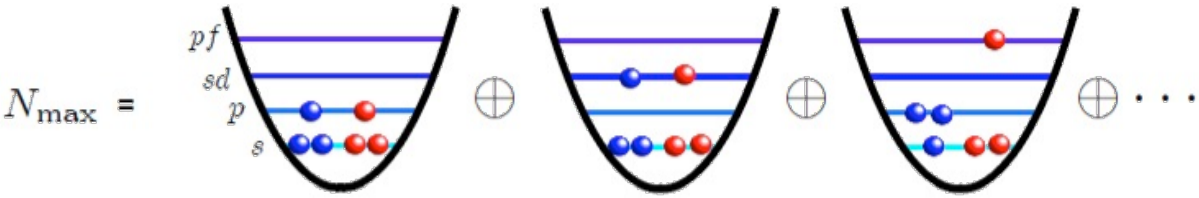
$$\mathrm{Sp}(3,\mathbb{R}) \supset U(3) \supset \mathrm{SO}(3) \supset SO(2)$$

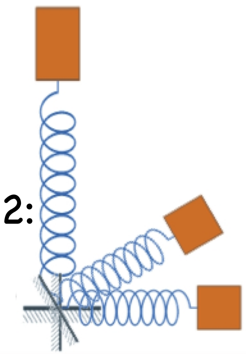
Body-fixed frame 

 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:

$$\frac{1}{N}\left[a^{\dagger}_{(n_1 0)st}\times a^{\dagger}_{(n_2 0)st}\right]^{(\lambda\mu)\kappa(LS)JM;TT_0}|0\rangle$$

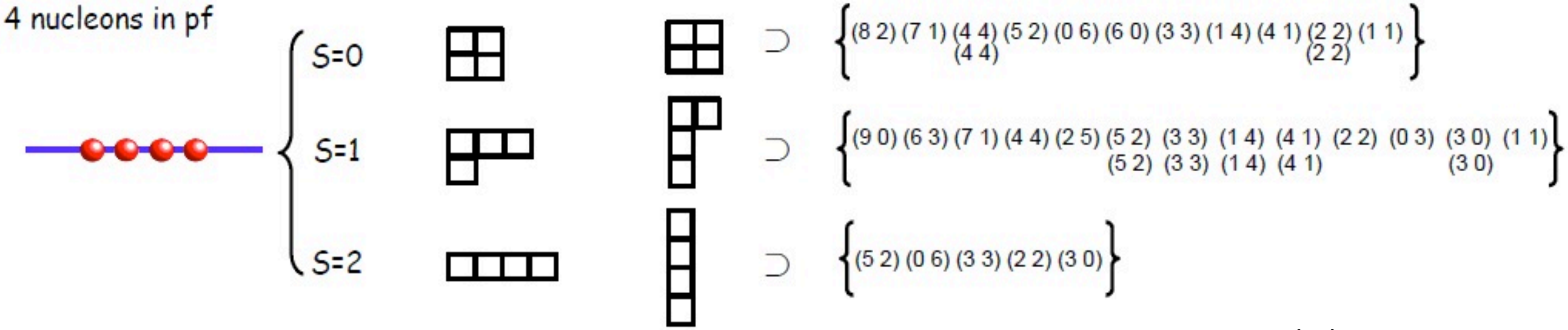
[…not used]

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

Fast basis construction! … based on Gel'fand patterns

	U(2)	⊗	U(10)	⊃	SU(3)
quantum labels:	S		[f]	α	$(\lambda\ \mu)$

- 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 $\langle(\chi\omega ST)_f \| V^{\omega_0 S_0 T_0=0} \| (\chi\omega ST)_i\rangle_{\rho_0}$

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

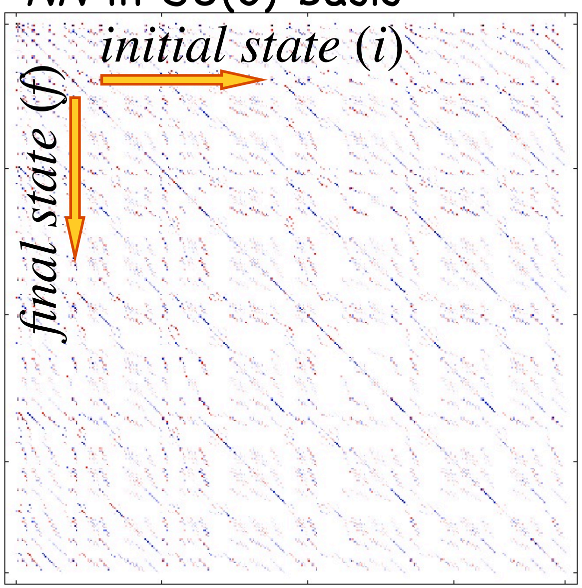
$$= (-)^{S_f+S_0}\Pi_{TS_0}\frac{\dim\omega_0}{\dim\omega_f}\sum_{J(\kappa L)_{if}}\begin{Bmatrix} L_f & S_f & J \\ S_i & L_i & S_0 \end{Bmatrix}\langle\omega_i\kappa_i L_i;\omega_0\kappa_0 L_0\|\omega_f\kappa_f L_f\rangle_{\rho_0}\times$$

$$(-)^{L_i+J}\Pi_{J^2L_f}\Pi_{L_iL_fS_iS_f}\sum_{\substack{l_rl_sl_tl_u\\ j_rj_sj_tj_u}}\sqrt{\frac{(1+\delta_{rs})(1+\delta_{tu})}{(1+\delta_{\eta_r\eta_s})(1+\delta_{\eta_t\eta_u})}}\langle(\eta_r\,0)l_r;(\eta_s\,0)l_s\|(\omega\kappa L)_f\rangle\times$$

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

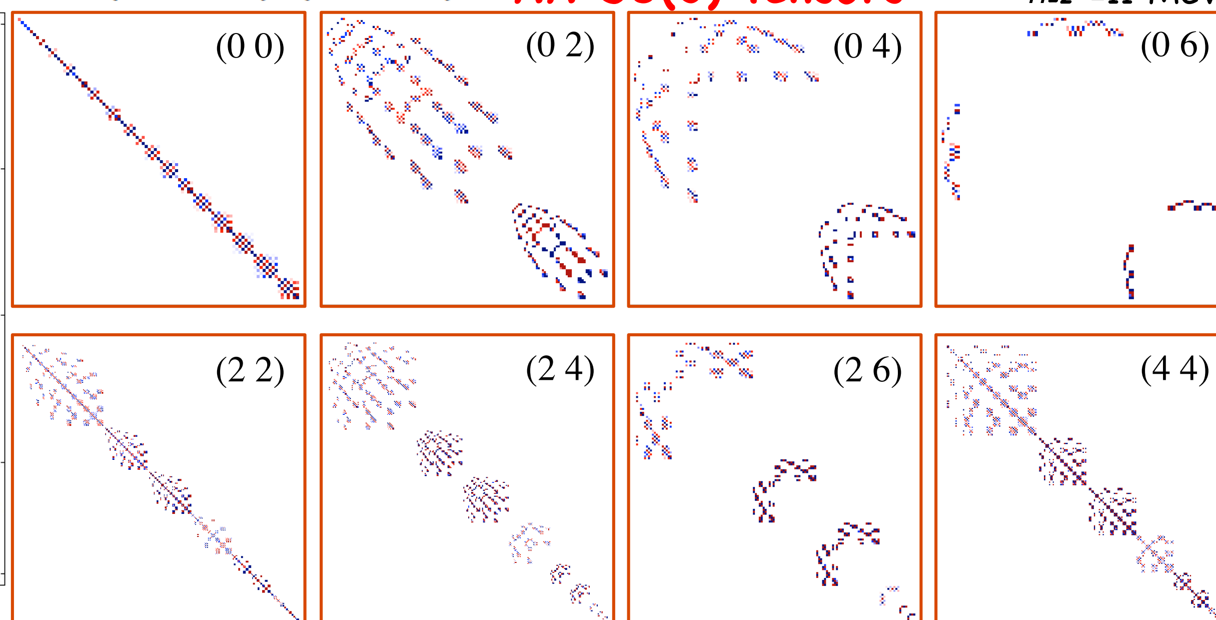
jj-coupled *NN*

NN in SU(3) basis

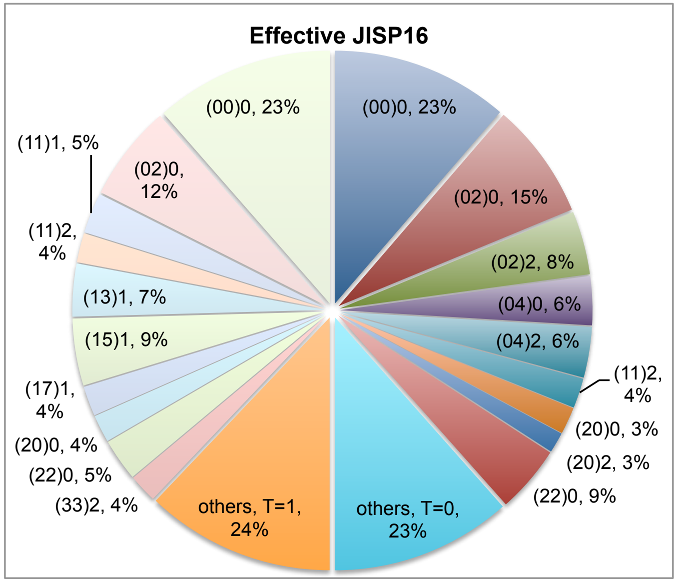


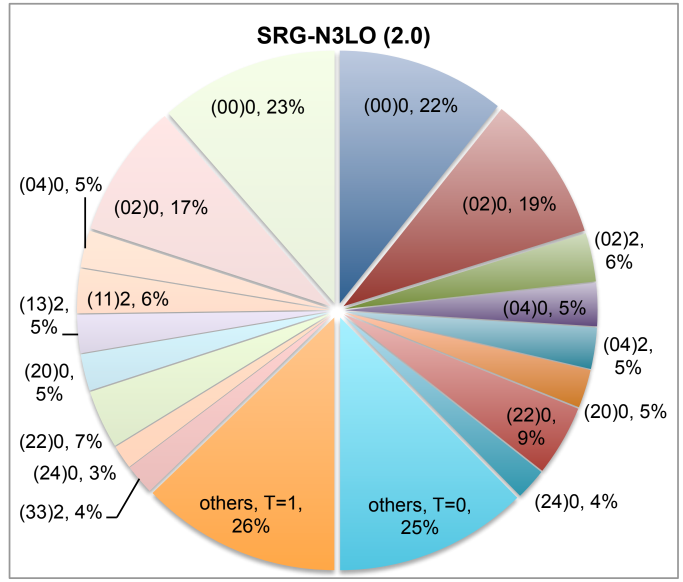
***NN* SU(3) Tensors**

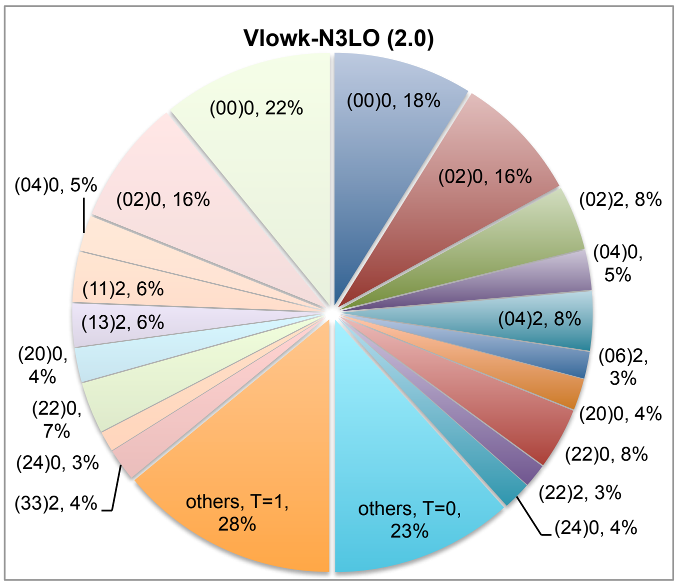
N3LO (N_{max}=6)
$\hbar\Omega$ =11 MeV

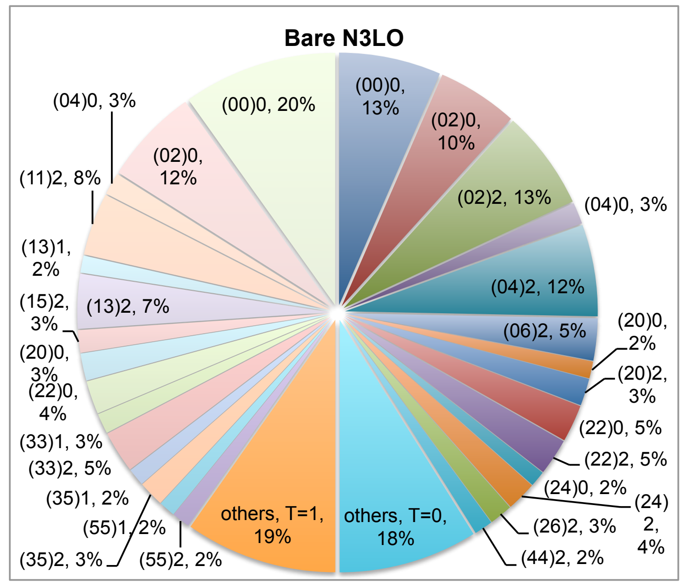


NN interaction SU(3) tensors









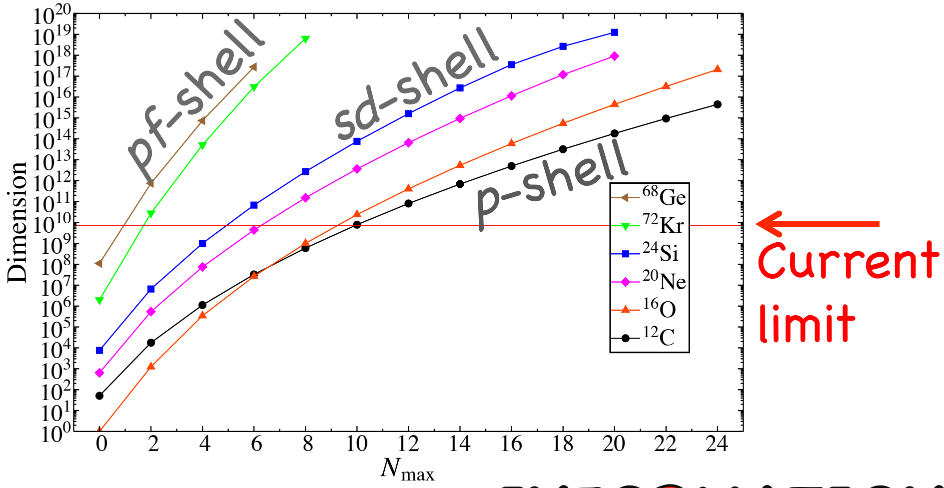
SA-NCSM … *Hamiltonian*

SA-NCSM:

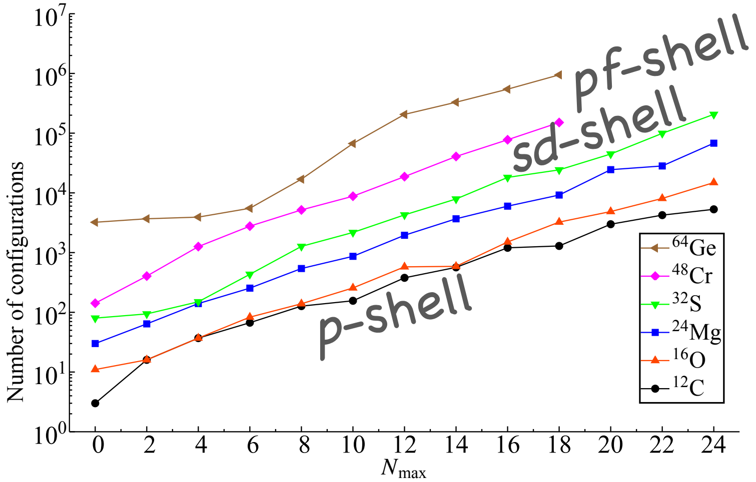
- SU(3)-coupled basis – fast construction (Gel'fand patterns)
- *NN* interaction SU(3) tensors – generated once per interaction
- Hamiltonian –
  - Wigner-Eckart theorem … reduced matrix elements (rme's)
  - Decoupling to single-shell tensors $Tn_1n_2n_1n_1$ -> Tn_2 x $Tn_1n_1n_1$
  - Important pieces of information … single-shell rme's

Important pieces of information (memory requirement)

NCSM



SA-NCSM

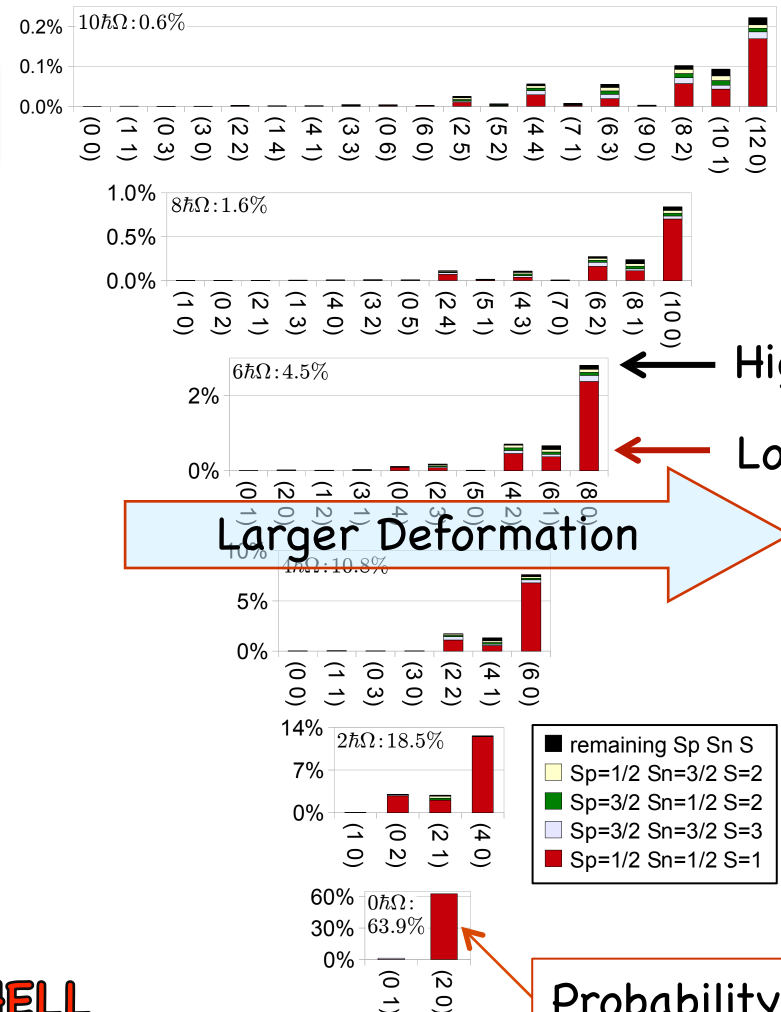


INFORMATION REDUCTION

Ab Initio SA-NCSM … The unique feature

^{6}Li 1^+ g.st. (JISP16, $\hbar\Omega$=20 MeV, N_{max}=10)

^{6}Li



Highest Spin

Lowest Spin

Larger Deformation

Probability (%)

First-principle:
light nuclei, low-lying states

Emergence of a simple pattern in complex nuclei

Novel feature

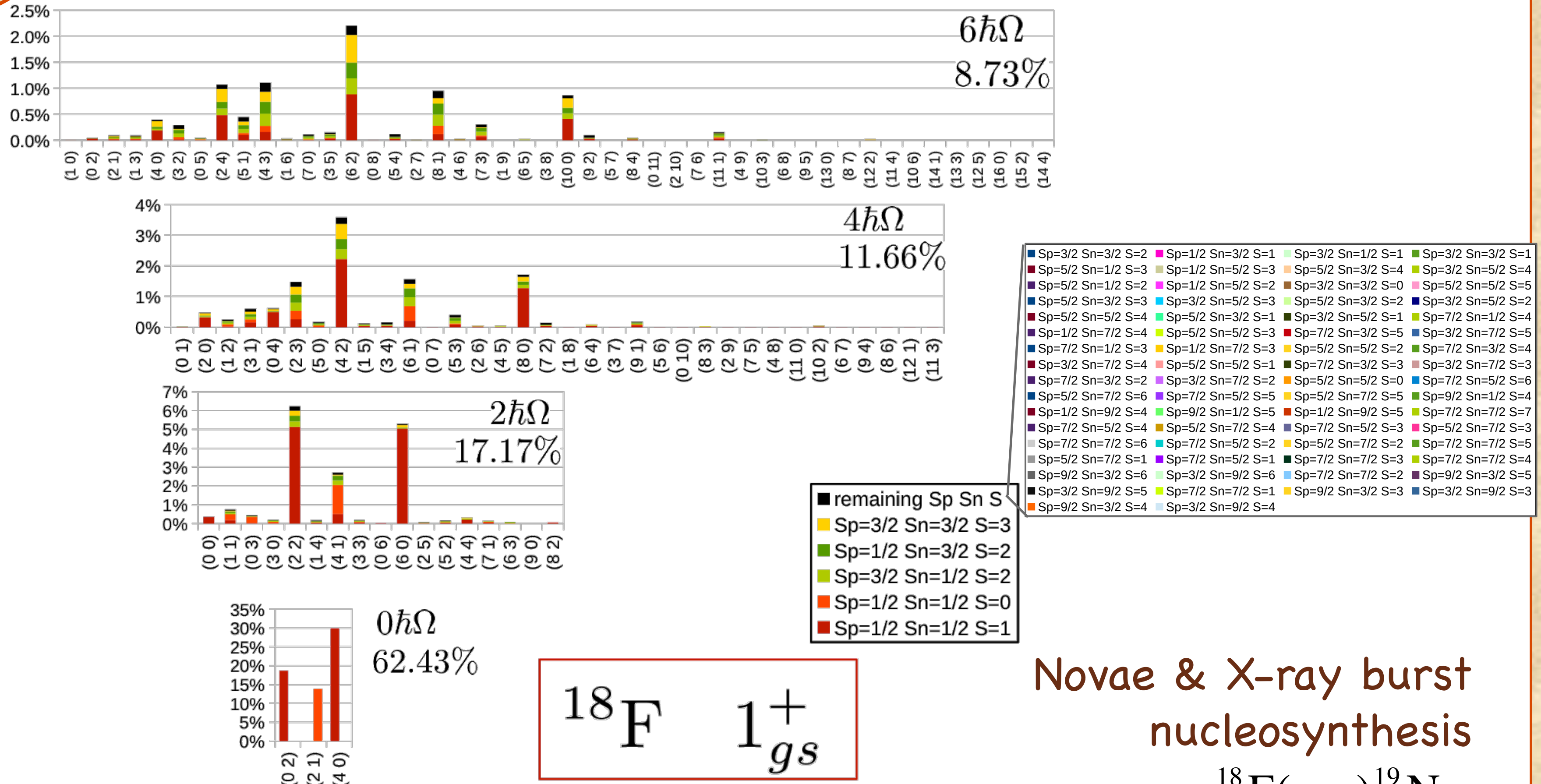
Large deformation
Low spin

P-SHELL NUCLEI

Dytrych, Launey, Draayer, et al., PRL 111 (2013) 252501

Ab Initio SA-NCSM … The unique feature

^{18}F 1$^+$ g.st. (N2LOopt, $\hbar\Omega$=20 MeV, N_{max}=6)



$$^{18}\mathrm{F} \quad 1^{+}_{gs}$$

Novae & X-ray burst nucleosynthesis

$^{18}\mathrm{F}(p,\gamma)^{19}\mathrm{Ne}$

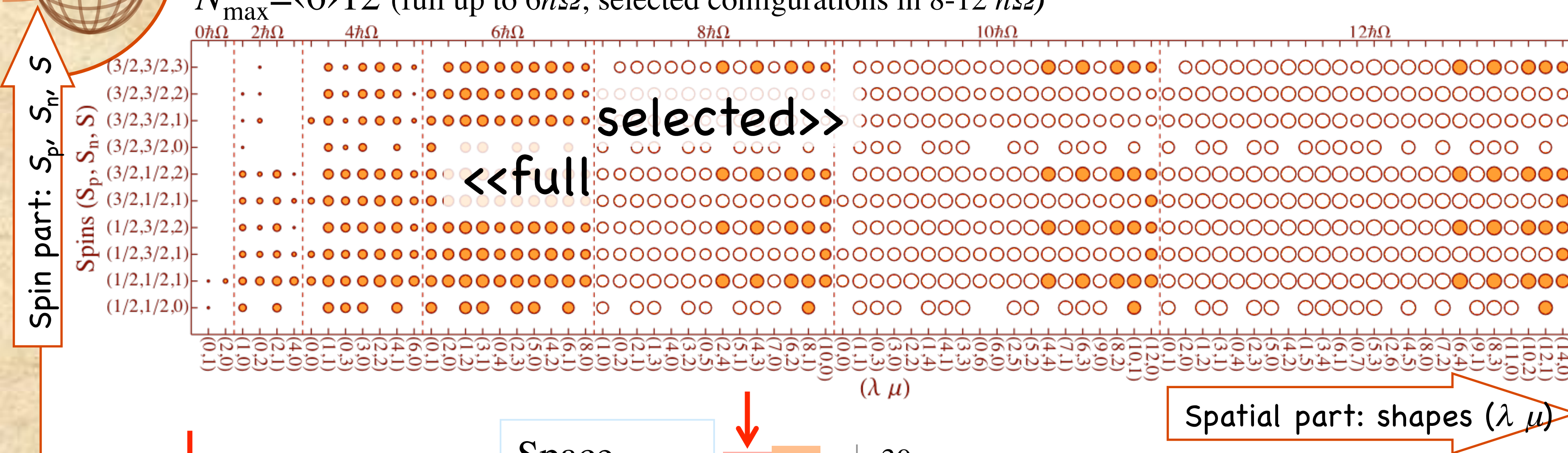
For input to NCSM/RGM (with P. Navratil)

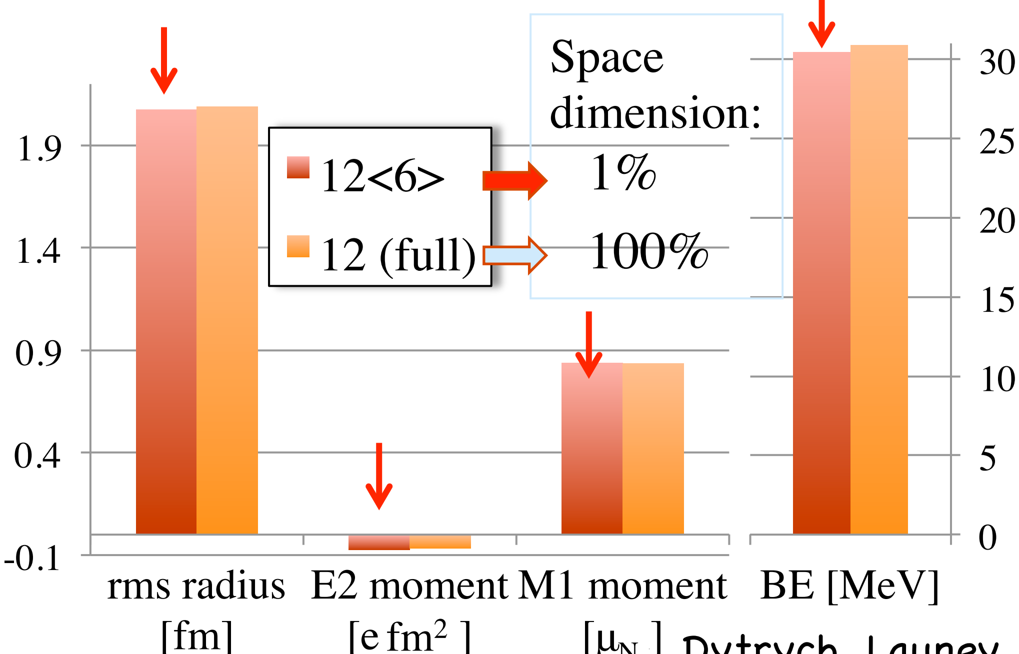
SD-SHELL NUCLEI

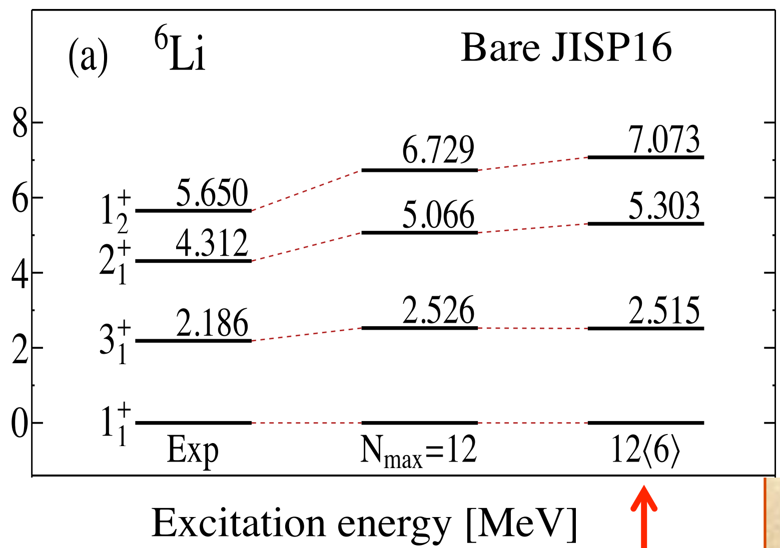
Symmetry-guided selected model space

^{6}Li

N_{max}=⟨6⟩12 (full up to 6$\hbar\Omega$; selected configurations in 8-12 $\hbar\Omega$)





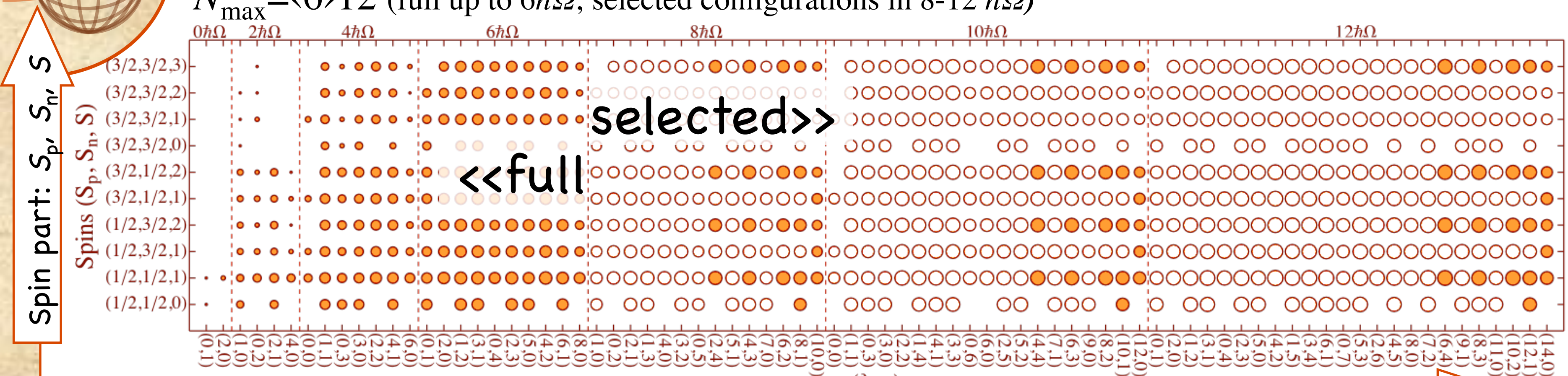


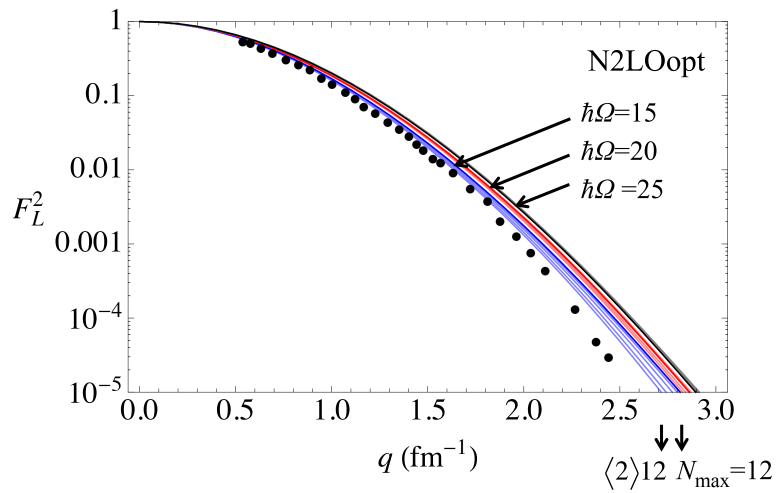
Dytrych, Launey, Draayer, et al., PRL 111 (2013) 252501

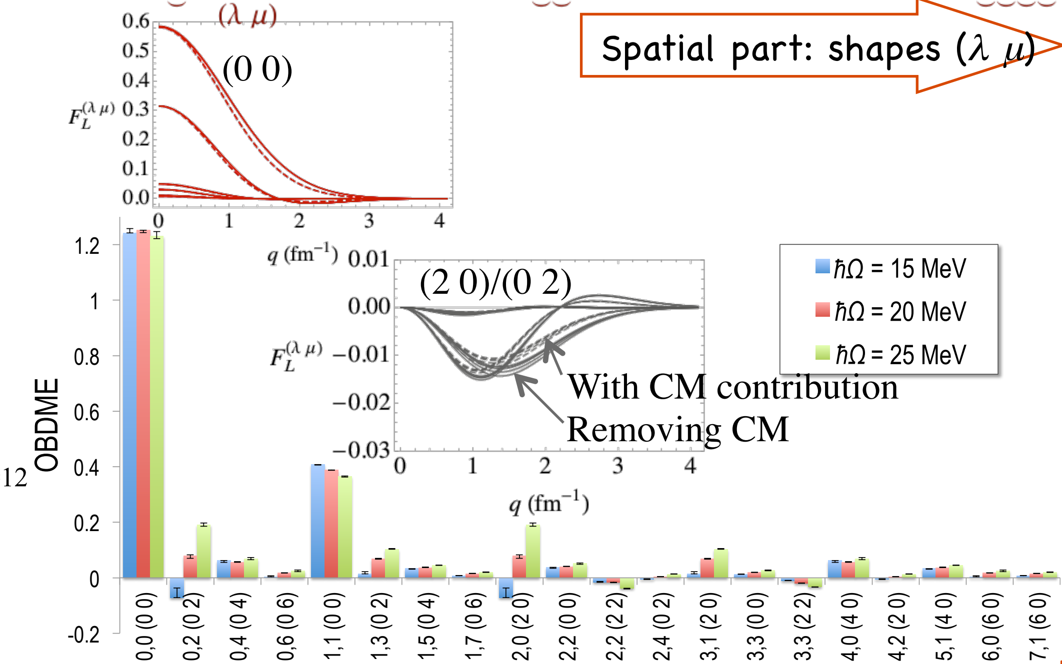
Li-6: Electron scattering off g.st.

^{6}Li

N_{max}=⟨6⟩12 (full up to 6$\hbar\Omega$; selected configurations in 8-12 $\hbar\Omega$)





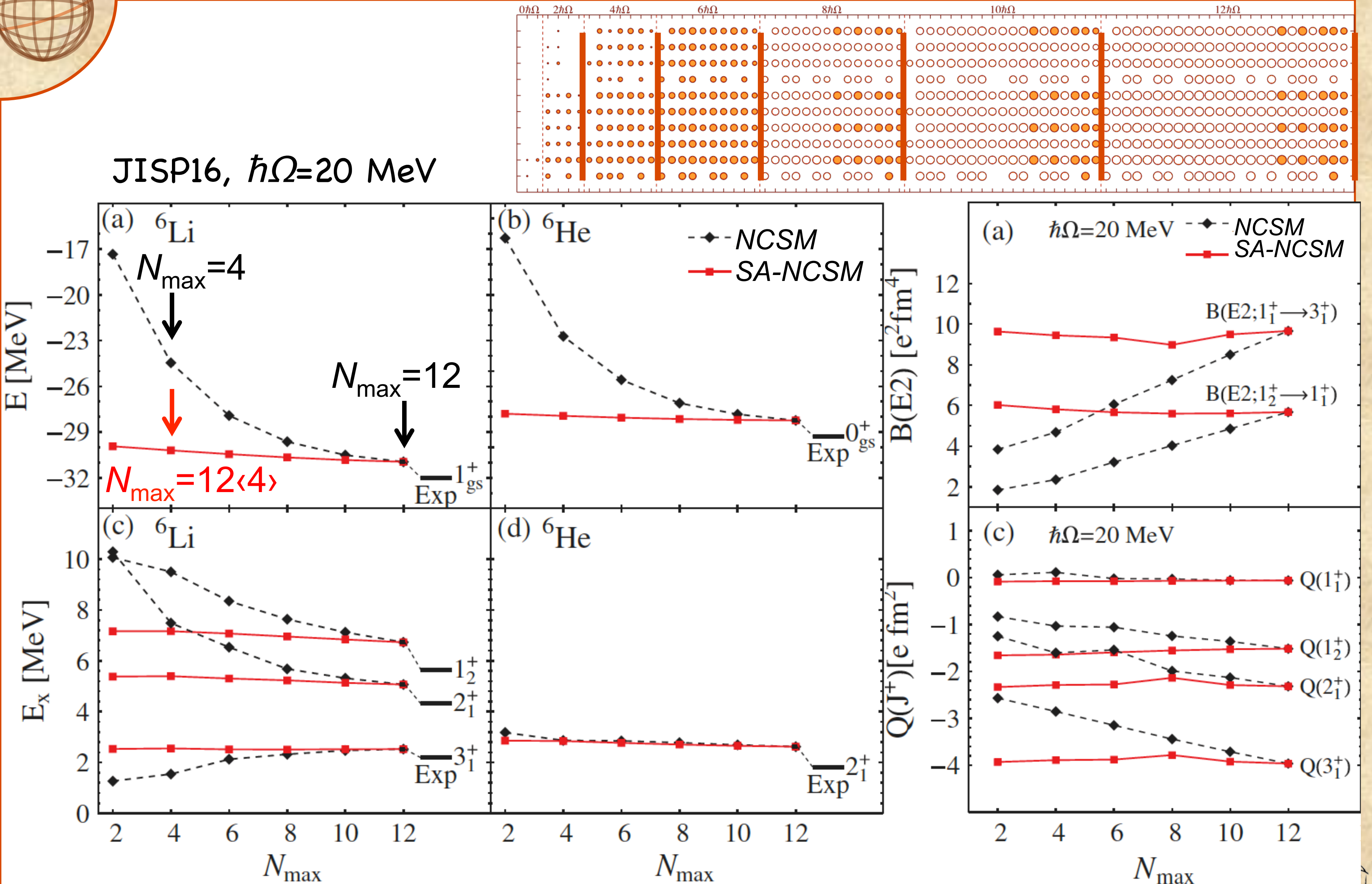


Phys. Rev. C 91 (2015) 024326
(with A. Hayes, LANL)

Agrees with GFMC results for q≲2 fm^{-1}
[Wiringa/Stoks/Schiavilla, Phys.Rev. C 51 (1995) 38]

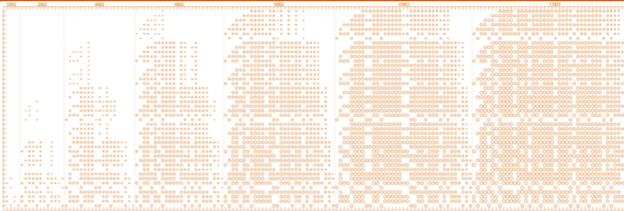
Symmetry-guided selected model space

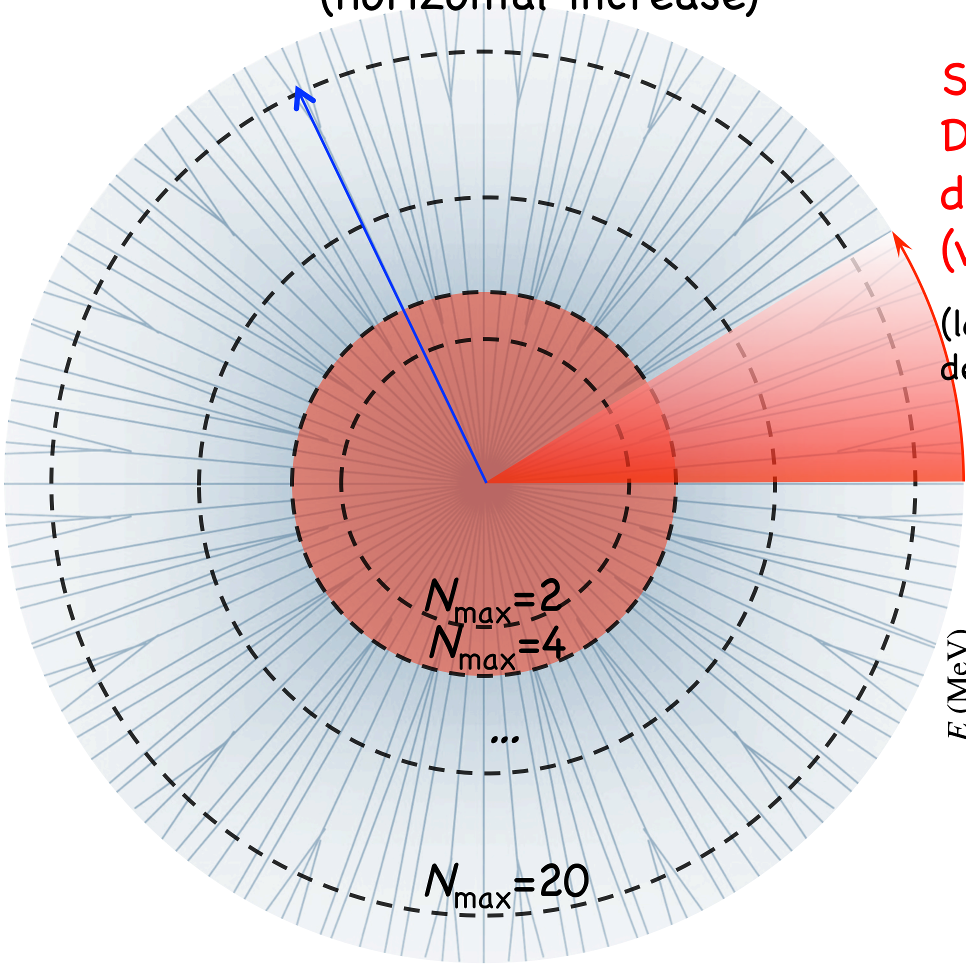
^{6}He, ^{6}Li



Symmetry-guided selected model space

NCSM:
Dependence on N_{max}
(horizontal increase)



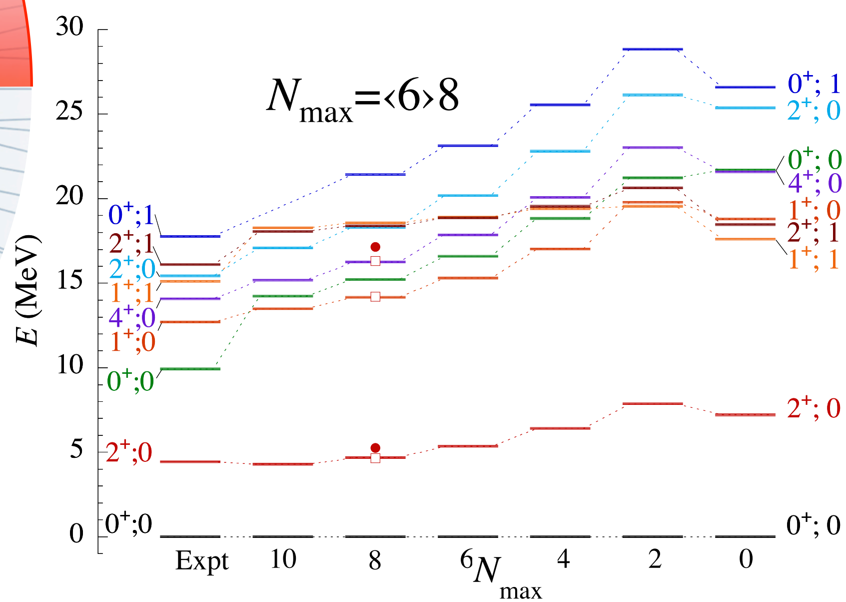


SA-NCSM:
Dependence on deformation cutoff
(vertical increase)

(largest bandhead deformation first)

^{12}C

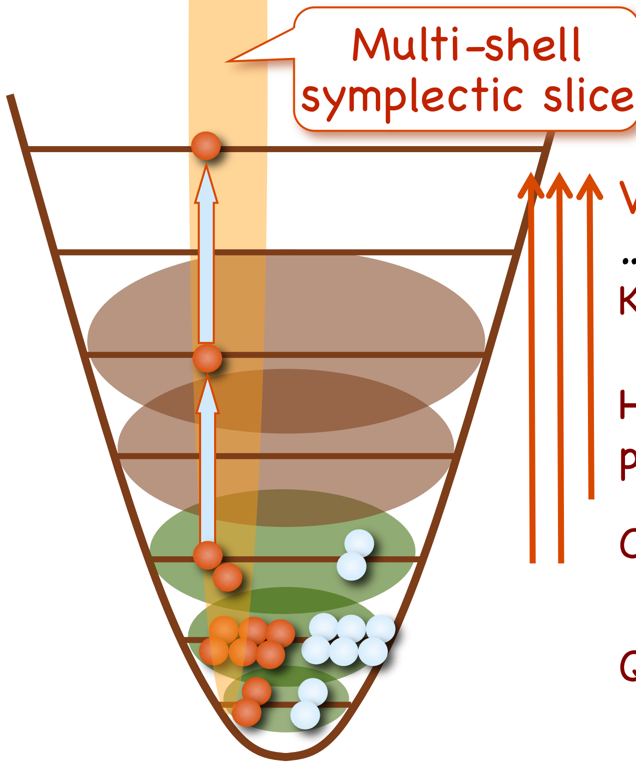
(JISP16, $\hbar\Omega$=20 MeV)



Dytrych, Maris, Launey, et al., in preparation

Going beyond – Symplectic basis

Horizontal shells
(all configurations)



Vertical (symplectic) slices

…are not mixed by:

Kinetic energy $\sum_n \frac{\mathbf{p}_n^2}{2m}$

Harmonic oscillator potential energy $\sum_n \frac{m\omega^2 \mathbf{r}_n^2}{2}$

Orbital angular momentum $\mathbf{L} = \sum_n \mathbf{r}_n \times \mathbf{p}_n$

Quadrupole momentum $Q_{ij} = \sum_n r_{ni} r_{nj}$

…based on the **Symplectic model**

Rosensteel & Rowe, PRL 38 (1977) 10

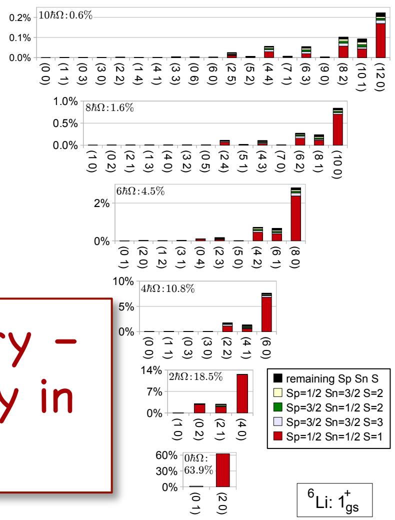
Going beyond – Symplectic basis

^{6}Li

^{6}Li g.st., JISP16

\# of configurations in N_{max}=12:

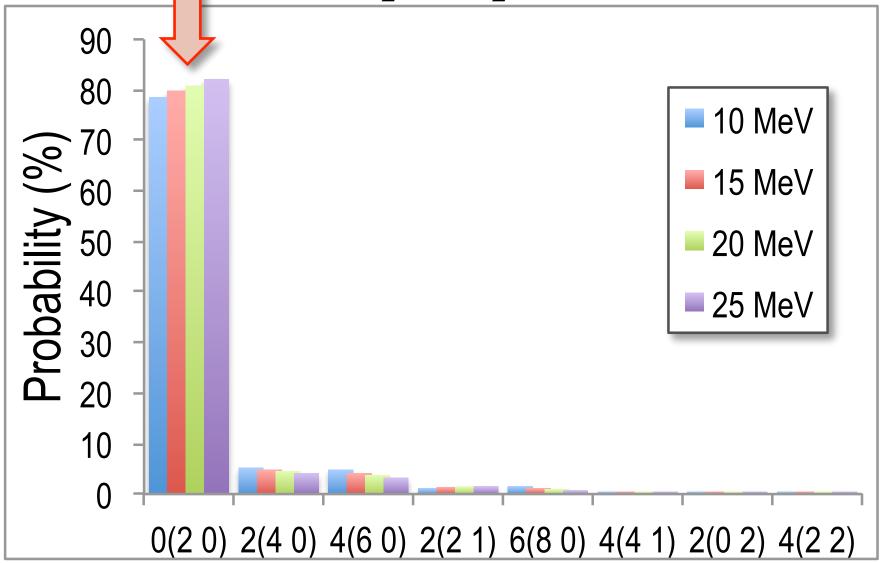
- *m*-scheme … 5x10^7
- *J*=1 … 4x10^6
- *J*=1 6<12> … 1.7x10^5
- Symplectic slices (95%) … 147



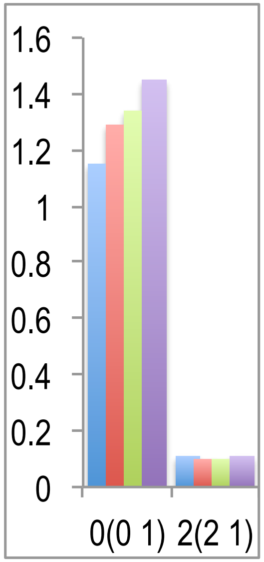
– Symplectic symmetry – *approximate* symmetry in nuclei

Symplectic slice starting at 0ħΩ (2 0) and expanding up to N_{max}=12

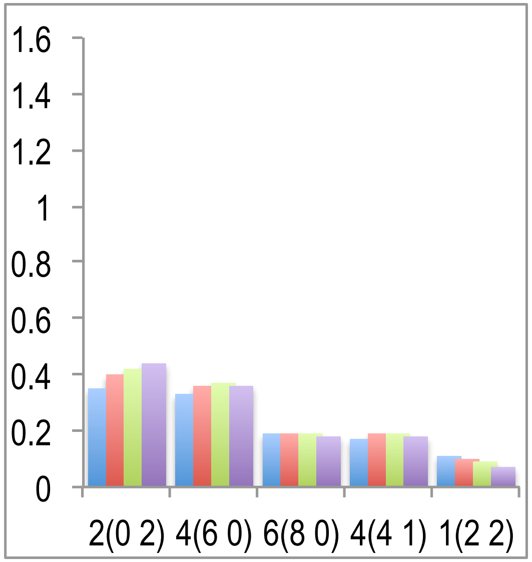
$S_p = \frac{1}{2} \quad S_n = \frac{1}{2} \quad S = 1$



$S_p = \frac{1}{2} \quad S_n = \frac{1}{2} \quad S = 0$

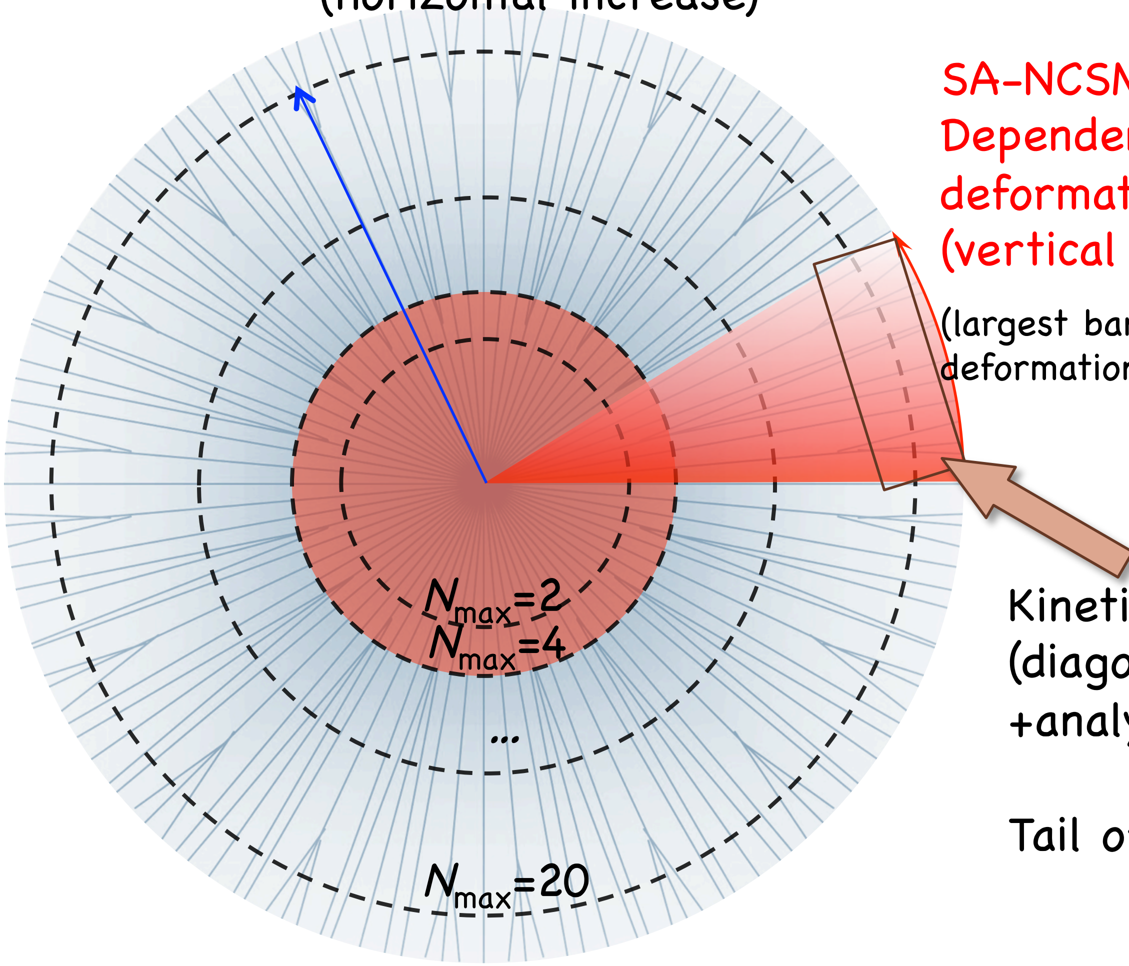


$S_p = \frac{3}{2} \quad S_n = \frac{3}{2} \quad S = 3$



Symmetry-guided selected model space

NCSM:
Dependence on N_{max}
(horizontal increase)



SA-NCSM:
Dependence on
deformation cutoff
(vertical increase)

(largest bandhead
deformation first)

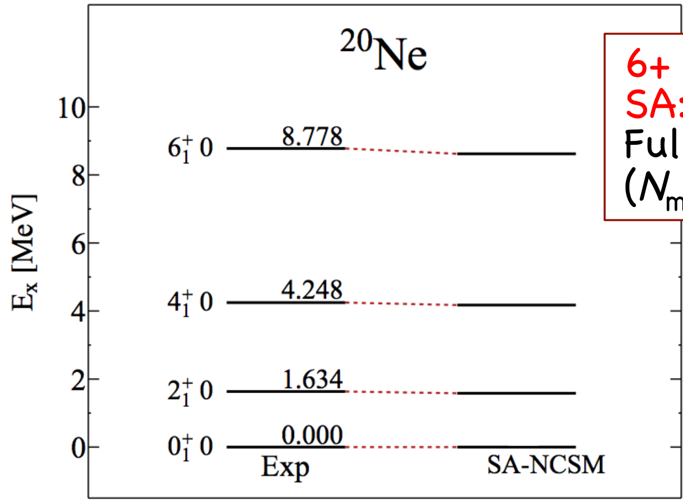
Kinetic energy
(diagonal in a symplectic slice
+analytic matrix elements)

Tail of wavefunctions

Ne Isotopes

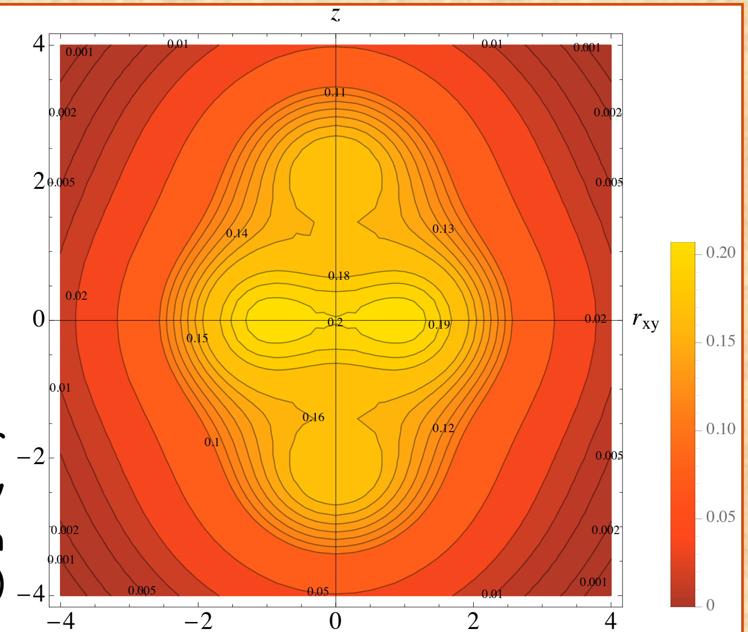
^{20}Ne

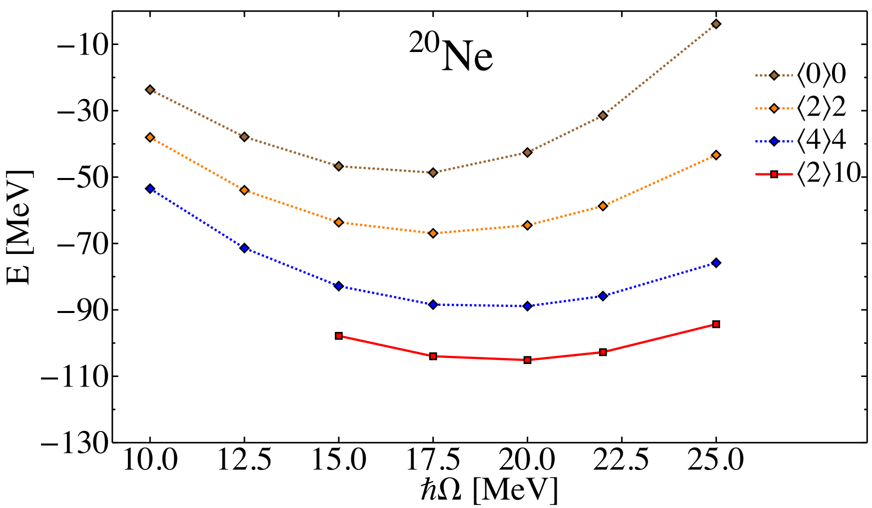
N2LOopt, $\hbar\Omega$=15 MeV, N_{max}=<2>10, 13 HO shells

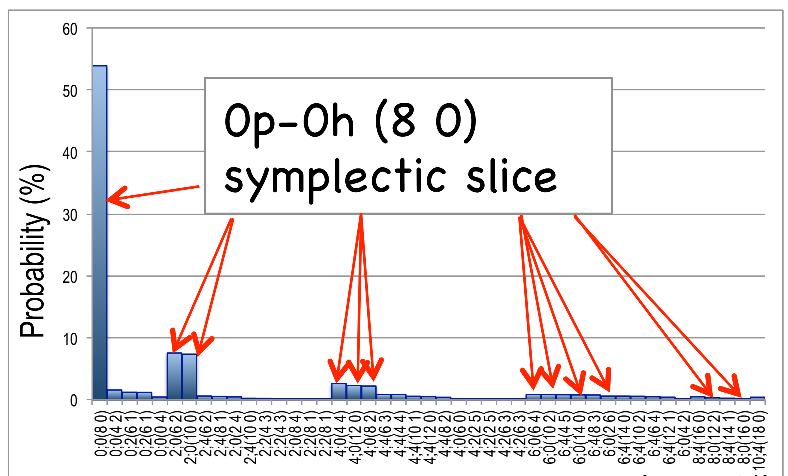


6+
SA: 51x10^6
Full: 4.4x10^{11}
(N_{max}=10: 1x10^{12})

Matter density (states with P>2.5%)







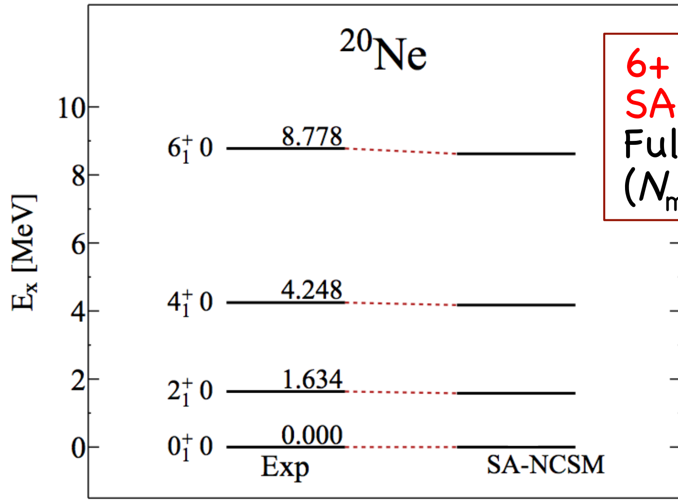
(P>0.1%)

Dytrych, Launey, Draayer, et al., LSU Preprint PA/NP2015-0002 (2015)

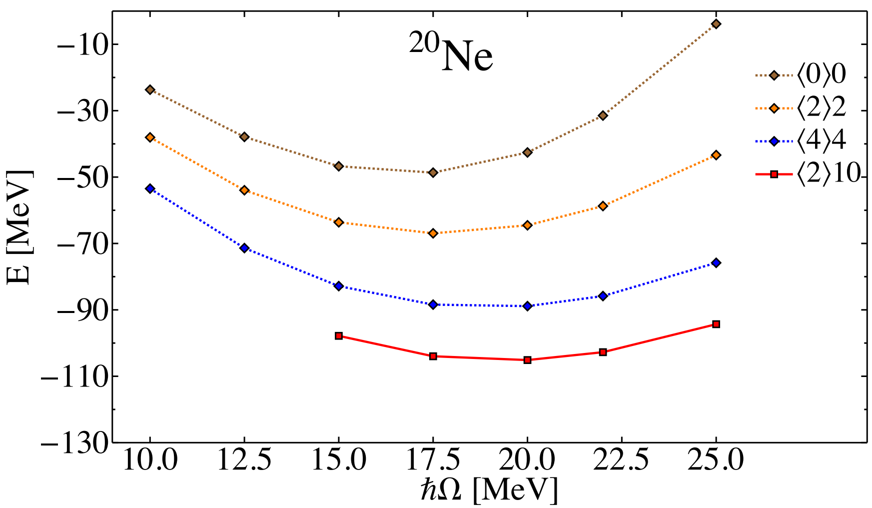
Ne Isotopes

^{20}Ne, ^{24}Ne, ^{32}Ne

N2LOopt, $\hbar\Omega$=15 MeV, N_{max}=<2>10, 13 HO shells

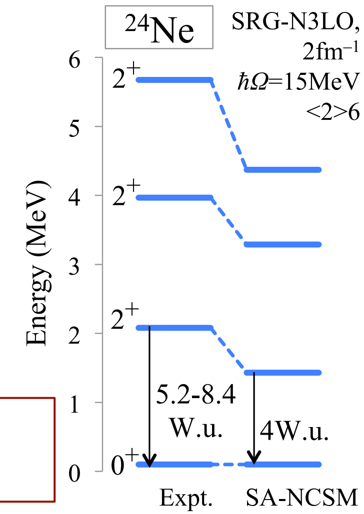


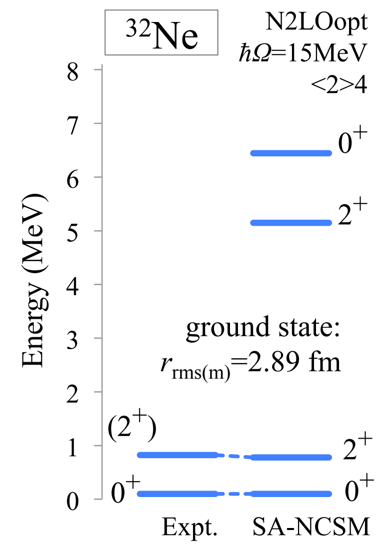
6+
SA: 51×10^6
Full: 4.4×10^{11}
(N_{max}=10: 1×10^{12})



SA: 3×10^6
Full: 8×10^9

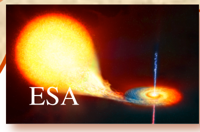
(pf)
SA: 0.5%





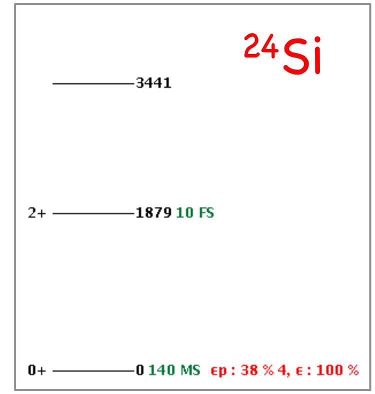
Robert Baker et al. (2015)

Ab initio modeling… New domains



X-ray burst nucleosynthesis

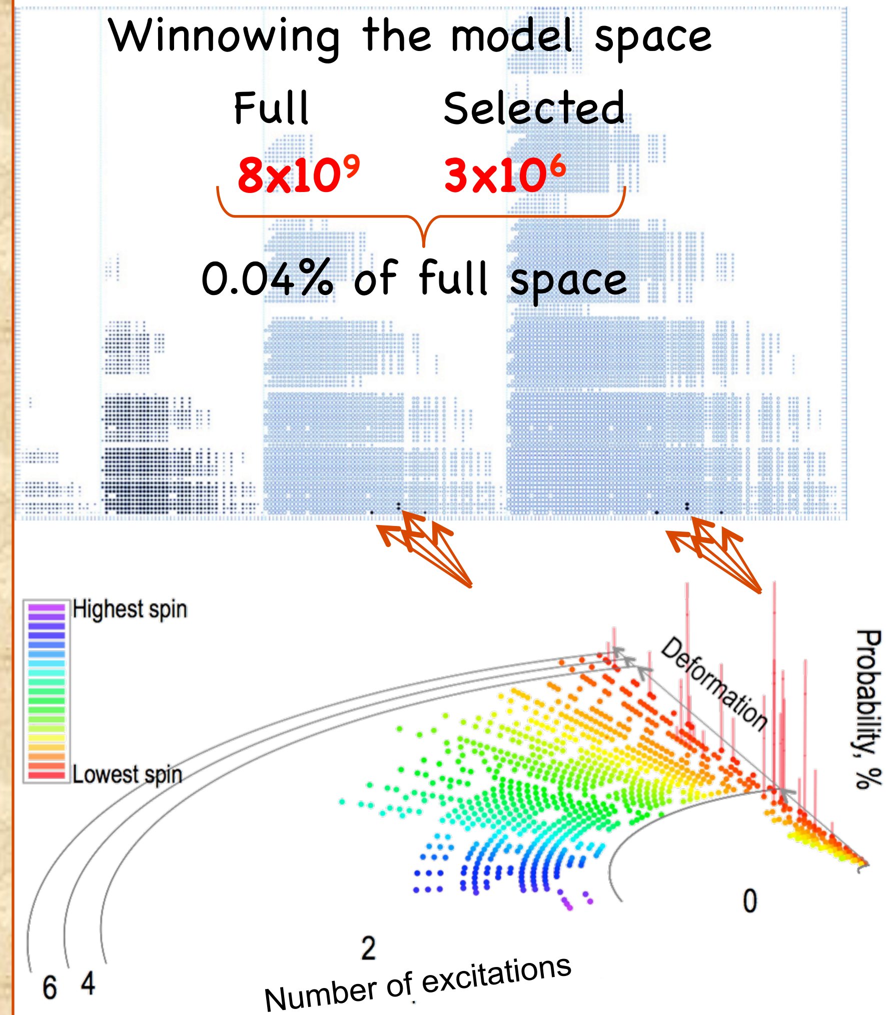
$^{23}Al(p,\gamma)^{24}Si$

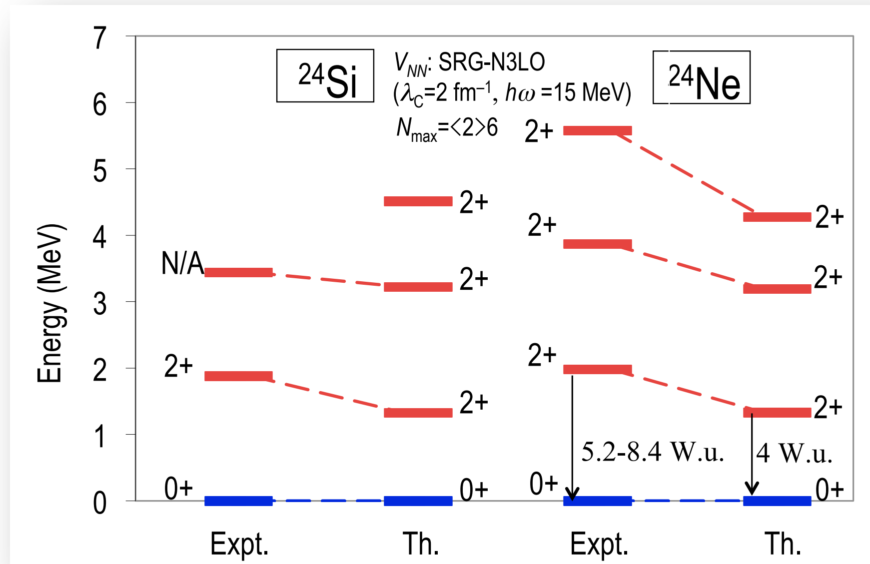


Winnowing the model space

Full 8×10^{9} Selected 3×10^{6}

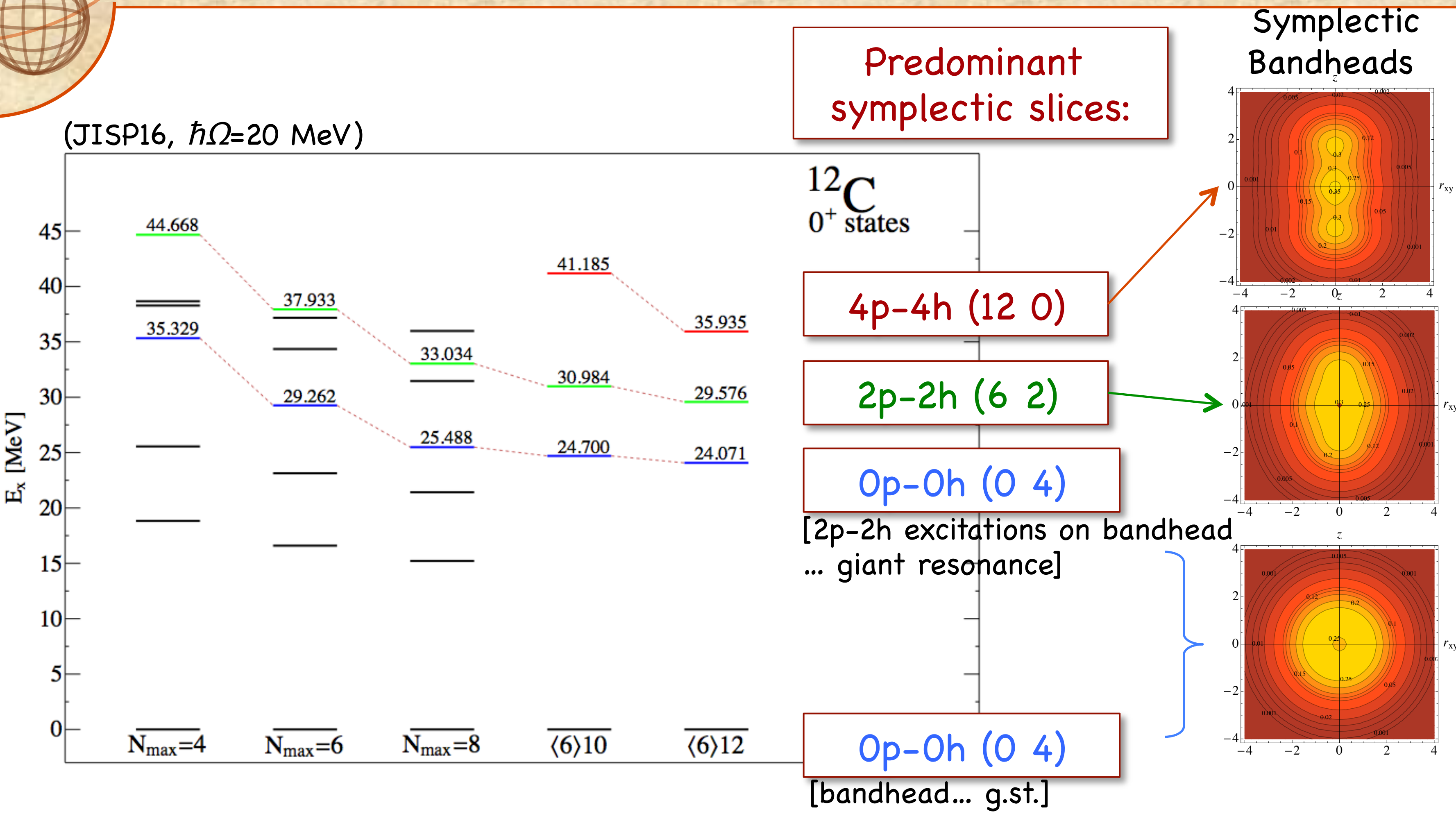
0.04% of full space





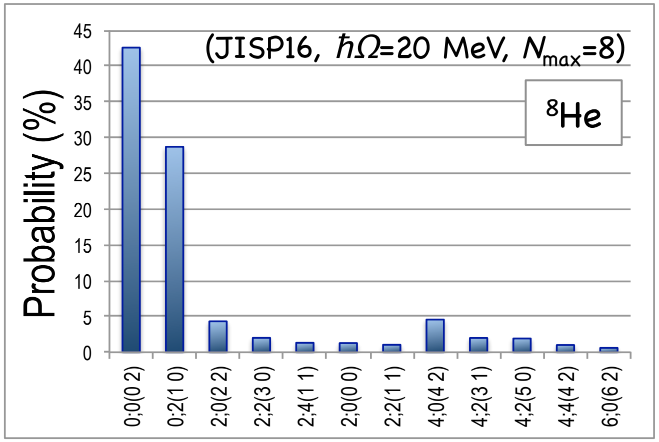
Yearbook of Science & Technology, YB140314, Dytrych, Launey, Draayer (2014)

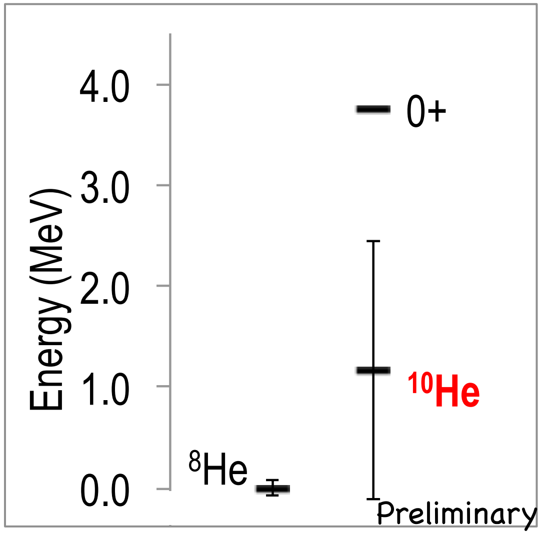
Ab initio SA-NCSM … the Hoyle state



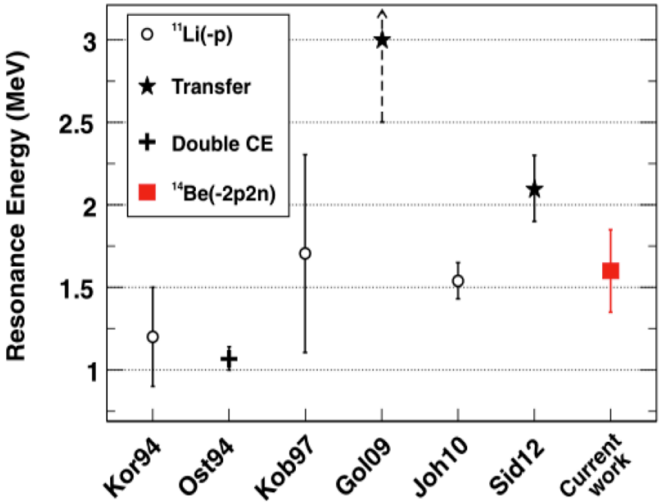
Neutron-rich He-10

B. Harvie,
REU, Summer 2014





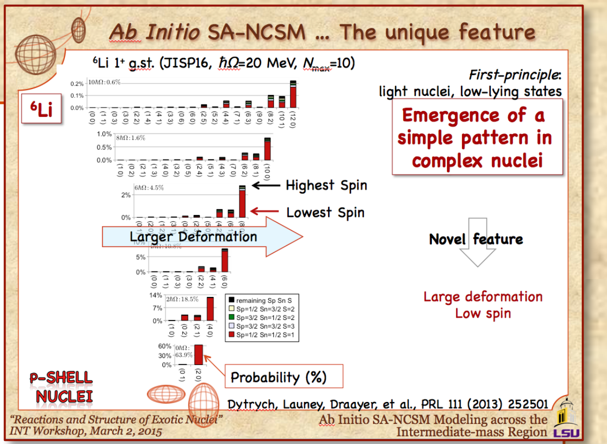
Extrapolations of SA-selected model spaces to full space [based on EFT-motivated approach … Furnstahl/Hagen/Papenbrock, Phys. Rev. C 86 (2012) 031301(R)]

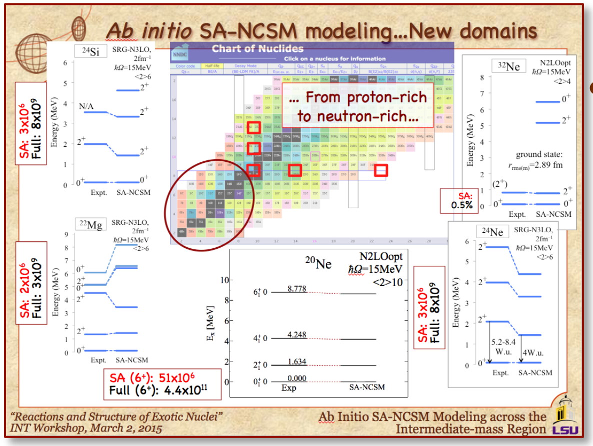


Z. Kohley et al. "Unresolved Question of the 10He Ground State Resonance", PRL 109 (2012) 232501

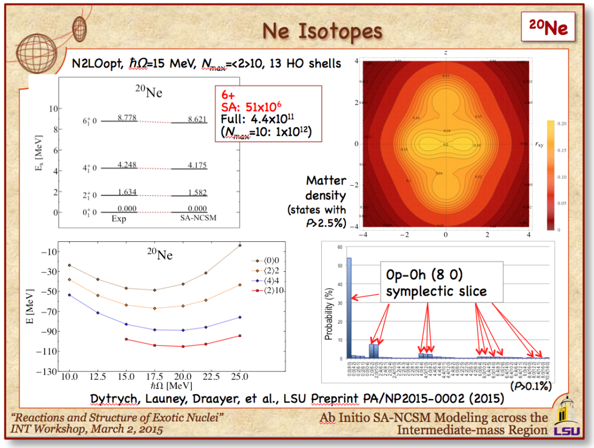
Summary

- The SA-framework: *ab (initio* + equal NCSM + efficient (physically relevant) organization of space + exact CM factorization





- SA-NCSM designed to reach ultra-large shell-model spaces … *ab initio* descriptions for sd (pf) shells/larger model spaces



- With a view toward studies of reactions, informed by *ab initio* SA-NCSM structure calculations