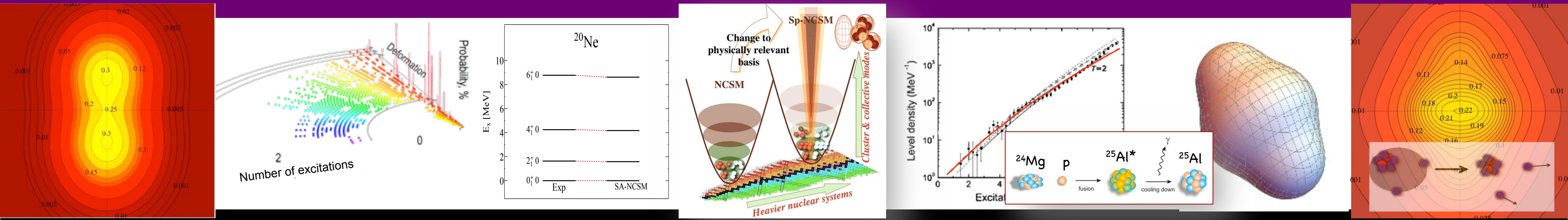
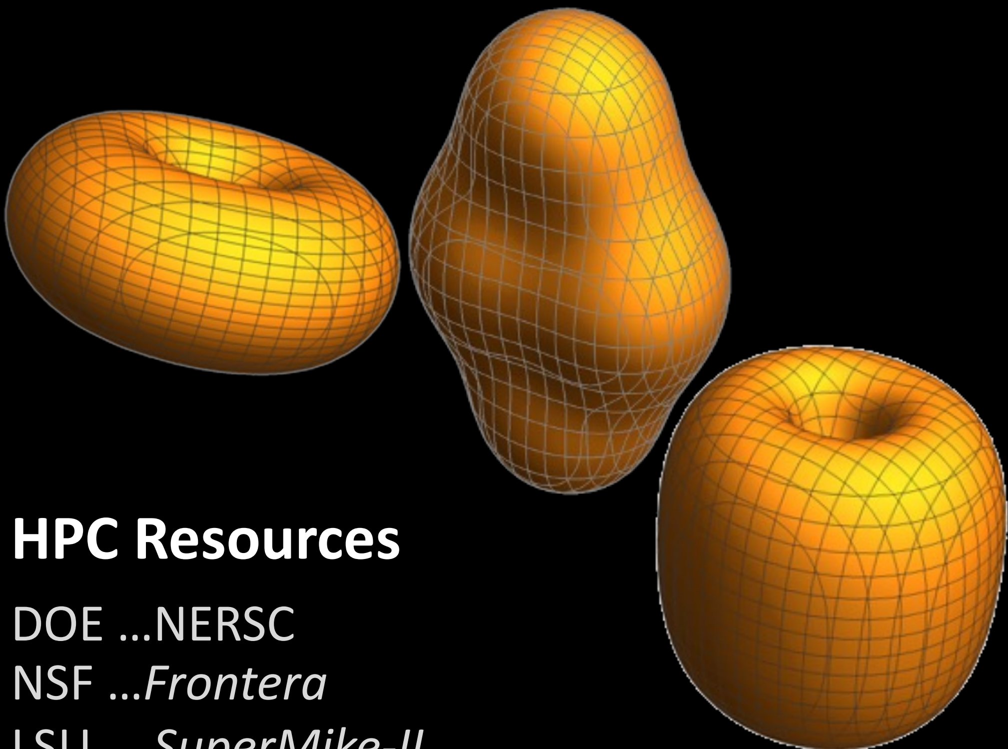


Eigenvector Continuation and Emulation With the Symmetry-Adapted No-Core Shell Model



Kevin Becker (LSU)

… In Collaboration With…

Kristina Launey (LSU), Andreas Ekström (Chalmers), Tomas Dytrych (Czech Ac. Sci.), Daniel Langr (Czech Ac. Sci.), Grigor Sargsyan (LLNL), Jerry Draayer (LSU)

HPC Resources

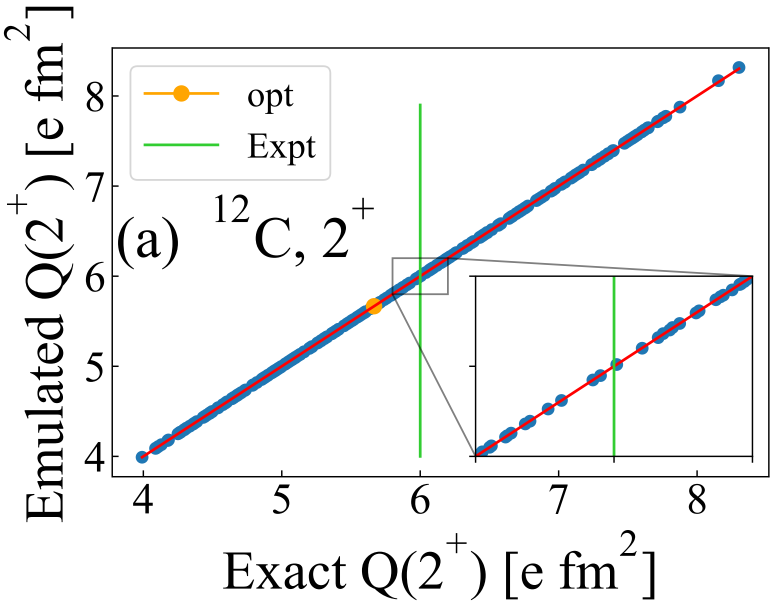
DOE …NERSC
NSF …*Frontera*
LSU … *SuperMike-II*

Supported by NSF & DOE

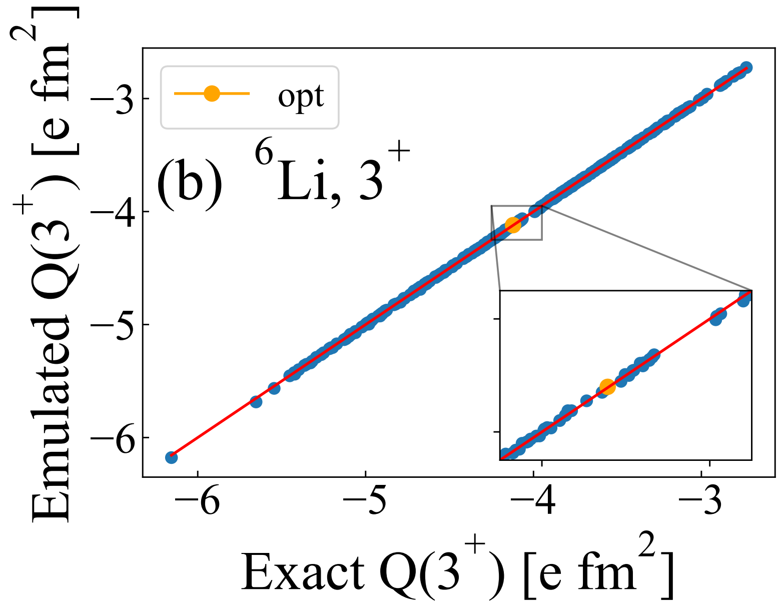
Emulators Work Great – But Why??

Becker et al., Frontiers in Nucl. Phys., 2023

Uniformly sample set of model parameters $\vec{c}$



32 x 32
matrices
1 process

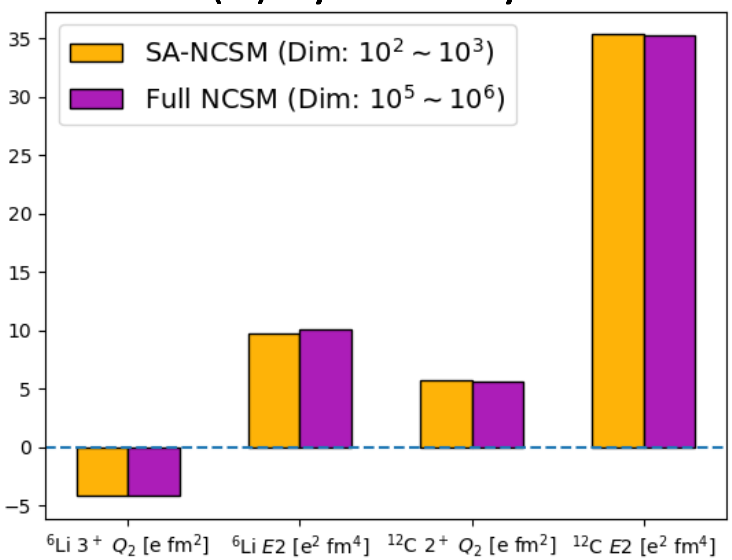


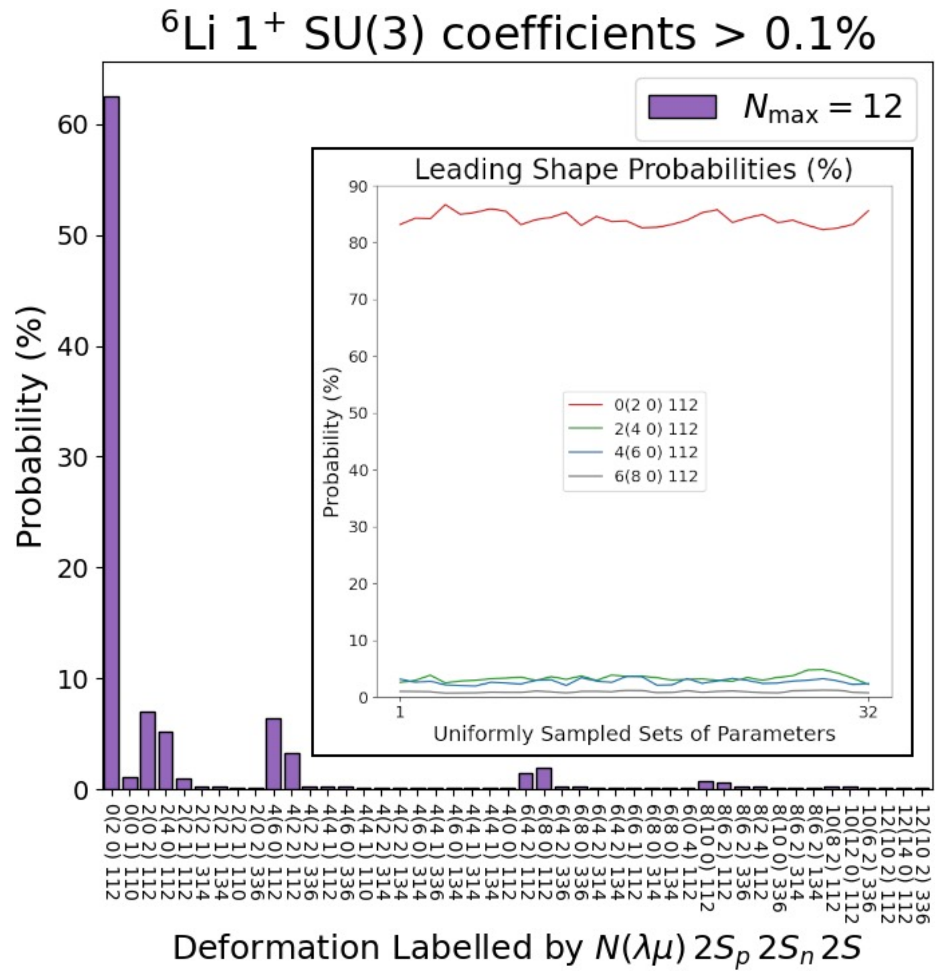
SA Basis:
238 x 238 matrices
Full basis:
5×10^6 x 5×10^6 matrices
10,584 parallel processes!!!

SA Basis:
9,108 x 9,108 matrices
Full basis:
3×10^5 x 3×10^5 matrices
168 parallel processes!

Group Theory and Near-Perfect Symmetry!

- Near-perfect Sp(3,R) symmetry guarantees wave functions depend smoothly on model parameters
- Very small subset of configurations contribute due to SU(3) symmetry

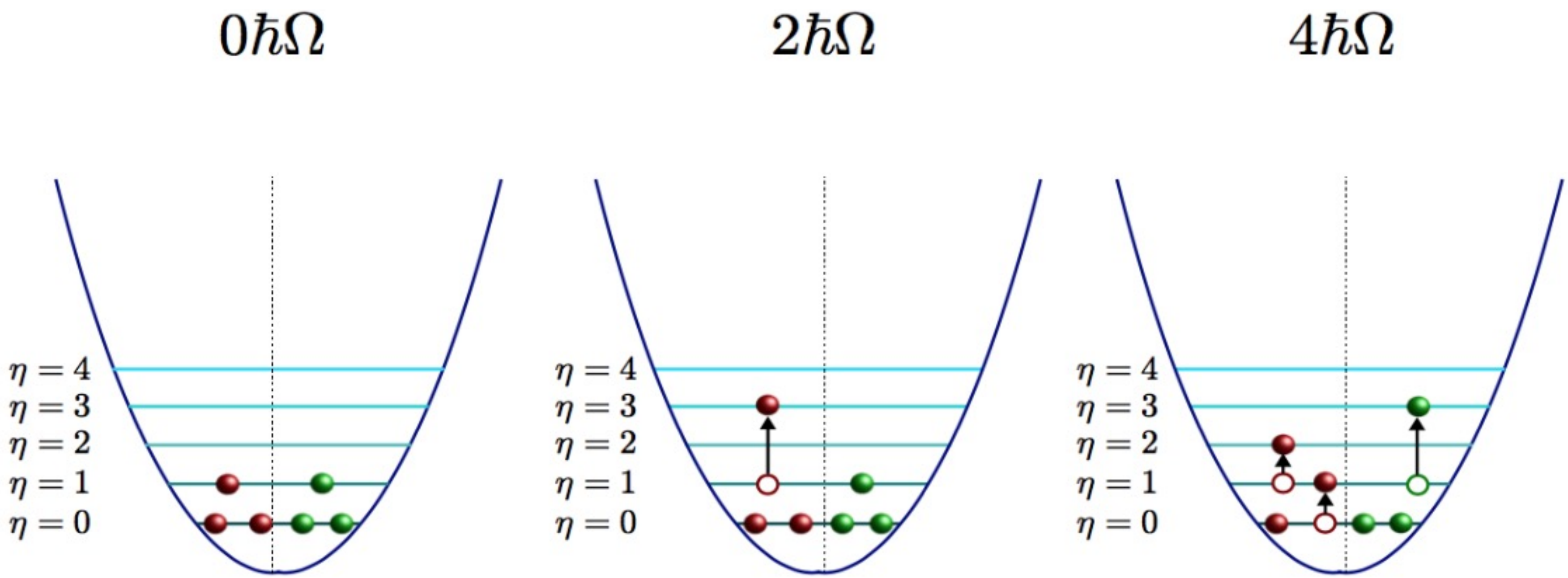




- Exploiting these symmetries provides an excellent emulator for the full many-body problem

Nuclear Many-Body Problem: No-Core Shell Model

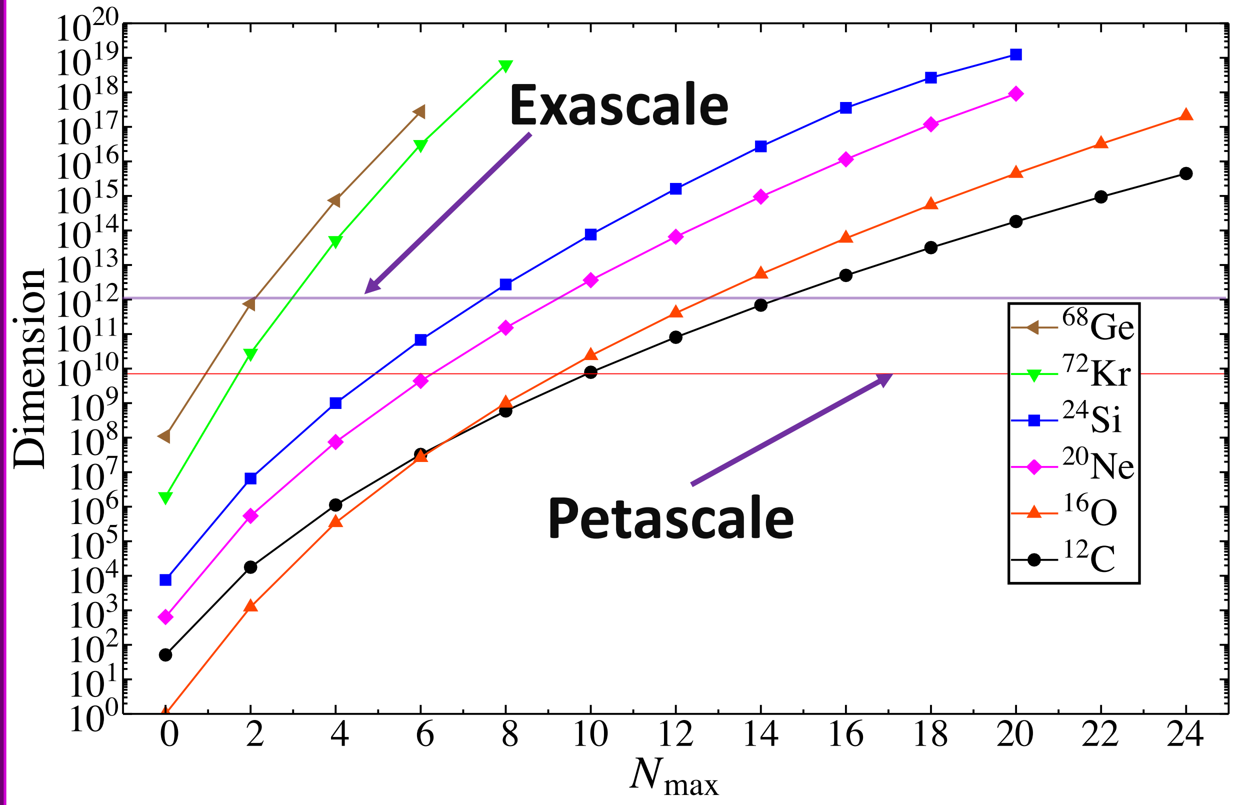
- Goal: solve the *A*-body Schrödinger equation for a nucleus with *A* particles
- Use antisymmetrized products of well-known single-particle 3D harmonic oscillator eigenstates

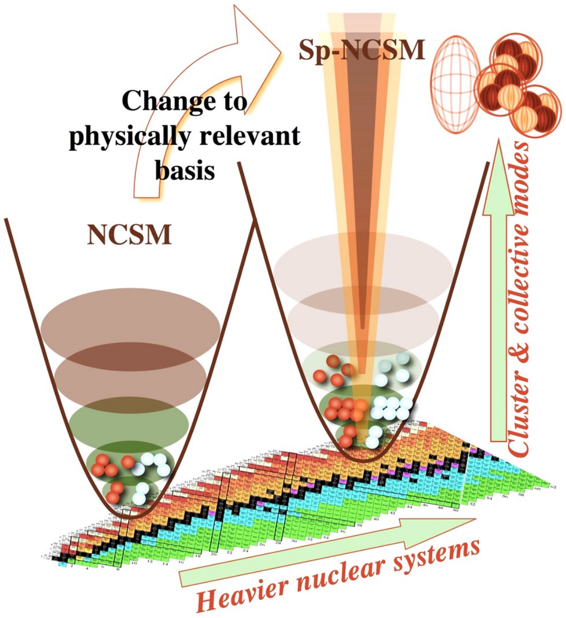


- Truncate infinite dimensional space up to cutoff in excitations: N_{max}

Solving the Many-Body Problem: No-Core Shell Model

- Principal difficulty: Dimension explodes combinatorically with A and N_{max}!





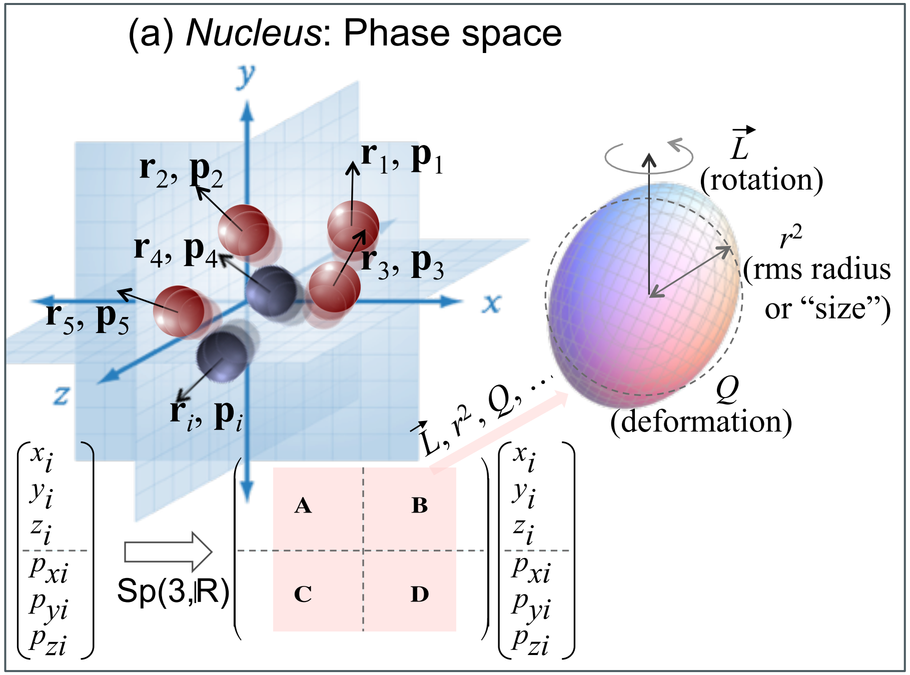
Sp(3,R) Algebra

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:

$$Q_{\alpha\beta} = \sum_{i=1}^{A} x_{i\alpha} x_{i\beta}$$

$$S_{\alpha\beta} = \sum_{i=1}^{A} (x_{i\alpha} p_{i\beta} + p_{i\alpha} x_{i\beta})$$

$$L_{\alpha\beta} = \sum_{i=1}^{A} (x_{i\alpha} p_{i\beta} - x_{i\beta} p_{i\alpha})$$

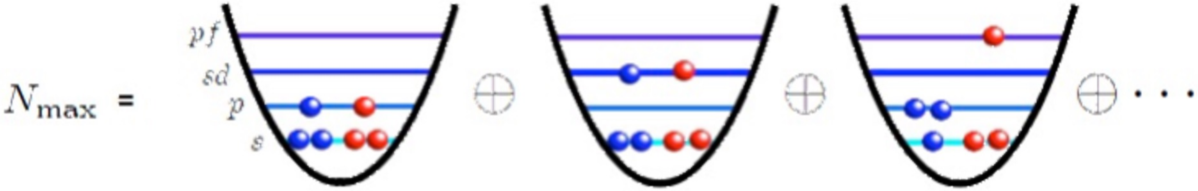
$$K_{\alpha\beta} = \sum_{i=1}^{A} p_{i\alpha} p_{i\beta}$$

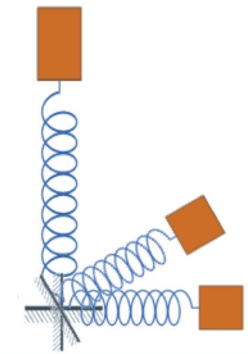
U(3)
in a HO shell
(Elliott, 1958)

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

Constructing the 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:

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

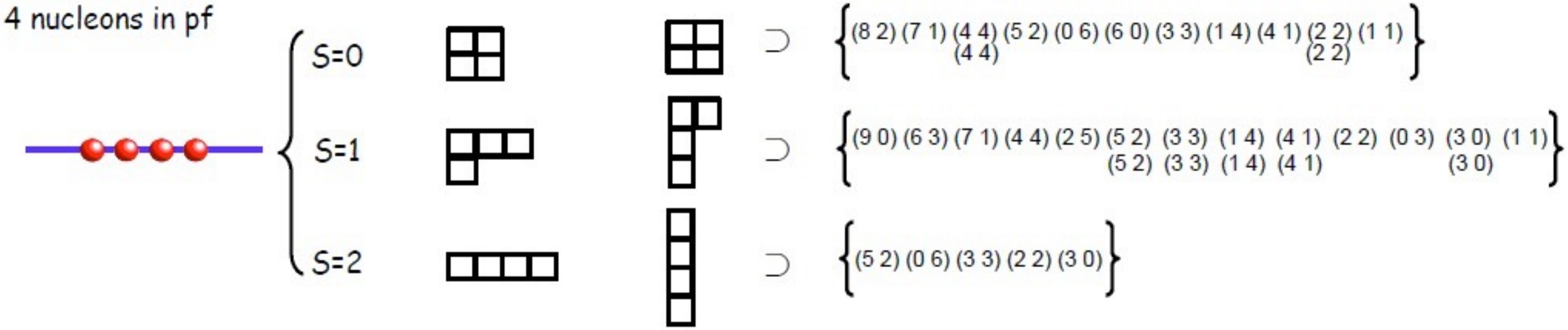
[…not used]

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

Fast basis construction! … based on Gel'fand patterns

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

- Example:
  4 nucleons in pf

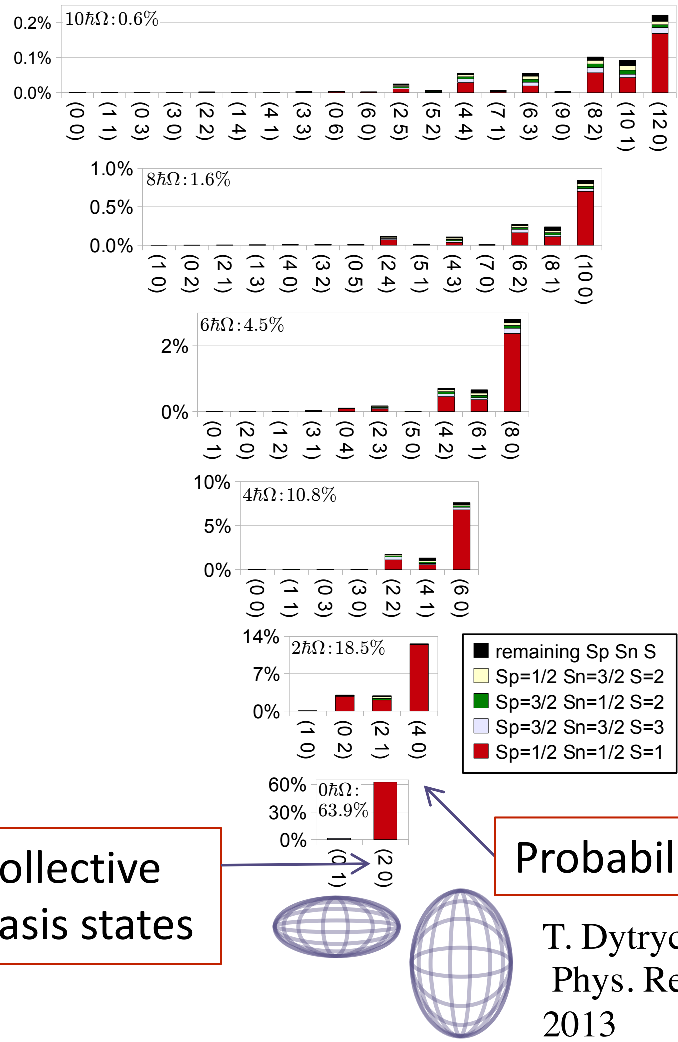


… followed by multi-shell coupling of SU(3) configurations

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

Wave Functions in the SA-NCSM

^{6}Li 1^+



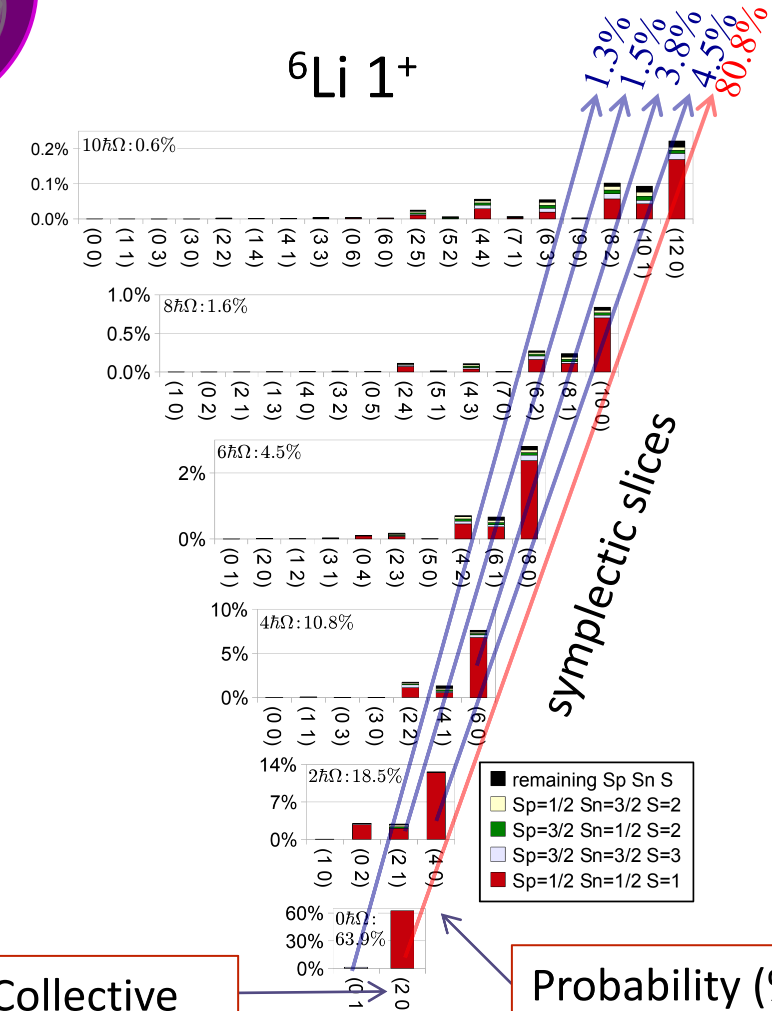
Collective basis states

Probability (%)

T. Dytrych,
Phys. Rev. Lett. 111, 252501
2013

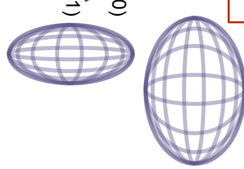
- Express nuclear wave functions in terms of states with definite deformation – SU(3)-adapted basis

Wave Functions in the SA-NCSM



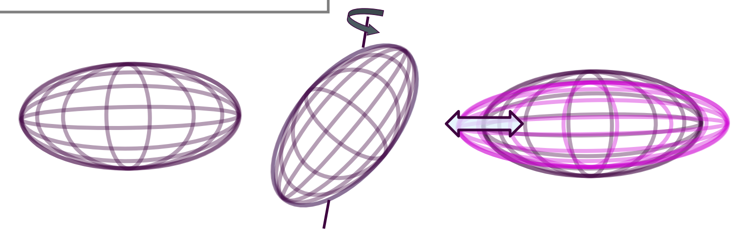
Collective basis states

Probability (%)



T. Dytrych, Phys. Rev. Lett. 111, 252501 2013

Symplectic slice:



- Express nuclear wave functions in terms of states with definite deformation – SU(3)-adapted basis
- Further organize SU(3) states into Sp(3,R) irreps – Sp(3,R)-adapted basis

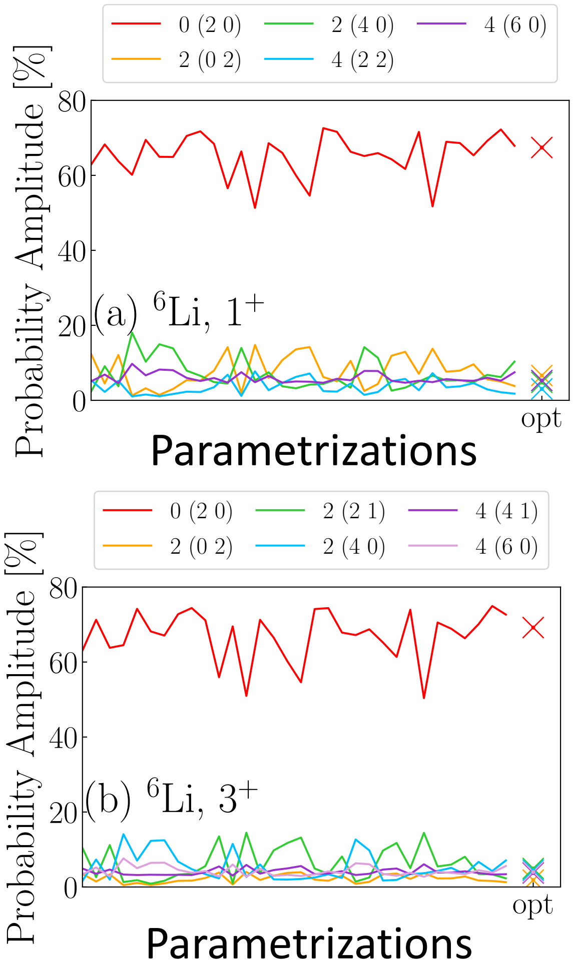
Approximate symplectic symmetry in nuclei

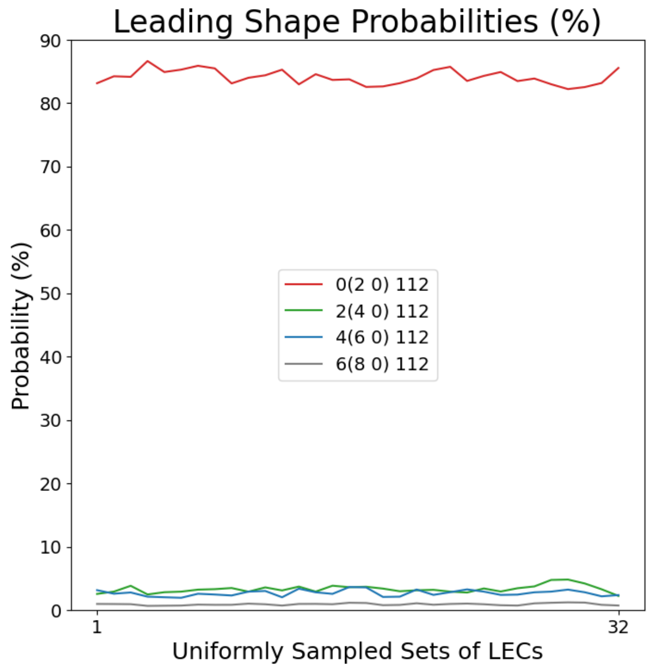
Model for the Nuclear Hamiltonian

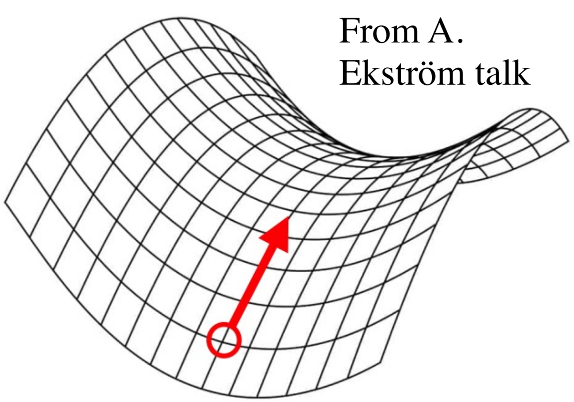
$$\hat{H} = \hat{H}_0 + \sum_{i=1}^{14} c_i \hat{H}_i$$

- $\hat{H}_0$: Kinetic Energy + Coulomb repulsion + parameter-independent terms
- $\hat{H}_i$: Realistic nucleon-nucleon interaction terms derived from chiral effective field theory at next-to-next-to-leading order
- c_i: Unknown **l**ow-**e**nergy **c**onstants (**LEC**s) that tie physics of nuclei to elementary particle interactions at low energies

The Ingredients of Eigenvector Continuation!







Wave function coefficients vary smoothly with parameters

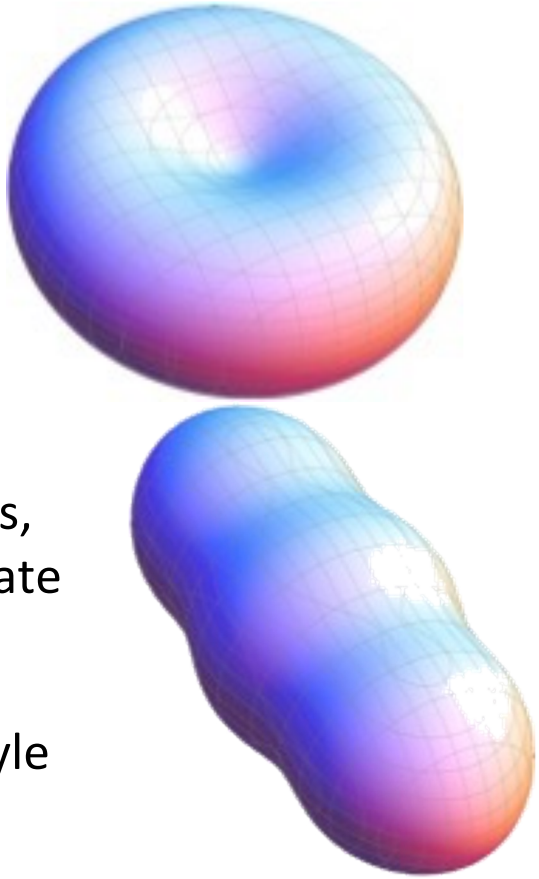
Out of thousands, only a few dozen contribute above 0.1%

An even smaller subset vary appreciably with parameters

The wave function traces out a trajectory in a low-dimensional subspace of the model

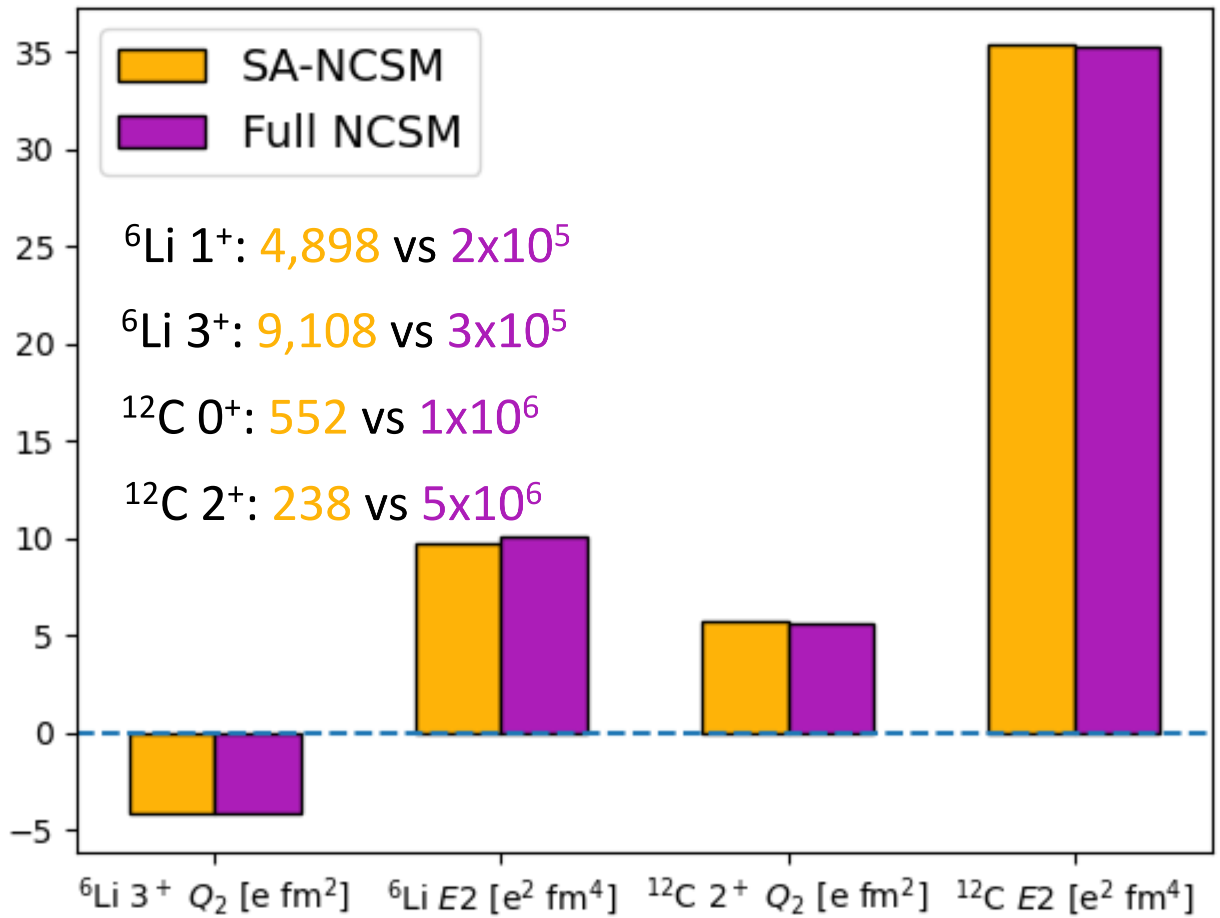
Becker et al., Frontiers in Nucl. Phys., 2023

Eigenvector Continuation: ^{12}C



- Consider the 0^+ ground state of ^{12}C: predominantly
- Emulator trained on g.s. wave functions can predict the next 0+: dominated by the same shapes
- The Hoyle state is described by very different physics, different shape. This may mix slightly into ground state only at very large N_{max}
- We need an emulator that includes ground AND Hoyle state physics, degrees of freedom!
- Difficulty of training EVC emulator scales ~ linearly with number of shapes; not too hard to train on both!

SA-NCSM Provides a Highly Effective Emulator!



Becker et al., Frontiers in Nucl. Phys., 2023

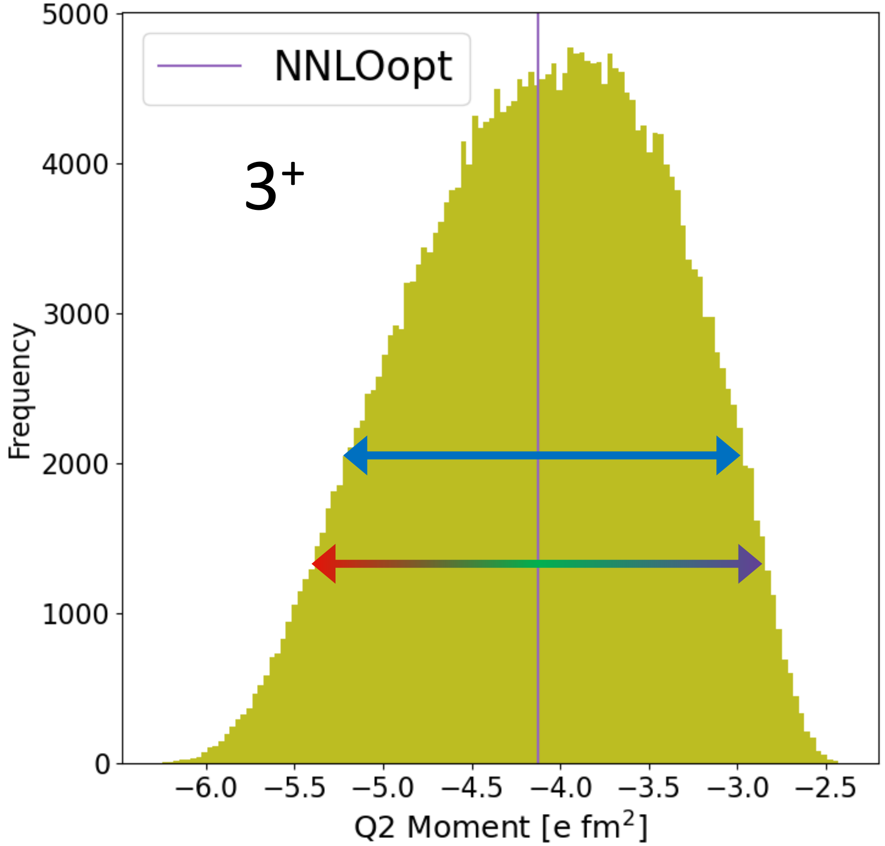
Which Parameters Are Most Important?

$$\hat{H} = \hat{H}_0 + \sum_{i=1}^{14} c_i \hat{H}_i$$

- **High-precision nuclear physics: accurate fitting and uncertainty quantifications of LECs c_i is required**
- **Question: Which (if any!) LECs have the greatest impact on collective properties of the nucleus?**

Global Sensitivity Analysis

Global Sensitivity Analysis: how does uncertainty in parameters cause uncertainty in nuclear observables?



Distribution of Q2 Moments in ^{6}Li, 10 HO Shells

Var[Q2]

Partial Variances

Break down width into contributions from different parameters

ANOVA Representation

- $Q_2 = f(\vec{c})$

- Expand f into the following series:

$$f_0 + \sum_{i=1}^{d} f_i(c_i) + \sum_{i<j}^{d} f_{ij}(c_i, c_j) + \sum_{i<j<k}^{d} f_{ijk}(c_i, c_j, c_k) + \cdots + f_{1\ldots d}(\vec{c})$$

f_0	$f_i(c_i)$	$f_{ij}(c_i, c_j)$	$f_{ijk}(c_i, c_j, c_k)$	$f_{1\ldots d}(\vec{c})$
LEC-independent	single-variable contribution	two-variable contribution	three-variable contribution	*d*-variable contribution

Decomposition into Partial Variances

- One can show that

$$\int f^2(\vec{x})\,d\vec{x} - f_0^2 = \sum_{i=1}^{d} \int f_i^2(x_i) dx_i + \sum_{i<j}^{d} \int f_{ij}^2(x_i, x_j)\, dx_i dx_j + \cdots$$

Var(Q_2) | **Single-variable contribution V_i** | **Two-variable contribution V_{ij}**

- ***First-Order Sensitivity Index:***

$$S_i = \frac{V_i}{\mathrm{Var}(Q_2)}$$

How much of the output variance is due to variance of c_i only?

- ***Second-Order Sensitivity Index:***

$$S_{ij} = \frac{V_{ij}}{\mathrm{Var}(Q_2)}$$

How much of the output variance is due to correlated variance of c_i and c_j?

Total-Order Sensitivity Effect

- We are most interested in the total sensitivity across all orders of correlation for the parameter c_i:

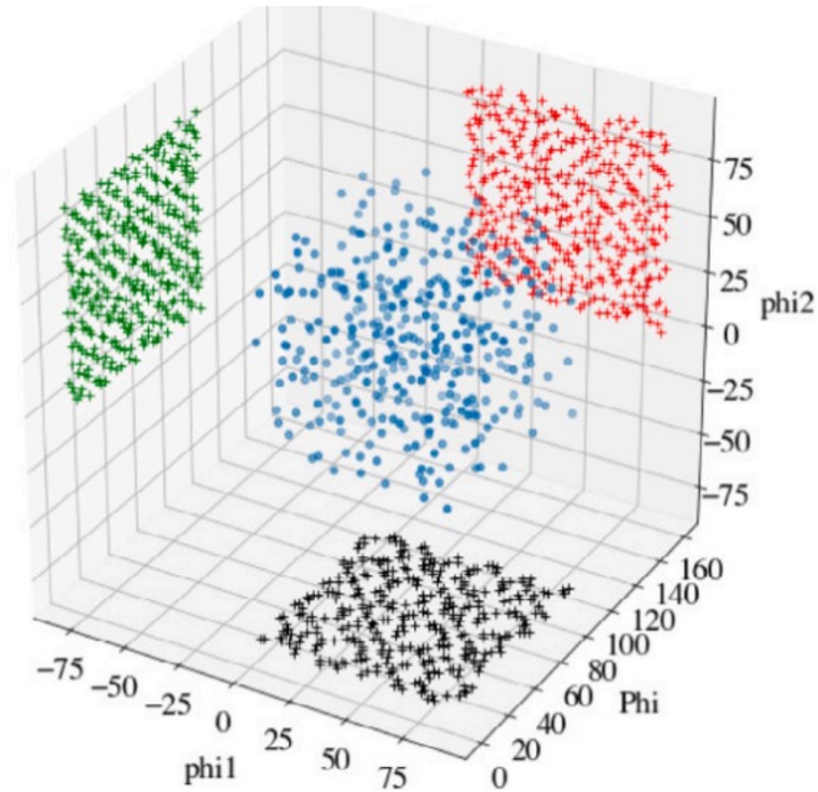
$$S_{Ti} = S_i + \sum_j S_{ij} + \sum_{jk} S_{ijk} + \cdots$$

- Each of the summands becomes progressively harder to evaluate…

- …But the total effect S_{Ti} can be well approximated with a single Monte Carlo integral

Saltelli Sampling Procedure

- A. Saltelli's method of drawing samples from a Sobol sequence
- Deterministic, based on number of parameters (14) and their ranges (±10% NNLOopt values)
- Evenly fill 14-dimensional hypercube *AND* **all** lower-dimensional hypersurfaces
- Huge number required for GSA convergence: $(d+1)\cdot 2^{d} \rightarrow$ 300,000



Ibragimova et al.,
Int. Journal of Plasticity,
103059, 2021

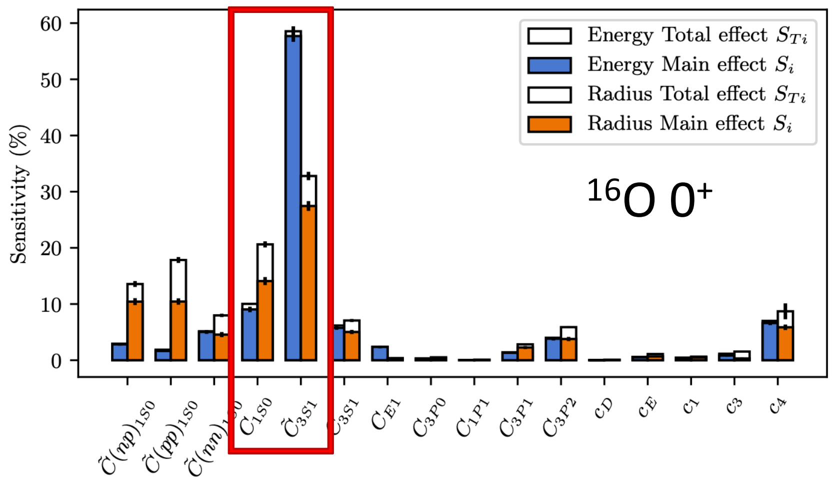
Enormous computational cost!

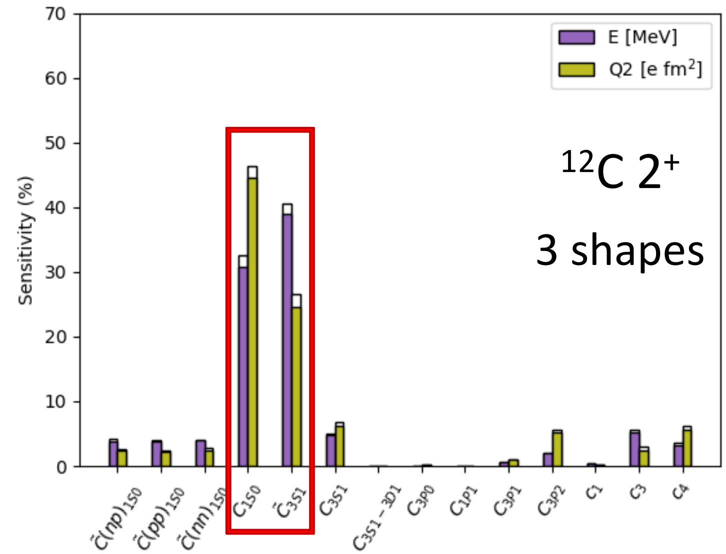
- ^{6}Li ground state, N_{max} = 8: dimension = 186,926
  - ~ 0.07 node-hours per evaluation: **21,000 for GSA**
- ^{6}Li ground state, N_{max} = 12: dimension = 3,948,000
  - ~ 9 node-hours per evaluation; **2.7 million for GSA!!**
- ^{12}C first excited 2^{+} state, N_{max} = 6: dimension = 5,025,653
  - ~ 18 node-hours per evaluation; **5.4 million for GSA!!**
- 12C first excited 2+ state, Nmax = 8: dimension = 78,814,670
  - ~3000 node-hours per evaluation! **900 million for GSA!!!!**

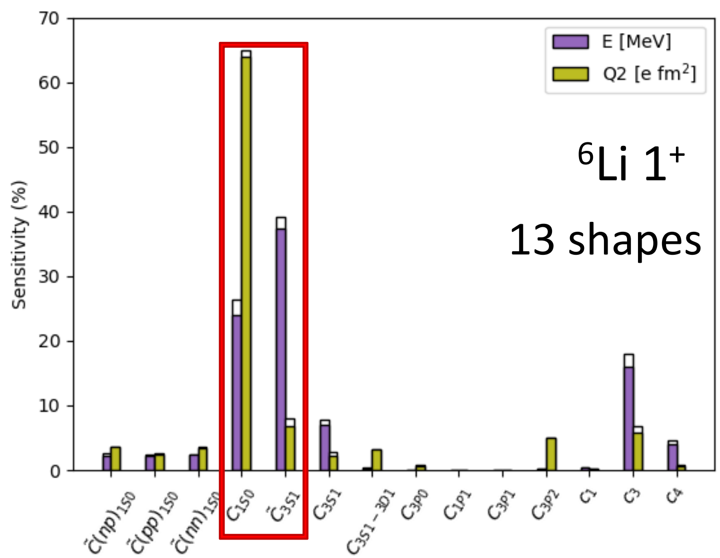
- Clearly, some kind of emulator is necessary to proceed!!
  - Or, combination of emulators…

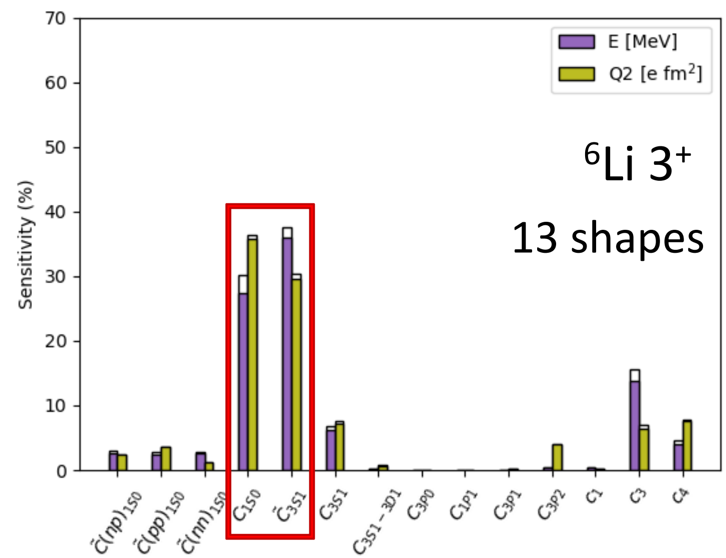
Sensitivity Indices: ^{16}O, ^{12}C, and ^{6}Li

A. Ekström
Phys. Rev. Lett. 123, 252501 (2019)



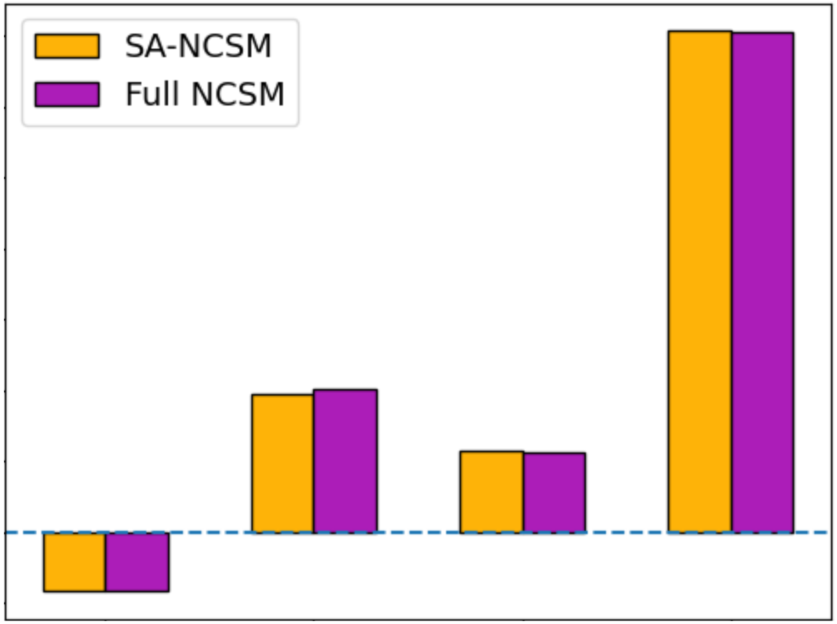


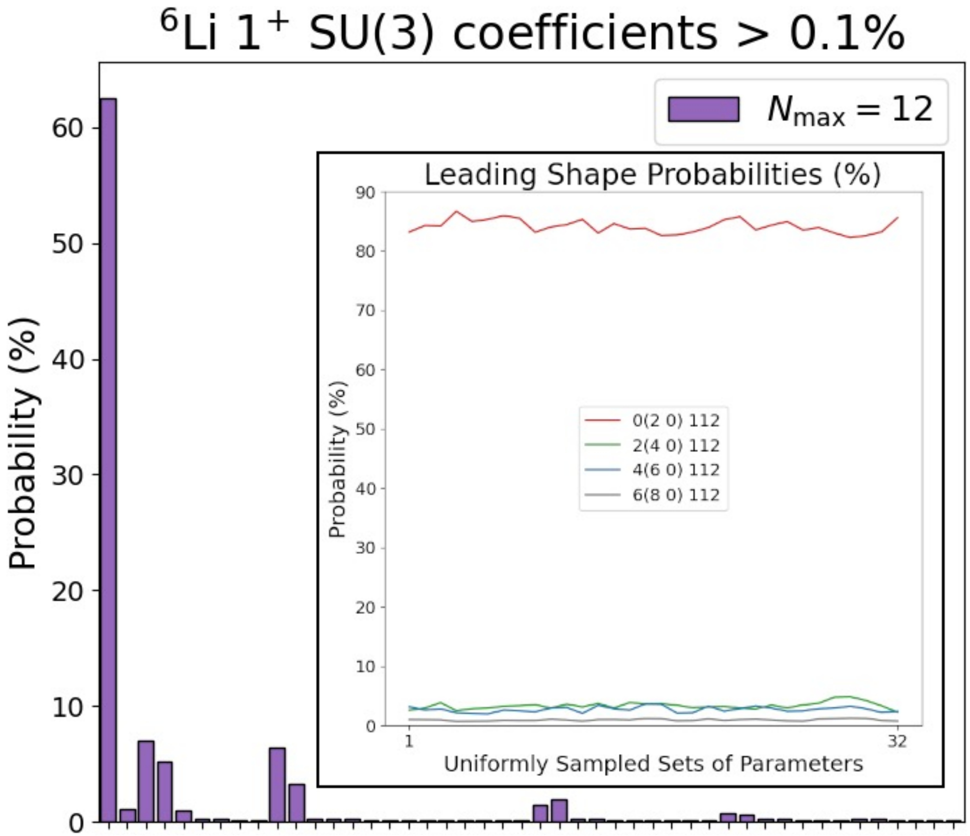




Summary

- Because of near-perfect symplectic symmetry and dominance of a small set of deformation…





- …The SA-NCSM is an effective emulator of the high-fidelity NCSM!