

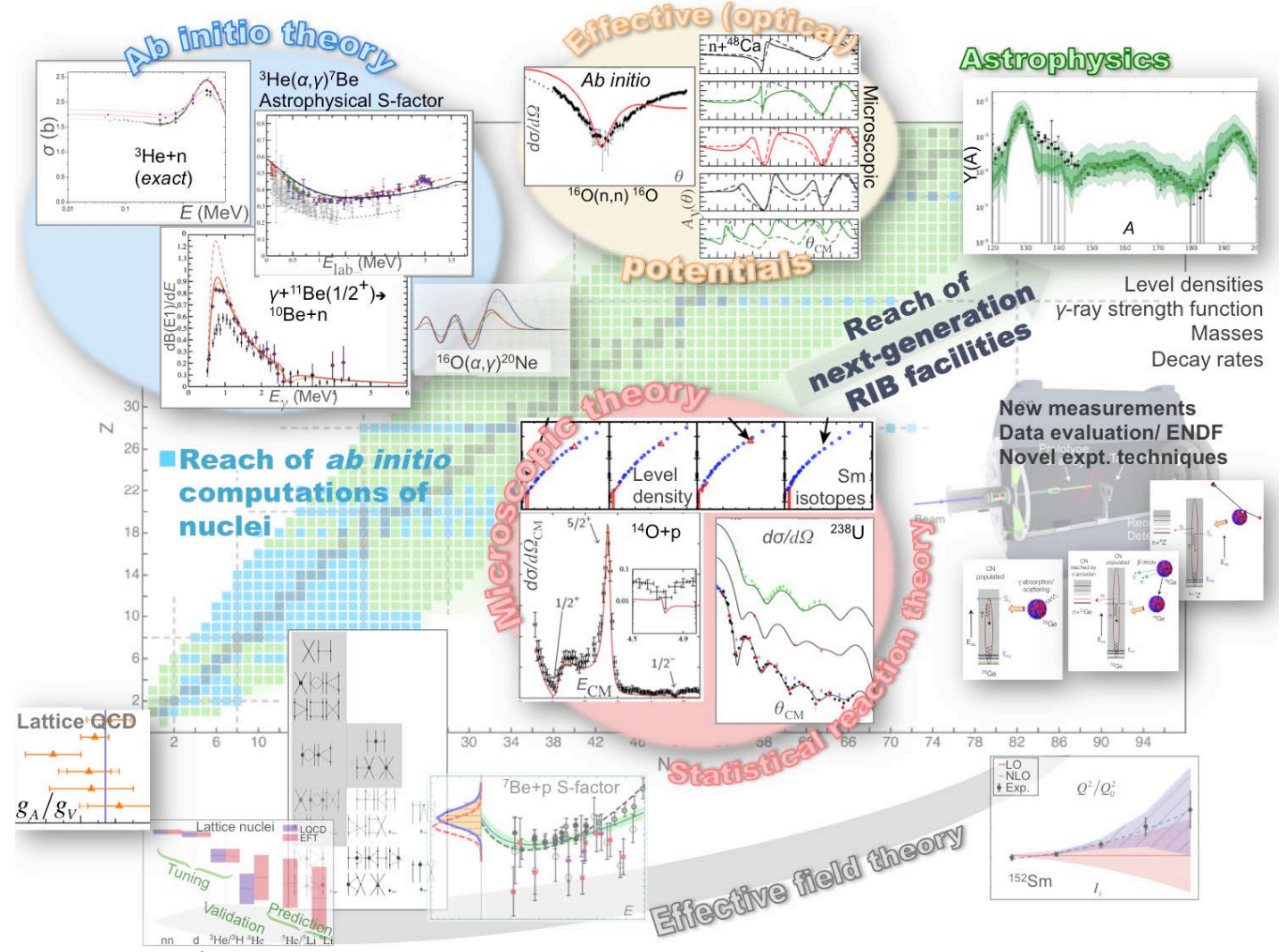
# Low Energy Nuclear Theory

KD Launey  
Louisiana State University

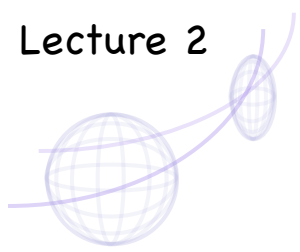


# Modeling nuclei: structure ...and reactions

I will focus on how to build on first principles (rooted in QCD)  
 ... EFT approaches are also powerful (halo-EFT, EFT for deformed nuclei, etc.)



From INT-17-1a program "Toward Predictive Theories of Nuclear Reactions Across the Isotopic Chart"



# Interaction Renormalization



Effective interactions...



# Effective interactions: renormalization

P+Q ... Infinite space

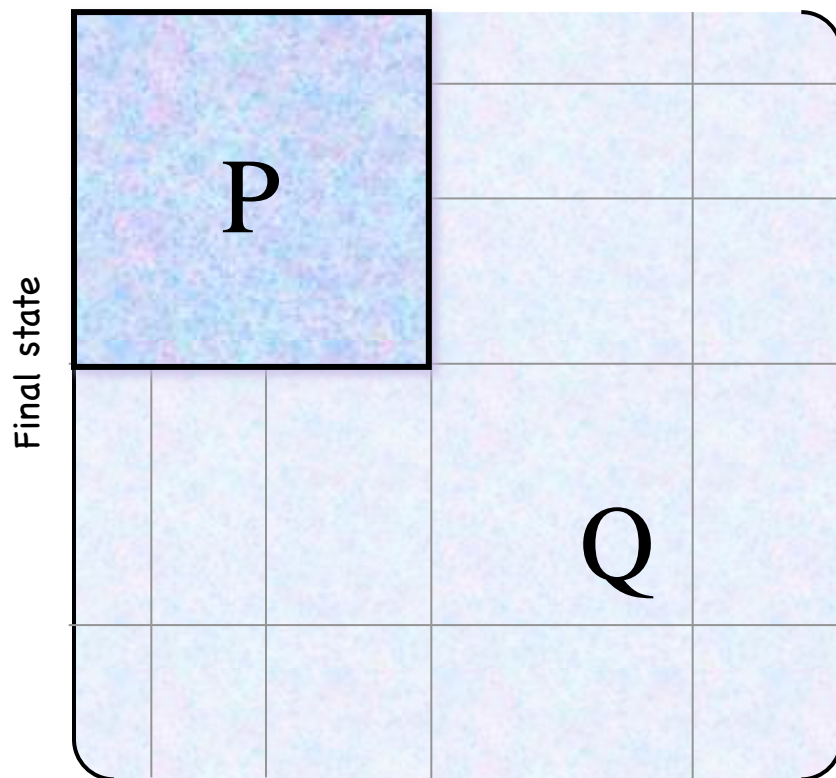


P ... Model space

$UHU^\dagger$

2 major techniques: Projection & Infinitesimal Rotations

Initial state



Excluded Space Q

$$H|\psi_k\rangle = E_k|\psi_k\rangle$$

$|\psi_k\rangle$

Model Space P  
 $H_{\text{eff}}|\xi_k\rangle = E_k|\xi_k\rangle$

$$|\xi_k\rangle = P|\psi_k\rangle$$

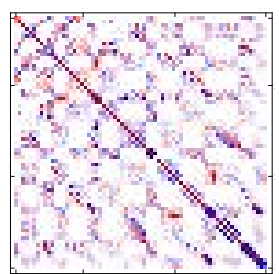
Lee-Suzuki technique:

Project to P space, while retaining the eigenvalues



# Similarity Renormalization Group (SRG)

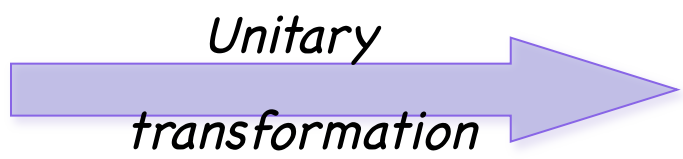
"Bare"  $H_{s=0}$



Large model space

"Simple" ... NN, 3N

$$H_s = U(s)H_{s=0}U^\dagger(s)$$

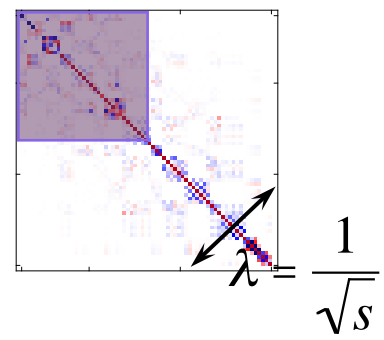


Many-body approach

Interaction

Renormalized...

$H_s$



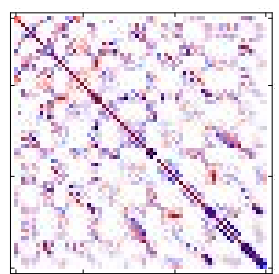
Small subspace

Complex ... many-body interactions (3b, 4b, 5b, etc.)

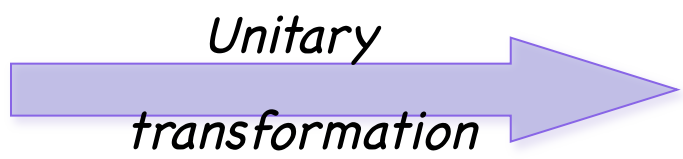


# Similarity Renormalization Group (SRG)

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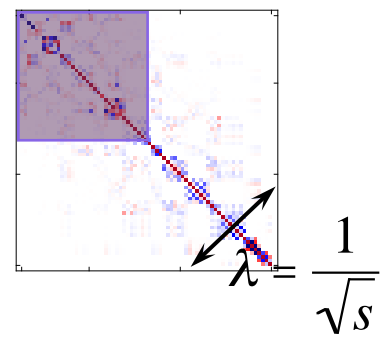


$$H_s = U(s)H_{s=0}U^\dagger(s)$$



Renormalized...

$H_s$

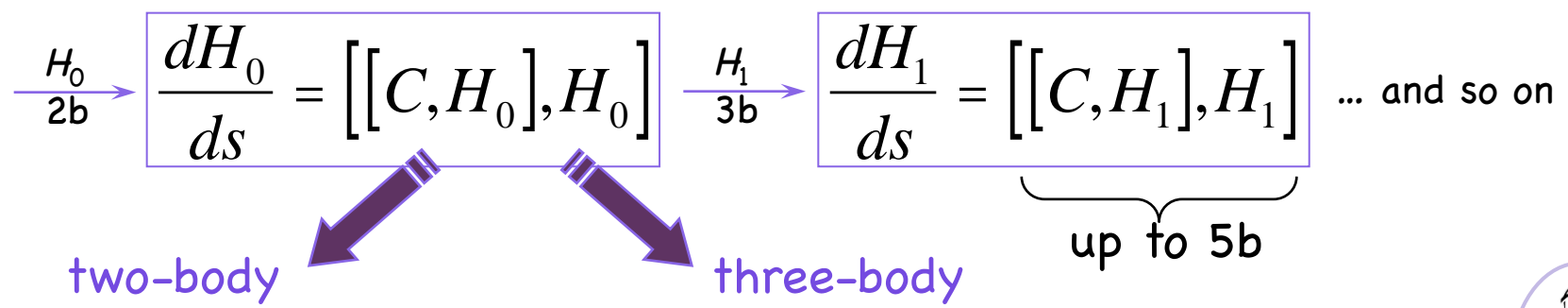


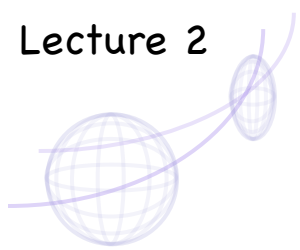
flow equation:

$$\frac{dH_s}{ds} = \left[ [C, H_s], H_s \right]$$

reference operators  
(C could be Trel, symmetry operator, etc.)

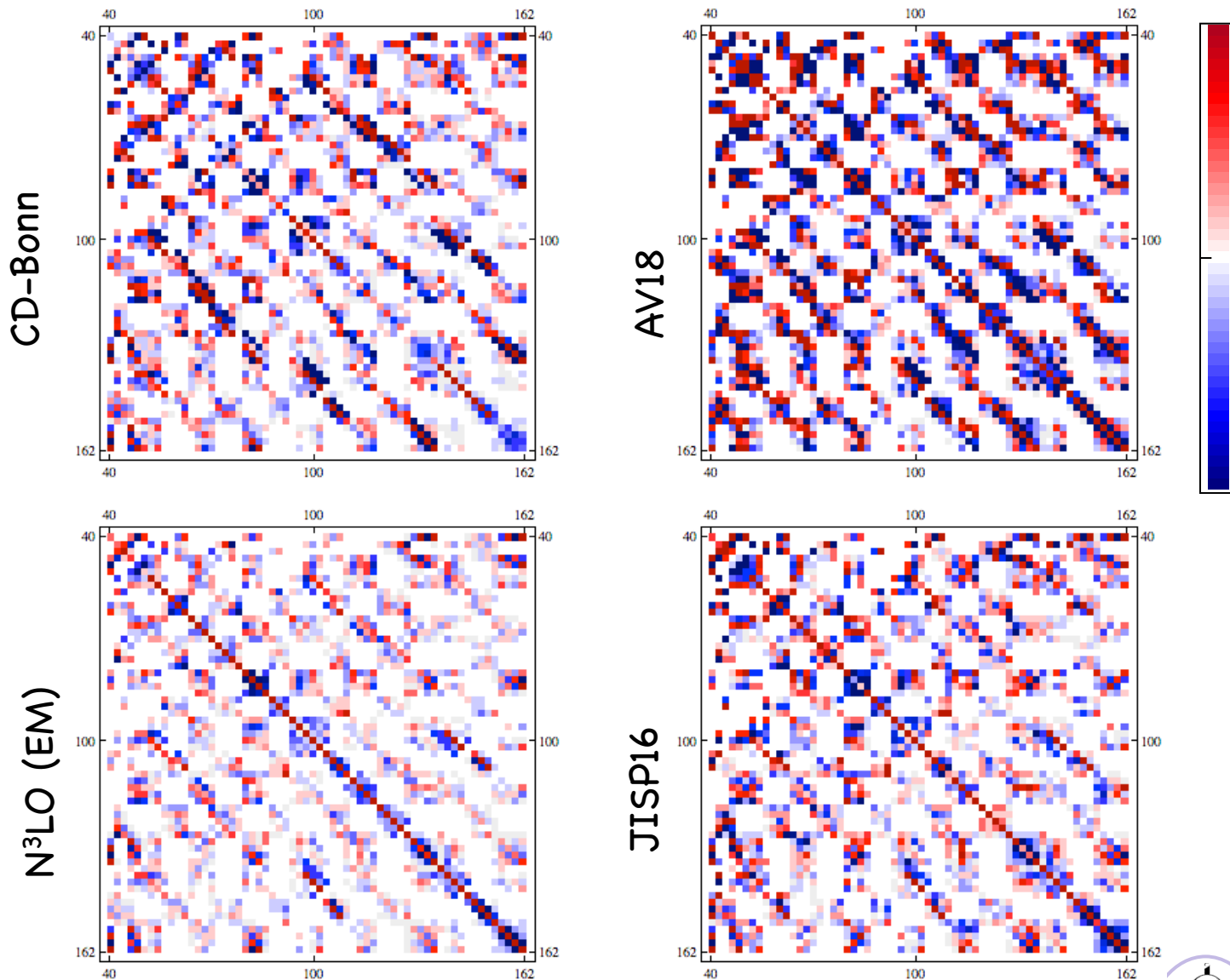
With  
1b C:





# SRG - Simple Illustration

- Bare NN+  
Relative  
Kinetic  
Energy
- Decouples  
model space

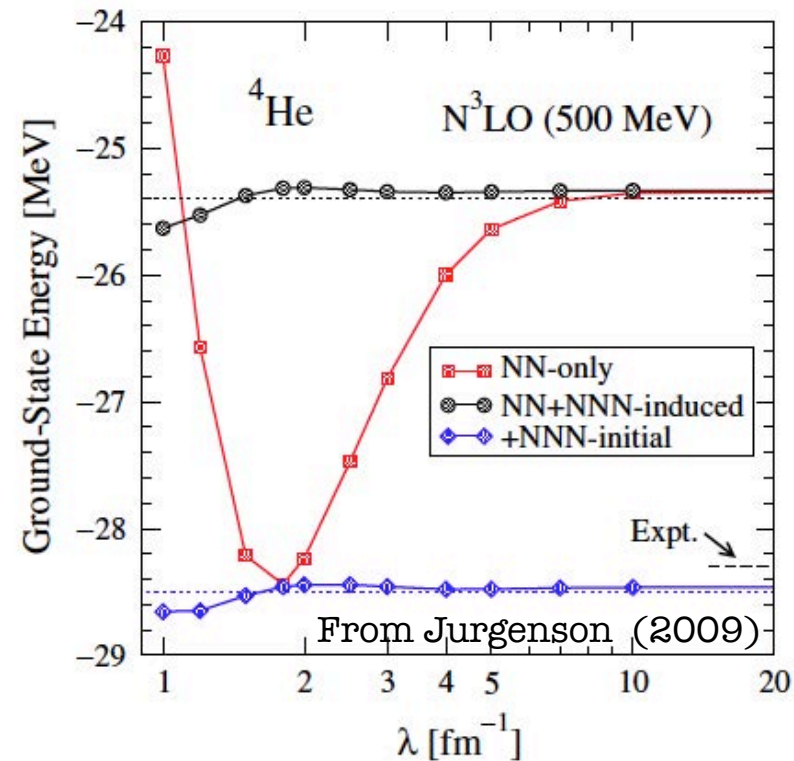




# Similarity Renormalization Group (SRG) for Nuclear Physics

## ❖ He-4

- ❖ SRG-evolved chiral potentials
  - ❖ 3-body important
  - ❖ 4-body negligible in He-4 (for binding energy)

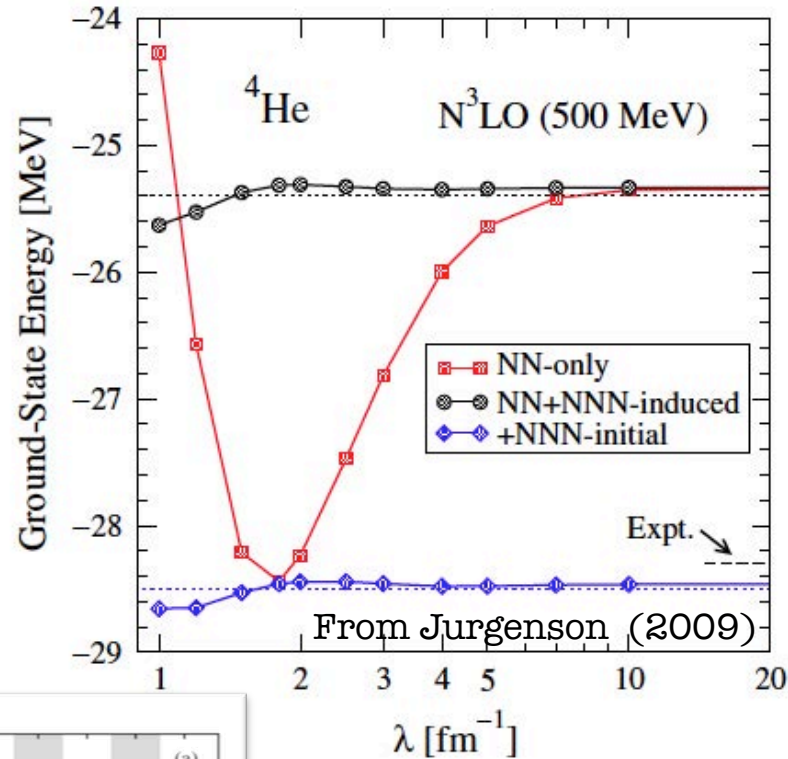


# Similarity Renormalization Group (SRG) for Nuclear Physics

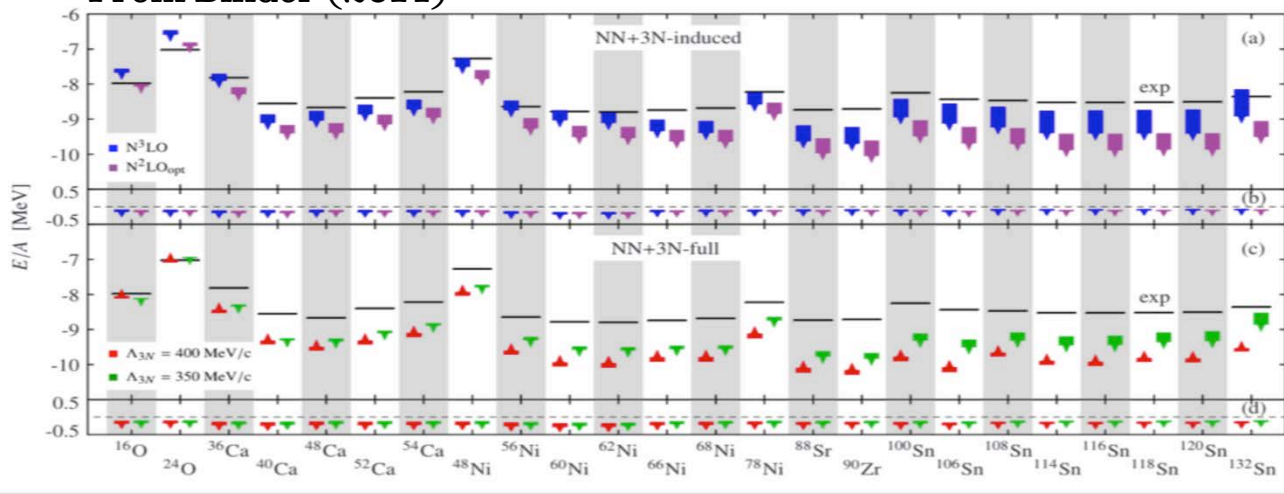
## ❖ He-4

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❖ SRG-induced interactions become important in heavy nuclei!



From Binder (2014)



# Similarity Renormalization Group (SRG) for Nuclear Physics

## ❖ He-4

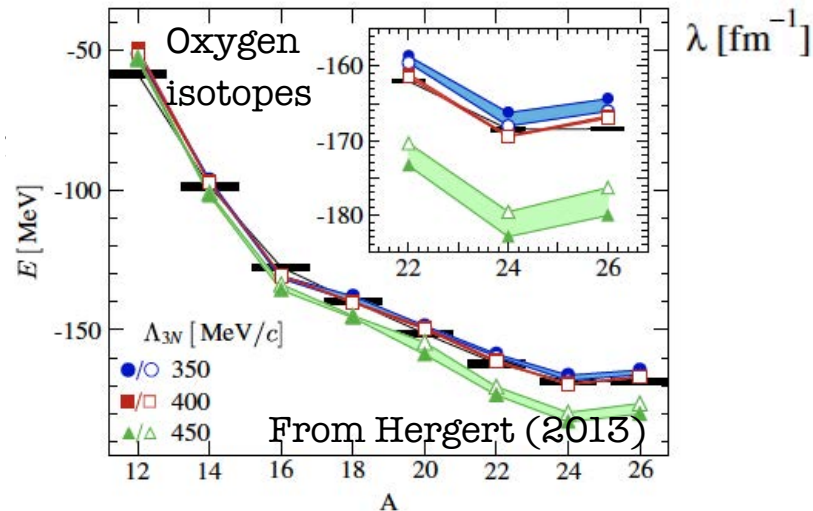
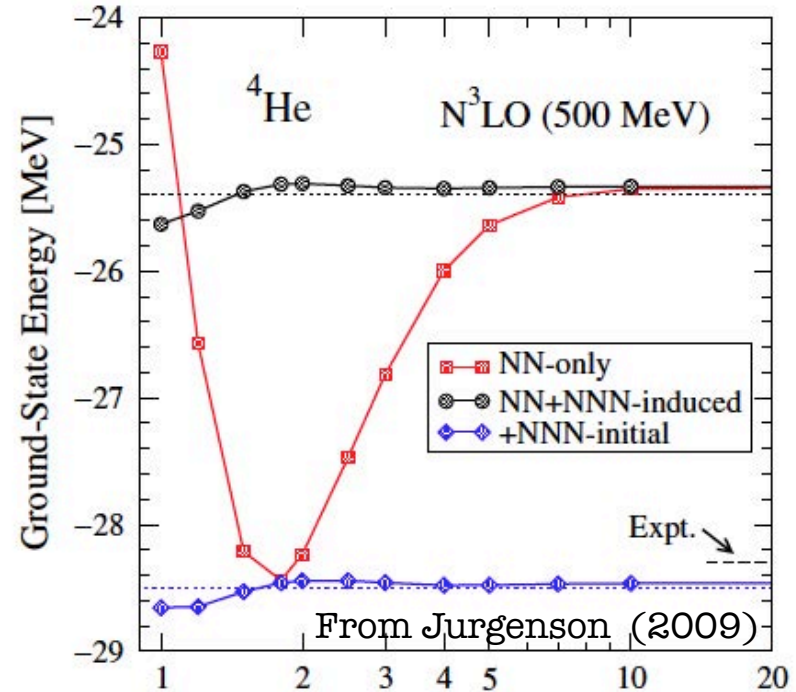
❖ SRG-evolved chiral potentials

❖ 3-body important

❖ 4-body negligible in He-4  
(for binding energy)

❖ SRG-induced interactions become important in heavy nuclei!

❖ SRG can evolve the entire nuclear Hamiltonian:  
In-medium SRG (IM-SRG)





# Similarity Renormalization Group (SRG) for Nuclear Physics

## ❖ He-4

### ❖ SRG-evolved chiral potentials

#### ❖ 3-body important

#### ❖ 4-body negligible in He-4 (for binding energy)

### ❖ SRG-induced interactions

become important in heavy nuclei!

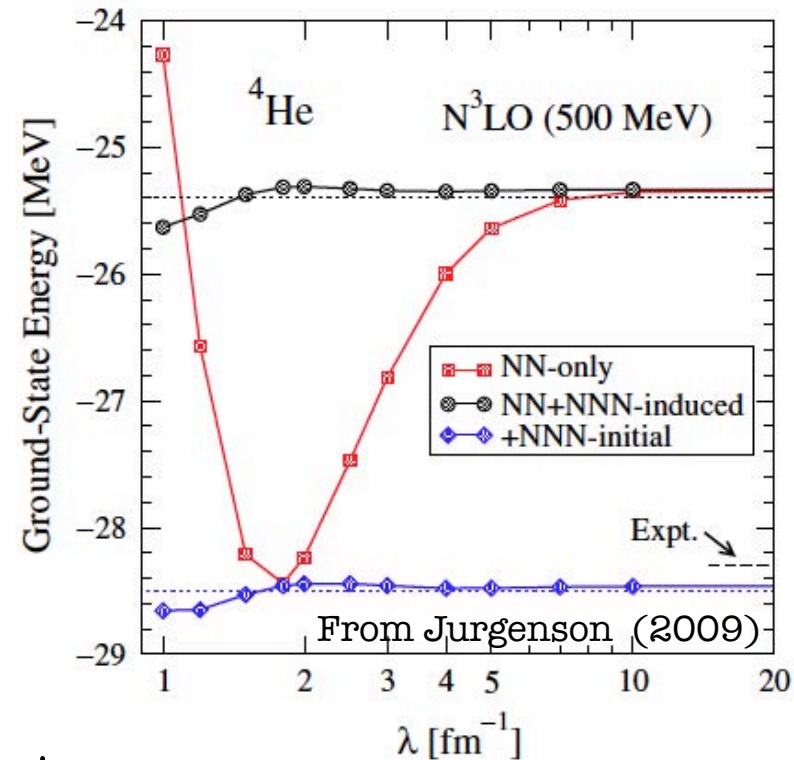
### ❖ Important: interaction renormalization changes

nuclear wave functions  $|\Psi_s\rangle$ ;

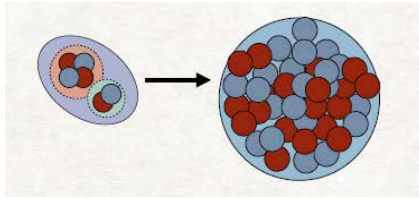
to calculate observables, the operators **need to be renormalized too**

### ❖ E.g., for rms radii, need to use $\langle \Psi_s | U(s) \left( \sum_i \hat{r}_i^2 \right) U^\dagger(s) | \Psi_s \rangle$

### ❖ Nontrivial (handling many-body operators)



# Effective interaction for reactions

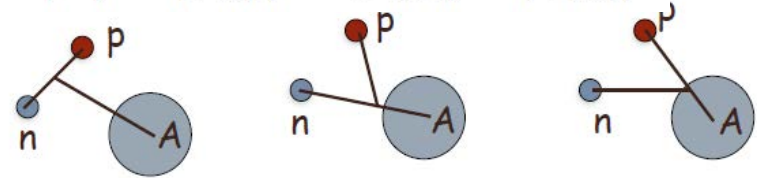


Many-body  
problem

Exact solutions...

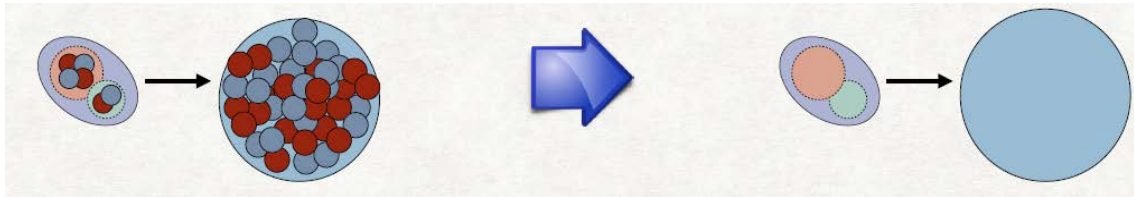
Faddeev equations ( $A=1$ ):

$$|\Psi\rangle = |\psi_{np}\rangle + |\psi_{nA}\rangle + |\psi_{pA}\rangle$$



Exact solutions exist to about 5 nucleons.

Can we use this technique for larger  $A$ ?

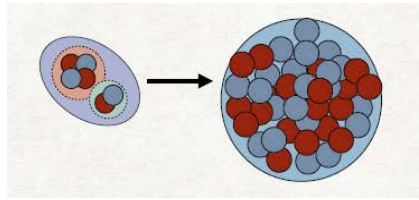


Many-body  
problem

Few-body  
problem

Reducing the many-body  
problem to a few-body problem  
induces effective interaction  
(optical potentials)

# Effective interaction for reactions

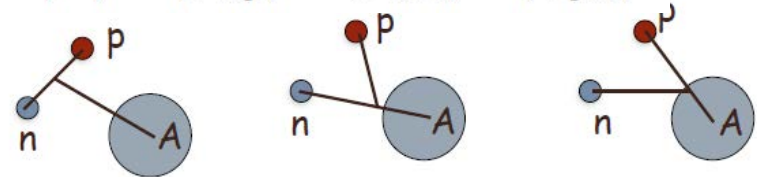


Many-body  
problem

Exact solutions...

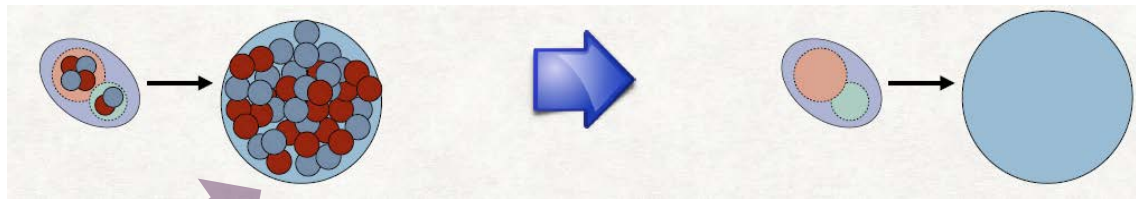
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Many-body  
problem

Few-body  
problem

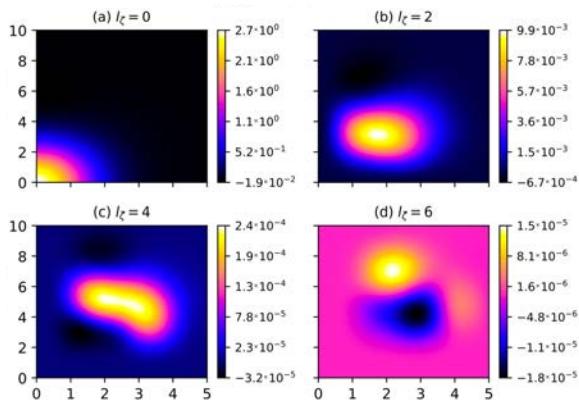
Use ab initio techniques to solve for the structure of target, and to derive effective interactions

Reducing the many-body problem to a few-body problem induces effective interaction (optical potentials)



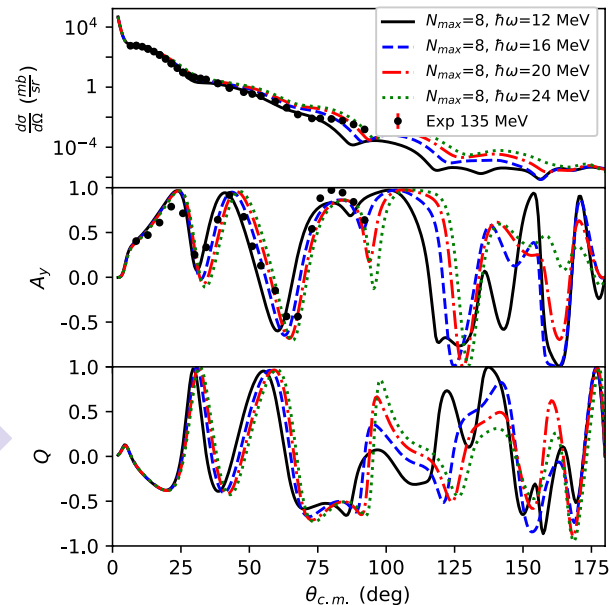
# Scattering observables from first principles

${}^6\text{Li}$ , ab initio densities

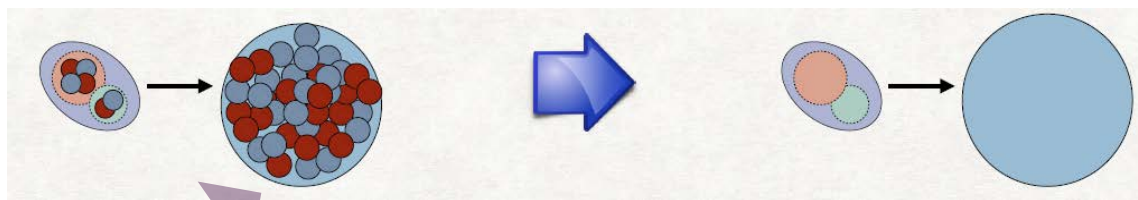


Proton scattering  
off target  ${}^{16}\text{O}$   
@ 135 MeV  
(NNLOopt)

First-principle derived  
effective interaction



From Burrows (2018, 2019)



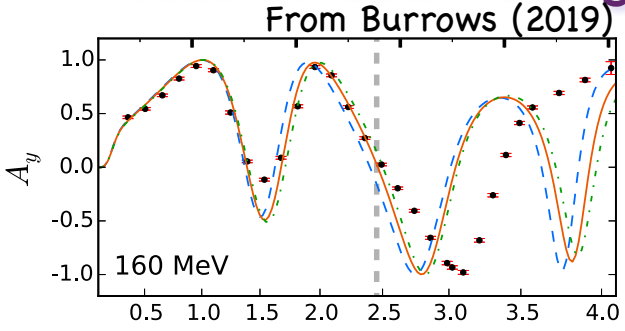
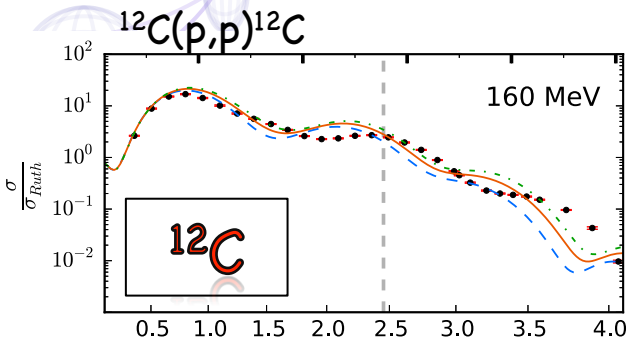
Many-body  
problem

Few-body  
problem

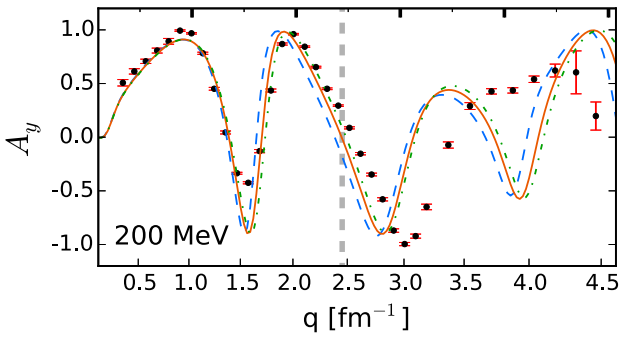
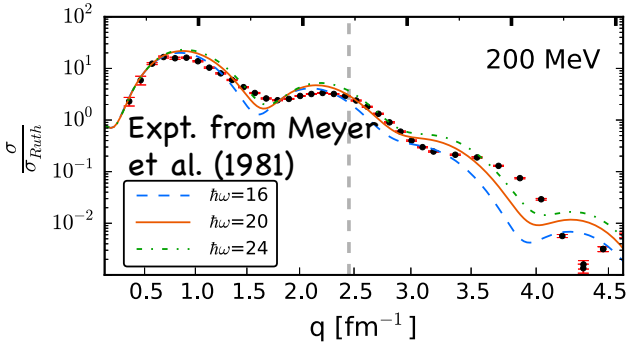
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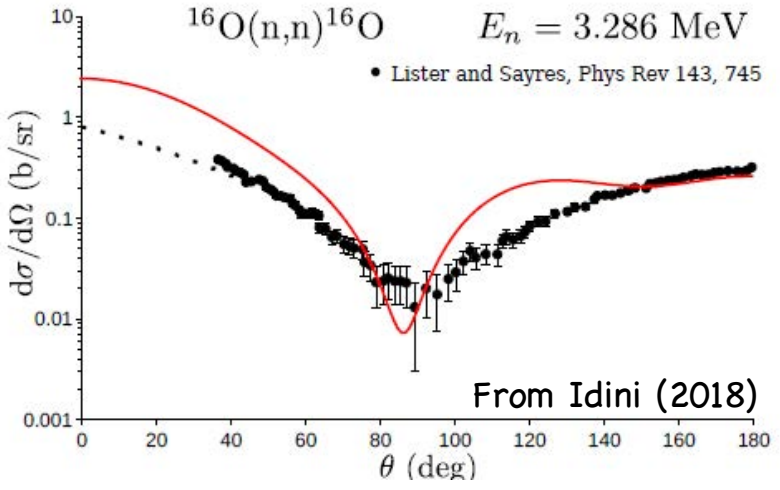
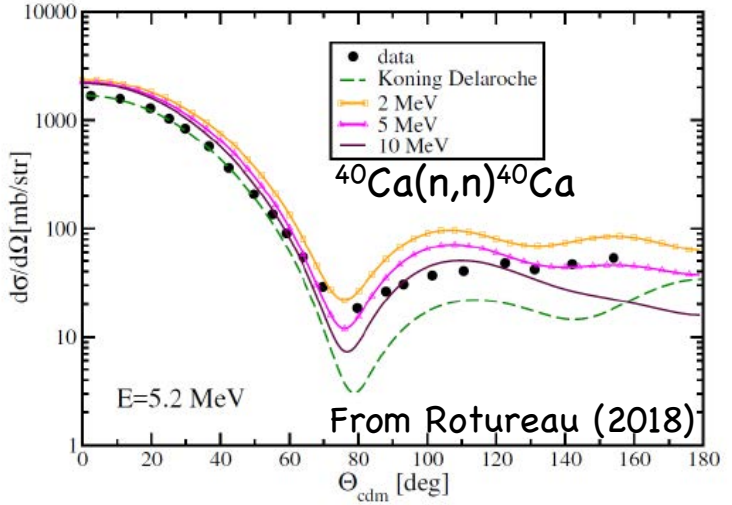
# Elastic scattering

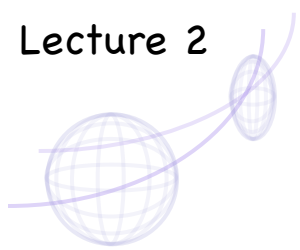


Higher energies  
(multiple scattering approach)

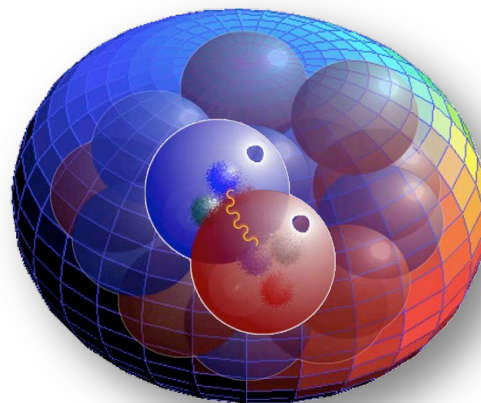


Low energy (~10 MeV)  
(Feshbach projection)





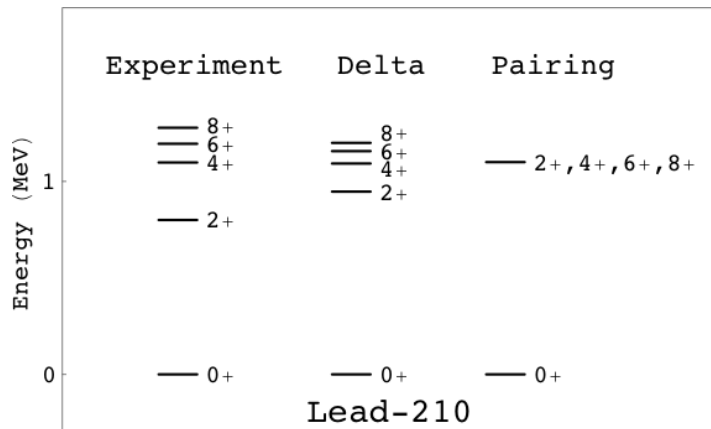
# Nuclei



Many-body approaches

# Inside the Nucleus ... the Insights

## Irrotational flow



### Nuclear "superfluidity":

- ❖ Pairing gap: higher first 2<sup>+</sup>.
- ❖ Two-particle (2n or 2p) transfer enhancement.
- ❖ Low moment of inertia

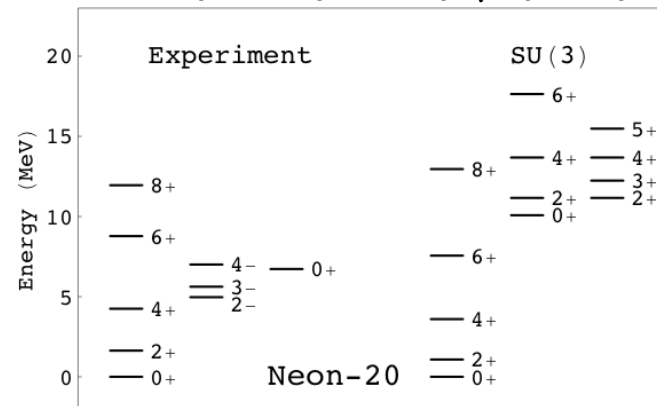
Irrotational-flow rotation



From Rowe (2013)

## Rotational modes

SU(3) model (Elliott model): shell model of deformation/rotations



### Nuclear "rigid rotor":

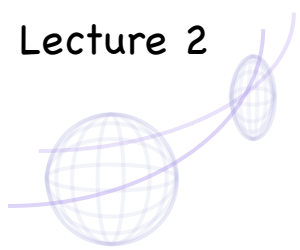
- ❖  $E_J \sim J(J+1) \Rightarrow E_{4+}/E_{2+} = 3.33$ : "3.33-rule"
- ❖ Rotations of deformation
- ❖ High moment of inertia

Rigid flow rotation



From Rowe (2013)

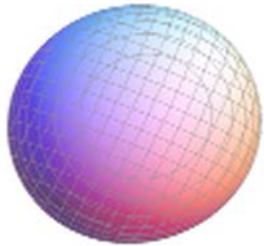




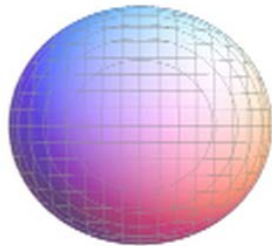
# Inside the Nucleus ... the Insights

## Vibrational modes

Intrinsic frame:

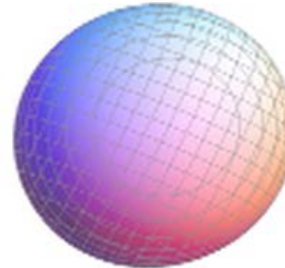


Giant resonance  
- monopole -  
(breathing mode)

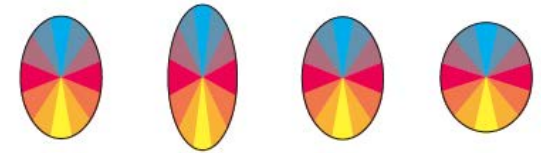


- quadrupole -

Lab frame:



Shape vibration



From Rowe (2013)

Nuclear compressibility  
rather stiff:  $\sim 80A^{-1/3}$  MeV

Low-energy vibrations not likely

Surface radius for  $\lambda$ -multipole vibrations (lab frame):

$$R(\theta, \varphi; t) = R_0 \left\{ 1 + \sum_{\lambda\mu} \alpha_{\lambda\mu}(t) Y_{\lambda\mu}(\theta, \varphi) \right\}$$



## The shell model

- ❖  $A$  nucleons of mass  $m_N$ ;  $\mathbf{r}_1, \mathbf{p}_1; \mathbf{r}_2, \mathbf{p}_2; \dots; \mathbf{r}_A, \mathbf{p}_A$

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A)$$

- ❖ Many-body Hamiltonian = kinetic energy + potential energy):

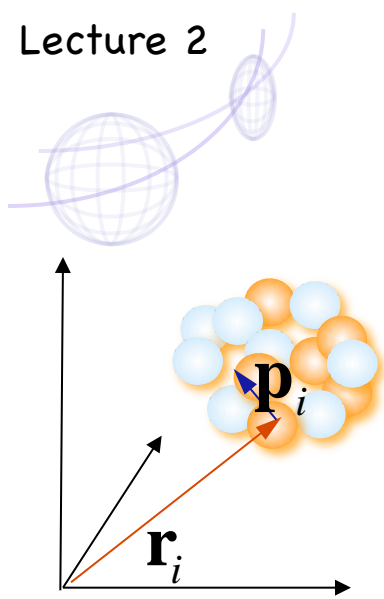
$$[\mathbf{p} = -i\hbar\nabla] \quad H = \sum_{i=1}^A \frac{\mathbf{p}_i^2}{2m_N} + \sum_{i,j=1(i<j)}^A V_{NN}(\mathbf{r}_i - \mathbf{r}_j) + \sum_{i<j<k} (V_{NNN})_{ijk} + \dots$$

- ❖ ...actually, relative kinetic energy:

$$\frac{1}{A} \sum_{i,j=1(i<j)}^A \frac{(\mathbf{p}_i - \mathbf{p}_j)^2}{2m_N}$$

- ❖ Solve Schrödinger equation

$$H\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A) = E\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A)$$



## The shell model

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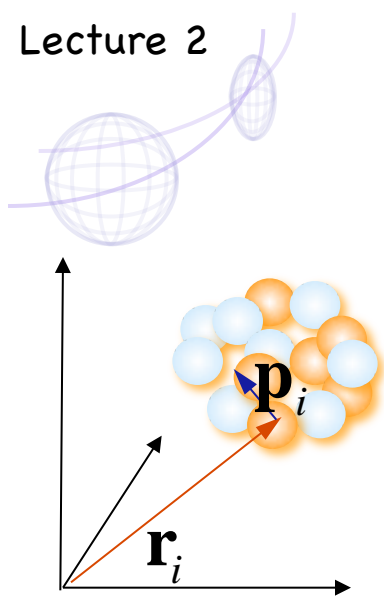
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- ❖ Solve Schrödinger equation

$$H\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A) = E\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A)$$

- ❖ Identify dominant average potential (mean field):  
dictates choice for s.p. states (basis states)

$$\sum_{i,j=1(i<j)}^A V_{NN}(\mathbf{r}_i - \mathbf{r}_j) = \sum_i V(\mathbf{r}_i) + \sum_{i,j=1(i<j)}^A V_{res}(\mathbf{r}_i - \mathbf{r}_j)$$



# The shell model

- ❖ Many-particle state  $\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2)\dots\varphi_d(\mathbf{r}_A)$
- ❖ Anti-symmetric many-particle **basis states** (Slater determinant):

Single-particle states  $\varphi_a, \varphi_b, \varphi_c, \varphi_d$  a b c d

Single-particle energies  $e_a, e_b, e_c, e_d$

$$\Phi_{ab\dots d}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \varphi_a(\mathbf{r}_1) & \varphi_a(\mathbf{r}_2) & \dots & \varphi_a(\mathbf{r}_A) \\ \varphi_b(\mathbf{r}_1) & \varphi_b(\mathbf{r}_2) & \dots & \varphi_b(\mathbf{r}_A) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_d(\mathbf{r}_1) & \varphi_d(\mathbf{r}_2) & \dots & \varphi_d(\mathbf{r}_A) \end{vmatrix}$$

State a

State b

State d

Particle 1

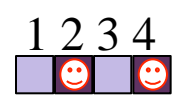
Particle 2

Particle A

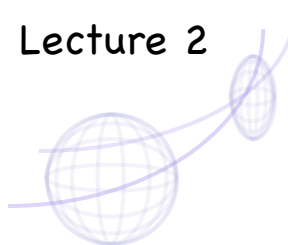
- ❖ Example for A=2 particles:

State:  $\Phi_{24}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} [\phi_2(\mathbf{r}_1)\phi_4(\mathbf{r}_2) - \phi_2(\mathbf{r}_2)\phi_4(\mathbf{r}_1)]$

$$E = e_2 + e_4$$







# The shell model

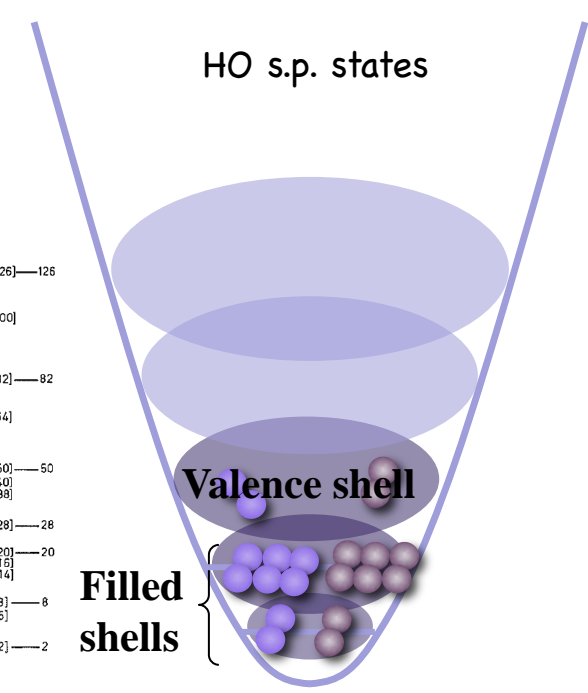
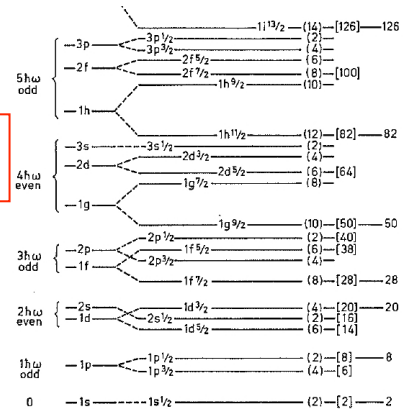
❖ Choice for s.p. states (basis states):  
often Harmonic Oscillator (HO)

❖ Solve Schrödinger equation: matrix eigenvalue problem

$$H\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A) = E\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A)$$

$$\Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A) = \sum_{k=1}^D C_k^\alpha \Phi_k(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A)$$

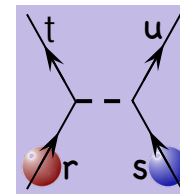
$$\begin{pmatrix} H_{11} & H_{12} & \dots & H_{1D} \\ H_{21} & H_{22} & \dots & H_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ H_{D1} & H_{D2} & \dots & H_{DD} \end{pmatrix} \begin{pmatrix} C_1^\alpha \\ C_2^\alpha \\ \vdots \\ C_D^\alpha \end{pmatrix} = E_\alpha \begin{pmatrix} C_1^\alpha \\ C_2^\alpha \\ \vdots \\ C_D^\alpha \end{pmatrix}$$



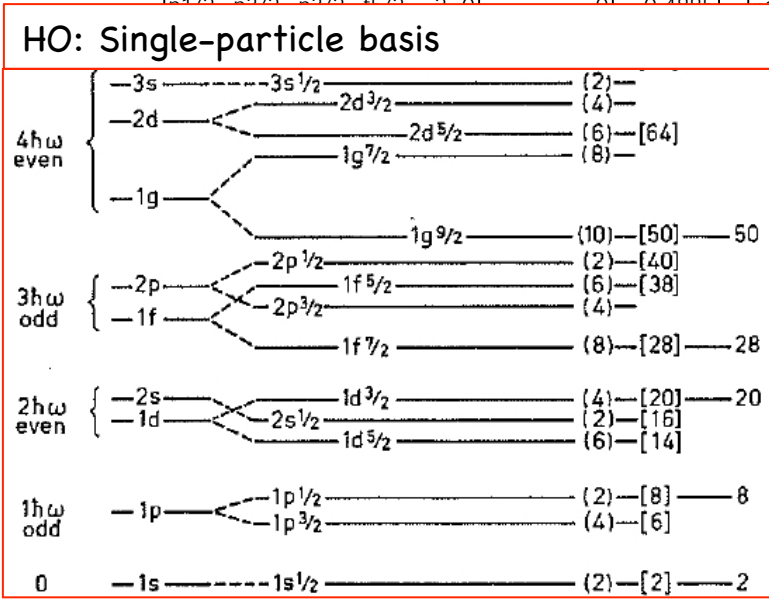
- ❖ ... in Hilbert space (infinite!)
- ❖ What is the best choice for basis?

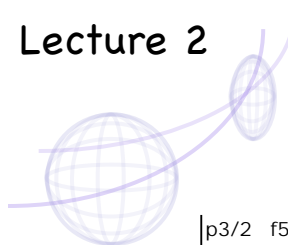


# Two-Body Matrix elements (TBME) fp shell



ir	js	jt	ju	J	T	Hsp4	GXPf1																
p1/2	p1/2	p1/2	p1/2	1	0	-1.077001	-1.2431	p1/2	f5/2	p3/2	p3/2	2	1	0	-0.1923	p3/2	p3/2	p3/2	p3/2	0	1	-0.523662	-1.1165
p1/2	p1/2	p1/2	p1/2	0	1	-0.209086	-0.4469	p1/2	f5/2	p3/2	f5/2	2	0	0	-0.354	p3/2	p3/2	p3/2	p3/2	2	1	0.105489	-0.0887
p1/2	p1/2	p1/2	p3/2	1	0	0	-0.849	p1/2	f5/2	p3/2	f5/2	3	0	0	1.0151	p3/2	p3/2	p3/2	f5/2	1	0	0	0.2373
p1/2	p1/2	p3/2	p3/2	1	0	0	0.7675	p1/2	f5/2	p3/2	f5/2	2	1	0	-0.4043	p3/2	p3/2	p3/2	f5/2	3	0	0	0.2276
p1/2	p1/2	p3/2	p3/2	0	1	-0.444876	-1.4928	p1/2	f5/2	p3/2	f5/2	3	1	0	-0.06	p3/2	p3/2	p3/2	f5/2	2	1	0	-0.4631
p1/2	p1/2	p3/2	f5/2	1	0	0	0.8137	p1/2	f5/2	p3/2	f7/2	2	0	0	1.0933	p3/2	p3/2	p3/2	f7/2	3	0	0	-0.4309
p1/2	p1/2	f5/2	f5/2	1	0	0	-0.3161	p1/2	f5/2	p3/2	f7/2	3	0	0	0.7227	p3/2	p3/2	p3/2	f7/2	2	1	0	-0.3738
p1/2	p1/2	f5/2	f5/2	0	1	-0.54486	-0.8093	p1/2	f5/2	p3/2	f7/2	2	1	0	-0.803	p3/2	p3/2	f5/2	f5/2	1	0	0	0.0483
p1/2	p1/2	f5/2	f7/2	1	0	0	-0.1928	p1/2	f5/2	p3/2	f7/2	3	1	0	-0.1814	p3/2	p3/2	f5/2	f5/2	3	0	0	-0.0546
p1/2	p1/2	f7/2	f7/2	1	0	0	0.0271	p1/2	f5/2	f5/2	f5/2	3	0	0	-0.6276	p3/2	p3/2	f5/2	f5/2	0	1	-0.770548	-1.2457
p1/2	p1/2	f7/2	f7/2	0	1	-0.816667	-0.38	p1/2	f5/2	f5/2	f5/2	2	1	0	-0.3208	p3/2	p3/2	f5/2	f5/2	2	1	0	0.0719
p1/2	p3/2	p1/2	p3/2	1	0	-1.077001	-2.5068	p1/2	f5/2	f5/2	f7/2	2	0	0	-0.5447	p3/2	p3/2	f5/2	f7/2	1	0	0	-0.8914
p1/2	p3/2	p1/2	p3/2	2	0	-1.077001	-2.3122	p1/2	f5/2	f5/2	f7/2	3	0	0	-0.6262	p3/2	p3/2	f5/2	f7/2	3	0	0	-0.6264
p1/2	p3/2	p1/2	p3/2	1	1	0.105489	-0.1594	p1/2	f5/2	f5/2	f7/2	2	1	0	0.1537	p3/2	p3/2	f5/2	f7/2	2	1	0	-0.0717
p1/2	p3/2	p1/2	p3/2	2	1	0.105489	-0.2938	p1/2	f5/2	f5/2	f7/2	3	1	0	-0.1105	p3/2	p3/2	f7/2	f7/2	1	0	0	-0.4313
p1/2	p3/2	p1/2	f5/2	2	0	0	-0.69	p1/2	f5/2	f7/2	f7/2	3	0	0	-0.1082	p3/2	p3/2	f7/2	f7/2	3	0	0	-0.3415
p1/2	p3/2	p1/2	f5/2	2	1	0	0.249	p1/2	f5/2	f7/2	f7/2	2	1	0	-0.1295	p3/2	p3/2	f7/2	f7/2	0	1	-1.154941	-0.7174
p1/2	p3/2	p3/2	p3/2	1	0	0	-1.8059	p1/2	f7/2	p1/2	f7/2	3	0	-1.638477	-1.6968	p3/2	p3/2	f7/2	f7/2	2	1	0	-0.2021
p1/2	p3/2	p3/2	p3/2	2	1	0	0.634	p1/2	f7/2	p1/2	f7/2	4	0	-1.638477	-1.0602	p3/2	f5/2	p3/2	f5/2	1	0	-1.077001	-2.7262
p1/2	p3/2	p3/2	f5/2	1	0	0	0.993	p1/2	f7/2	p1/2	f7/2	3	1	0.08819	0.4873	p3/2	f5/2	p3/2	f5/2	2	0	-1.077001	-1.511
p1/2	p3/2	p3/2	f5/2	2	0	0	0.4895	p1/2	f7/2	p1/2	f7/2	4	1	0.08819	-0.1347	p3/2	f5/2	p3/2	f5/2	3	0	-1.077001	-0.5859
p1/2	p3/2	p3/2	f5/2	3	0	0	0.4895	p1/2	f7/2	p3/2	p3/2	3	0	0	-0.6411	p3/2	f5/2	p3/2	f5/2	4	0	-1.077001	-1.0882
p1/2	p3/2	p3/2	f5/2	3	0	0	0.4895	p1/2	f7/2	p3/2	f5/2	3	0	0	0.0354	p3/2	f5/2	p3/2	f5/2	1	1	0.105489	0.3284
p1/2	p3/2	p3/2	f5/2	4	0	0	0.4895	p1/2	f7/2	p3/2	f5/2	4	0	0	-1.3607	p3/2	f5/2	p3/2	f5/2	2	1	0.105489	0.3608
p1/2	p3/2	p3/2	f5/2	3	1	0	0.4895	p1/2	f7/2	p3/2	f5/2	3	1	0	0.3891	p3/2	f5/2	p3/2	f5/2	3	1	0.105489	0.346
p1/2	p3/2	p3/2	f5/2	4	1	0	0.4895	p1/2	f7/2	p3/2	f5/2	4	1	0	0.6111	p3/2	f5/2	p3/2	f5/2	4	1	0.105489	-0.2584
p1/2	p3/2	p3/2	f7/2	3	0	0	0.4895	p1/2	f7/2	p3/2	f7/2	3	0	0	-1.685	p3/2	f5/2	p3/2	f7/2	2	0	0	1.2708
p1/2	p3/2	p3/2	f7/2	4	0	0	0.4895	p1/2	f7/2	p3/2	f7/2	4	0	0	-0.1706	p3/2	f5/2	p3/2	f7/2	3	0	0	0.579
p1/2	p3/2	p3/2	f7/2	3	1	0	0.4895	p1/2	f7/2	p3/2	f7/2	3	1	0	0.1048	p3/2	f5/2	p3/2	f7/2	4	0	0	0.7103
p1/2	p3/2	p3/2	f7/2	4	1	0	0.4895	p1/2	f7/2	p3/2	f7/2	4	1	0	0.3351	p3/2	f5/2	p3/2	f7/2	2	1	0	-0.5436
p1/2	p3/2	p3/2	f7/2	3	0	0	0.4895	p1/2	f7/2	f5/2	f5/2	3	0	0	0.2621	p3/2	f5/2	p3/2	f7/2	3	1	0	-0.1836
p1/2	p3/2	p3/2	f7/2	4	1	0	0.4895	p1/2	f7/2	f5/2	f5/2	4	1	0	0.2248	p3/2	f5/2	p3/2	f7/2	4	1	0	-0.4546
p1/2	p3/2	p3/2	f7/2	3	0	0	0.4895	p1/2	f7/2	f5/2	f7/2	3	0	0	-0.4252	p3/2	f5/2	f5/2	f5/2	1	0	0	0.477
p1/2	p3/2	p3/2	f7/2	4	0	0	0.4895	p1/2	f7/2	f5/2	f7/2	4	0	0	-0.3789	p3/2	f5/2	f5/2	f5/2	3	0	0	0.32
p1/2	p3/2	p3/2	f7/2	3	1	0	0.4895	p1/2	f7/2	f5/2	f7/2	3	1	0	0.3224	p3/2	f5/2	f5/2	f5/2	2	1	0	-0.056
p1/2	p3/2	p3/2	f7/2	4	1	0	0.4895	p1/2	f7/2	f5/2	f7/2	4	1	0	0.1907	p3/2	f5/2	f5/2	f5/2	4	1	0	-0.3615
p1/2	p3/2	p3/2	f7/2	3	0	0	0.4895	p1/2	f7/2	f7/2	f7/2	3	0	0	-0.8883	p3/2	f5/2	f5/2	f7/2	1	0	0	1.2721
p1/2	p3/2	p3/2	f7/2	4	1	0	0.4895	p1/2	f7/2	f7/2	f7/2	4	1	0	0.2096	p3/2	f5/2	f5/2	f7/2	2	0	0	-0.598
p1/2	p3/2	p3/2	p3/2	1	0	-1.077001	-0.6308	p1/2	p3/2	p3/2	p3/2	1	0	-1.077001	-0.6308	p3/2	f5/2	f5/2	f7/2	3	0	0	0.7716
p1/2	p3/2	p3/2	p3/2	3	0	-1.077001	-2.289	p1/2	p3/2	p3/2	p3/2	3	0	-1.077001	-2.289	p3/2	f5/2	f5/2	f7/2	4	0	0	-0.6408





# ... and more two-body matrix elements

p3/2	f5/2	f5/2	f7/2	1	1	0	0.0521	f5/2	f5/2	f5/2	f7/2	5	0	0	-1.1302
p3/2	f5/2	f5/2	f7/2	2	1	0	0.4247	f5/2	f5/2	f5/2	f7/2	2	1	0	0.5022
p3/2	f5/2	f5/2	f7/2	3	1	0	-0.0268	f5/2	f5/2	f5/2	f7/2	4	1	0	0.2709
p3/2	f5/2	f5/2	f7/2	4	1	0	0.2699	f5/2	f5/2	f7/2	f7/2	1	0	0	0.6511
p3/2	f5/2	f7/2	f7/2	1	0	0	-0.0907	f5/2	f5/2	f7/2	f7/2	3	0	0	0.4358
p3/2	f5/2	f7/2	f7/2	3	0	0	0.0752	f5/2	f5/2	f7/2	f7/2	5	0	0	0.1239
p3/2	f5/2	f7/2	f7/2	2	1	0	-0.1725	f5/2	f5/2	f7/2	f7/2	0	1	-1.414508	-1.3832
p3/2	f5/2	f7/2	f7/2	4	1	0	-0.2224	f5/2	f5/2	f7/2	f7/2	2	1	0	-0.2038
p3/2	f7/2	p3/2	f7/2	2	0	-1.638477	-0.5391	f5/2	f5/2	f7/2	f7/2	4	1	0	-0.0331
p3/2	f7/2	p3/2	f7/2	3	0	-1.638477	-1.0055	f5/2	f7/2	f5/2	f7/2	1	0	-1.638477	-4.5802
p3/2	f7/2	p3/2	f7/2	4	0	-1.638477	-0.3695	f5/2	f7/2	f5/2	f7/2	2	0	-1.638477	-3.252
p3/2	f7/2	p3/2	f7/2	5	0	-1.638477	-2.967	f5/2	f7/2	f5/2	f7/2	3	0	-1.638477	-1.4019
p3/2	f7/2	p3/2	f7/2	2	1	0.08819	-0.6081	f5/2	f7/2	f5/2	f7/2	4	0	-1.638477	-2.2583
p3/2	f7/2	p3/2	f7/2	3	1	0.08819	0.1561	f5/2	f7/2	f5/2	f7/2	5	0	-1.638477	-0.6084
p3/2	f7/2	p3/2	f7/2	4	1	0.08819	-0.1398	f5/2	f7/2	f5/2	f7/2	6	0	-1.638477	-3.0351
p3/2	f7/2	p3/2	f7/2	5	1	0.08819	0.5918	f5/2	f7/2	f5/2	f7/2	1	1	0.08819	-0.0889
p3/2	f7/2	f5/2	f5/2	3	0	0	0.166	f5/2	f7/2	f5/2	f7/2	2	1	0.08819	-0.175
p3/2	f7/2	f5/2	f5/2	5	0	0	0.0334	f5/2	f7/2	f5/2	f7/2	3	1	0.08819	0.6302
p3/2	f7/2	f5/2	f5/2	2	1	0	0.088	f5/2	f7/2	f5/2	f7/2	4	1	0.08819	0.4763
p3/2	f7/2	f5/2	f5/2	4	1	0	-0.2146	f5/2	f7/2	f5/2	f7/2	5	1	0.08819	0.7433
p3/2	f7/2	f5/2	f7/2	2	0	0	0.6381	f5/2	f7/2	f5/2	f7/2	6	1	0.08819	-0.9916
p3/2	f7/2	f5/2	f7/2	3	0	0	-0.254	f5/2	f7/2	f7/2	f7/2	1	0	0	-1.8998
p3/2	f7/2	f5/2	f7/2	4	0	0	-0.1951	f5/2	f7/2	f7/2	f7/2	3	0	0	-1.0917
p3/2	f7/2	f5/2	f7/2	5	0	0	-0.6743	f5/2	f7/2	f7/2	f7/2	5	0	0	-1.2853
p3/2	f7/2	f5/2	f7/2	2	1	0	-0.0959	f5/2	f7/2	f7/2	f7/2	2	1	0	-0.2167
p3/2	f7/2	f5/2	f7/2	3	1	0	0.523	f5/2	f7/2	f7/2	f7/2	4	1	0	0.4999
p3/2	f7/2	f5/2	f7/2	4	1	0	0.2486	f5/2	f7/2	f7/2	f7/2	6	1	0	0.5643
p3/2	f7/2	f5/2	f7/2	5	1	0	0.481	f7/2	f7/2	f7/2	f7/2	1	0	-2.078472	-1.2838
p3/2	f7/2	f7/2	f7/2	3	0	0	-0.8807	f7/2	f7/2	f7/2	f7/2	3	0	-2.078472	-0.8418
p3/2	f7/2	f7/2	f7/2	5	0	0	-0.4265	f7/2	f7/2	f7/2	f7/2	5	0	-2.078472	-0.7839
p3/2	f7/2	f7/2	f7/2	2	1	0	-0.516	f7/2	f7/2	f7/2	f7/2	7	0	-2.078472	-2.6661
p3/2	f7/2	f7/2	f7/2	4	1	0	-0.2969	f7/2	f7/2	f7/2	f7/2	0	1	-1.845204	-2.4385
f5/2	f5/2	f5/2	f5/2	1	0	-1.077001	-0.8551	f7/2	f7/2	f7/2	f7/2	2	1	0.062016	-0.9352
f5/2	f5/2	f5/2	f5/2	3	0	-1.077001	-0.5599	f7/2	f7/2	f7/2	f7/2	4	1	0.062016	-0.1296
f5/2	f5/2	f5/2	f5/2	5	0	-1.077001	-2.2816	f7/2	f7/2	f7/2	f7/2	6	1	0.062016	0.2783
f5/2	f5/2	f5/2	f5/2	0	1	-0.838236	-1.2081								
f5/2	f5/2	f5/2	f5/2	2	1	0.105489	-0.4621								
f5/2	f5/2	f5/2	f5/2	4	1	0.105489	-0.1624								
f5/2	f5/2	f5/2	f7/2	1	0	0	0.2735								
f5/2	f5/2	f5/2	f7/2	3	0	0	-0.6378								

## Empirical interactions: from available data

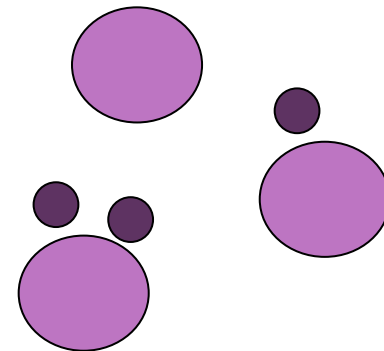
### Question

Binding Energies: 342.05 MeV (Ca-40)  
 350.41 MeV (Ca-41, 7/2<sup>-</sup>) + 1 neutron in f7/2  
 361.90 MeV (Ca-42, 0<sup>+</sup>) + 2 neutrons in f7/2

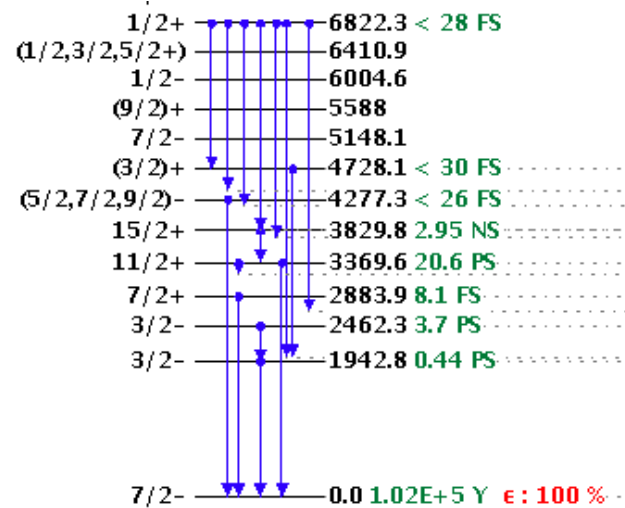
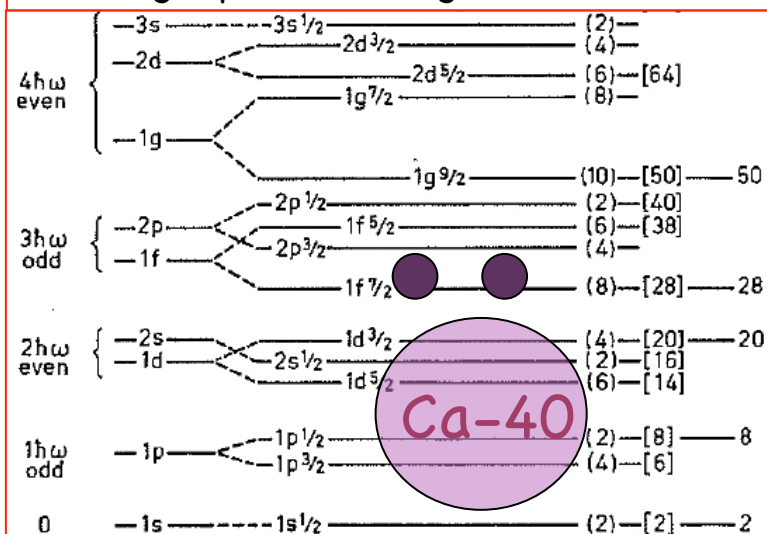
$E_c = ?$  (energy due to core)

$e_{f7/2} = ?$  (energy of single nucleon)

$V_{f7/2f7/2f7/2f7/2}^{01} = ?$  (energy of two nucleons,  $J=0, T=1$ )



### HO: Single-particle energies (SPE)



Ca-41



# Ca Isotopes

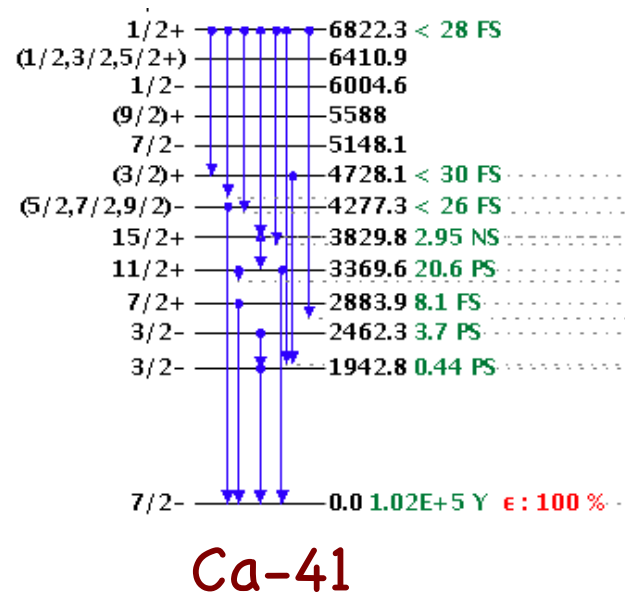
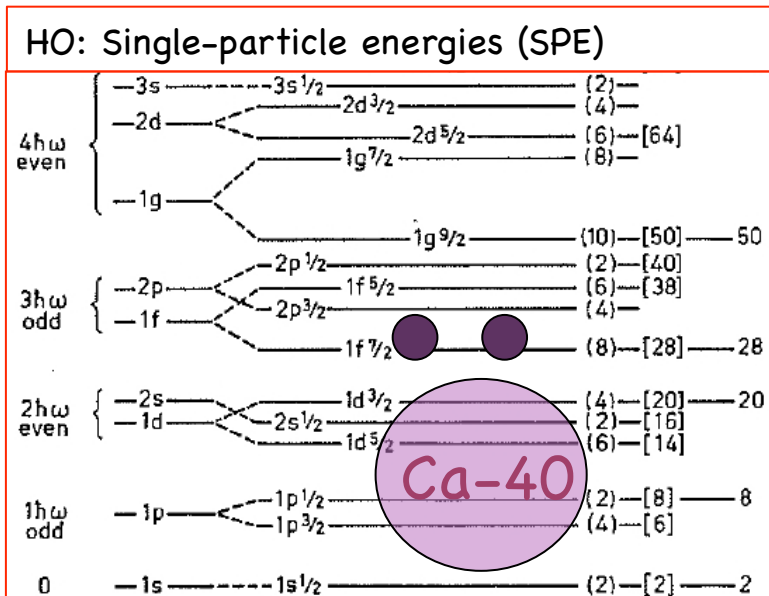
## Empirical interactions: from available data

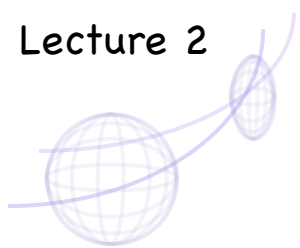
Binding Energies: 342.05 MeV (Ca-40)  $\updownarrow$  -8.36 MeV  $\updownarrow$  -19.84 MeV  
 350.41 MeV (Ca-41, 7/2-) + 1 neutron in f7/2  
 361.90 MeV (Ca-42, 0+) + 2 neutrons in f7/2

$E_c = -342.05$  MeV (energy due to core)

$e_{f7/2} = -350.41 - (-342.05) = -8.36$  MeV

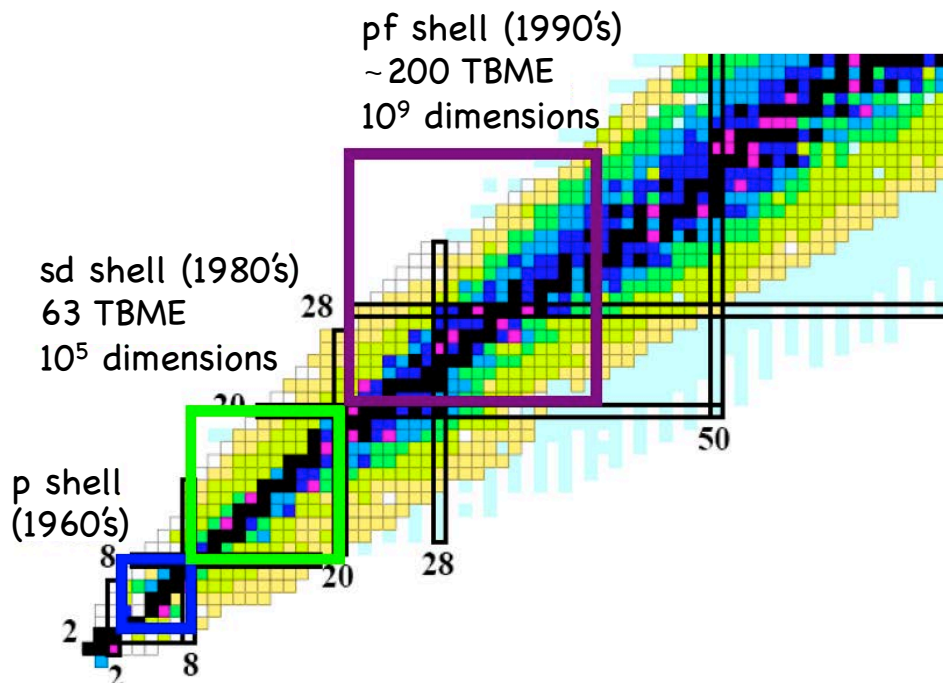
$V_{f7/2f7/2f7/2f7/2}^{01} = -361.90 - (-342.05) - 2*(e_{f7/2}) = -3.12$  MeV ( $J=0, T=1$ )





# Valence shell model

At present: large-scale SM calculations, pfg<sub>9/2</sub> shell

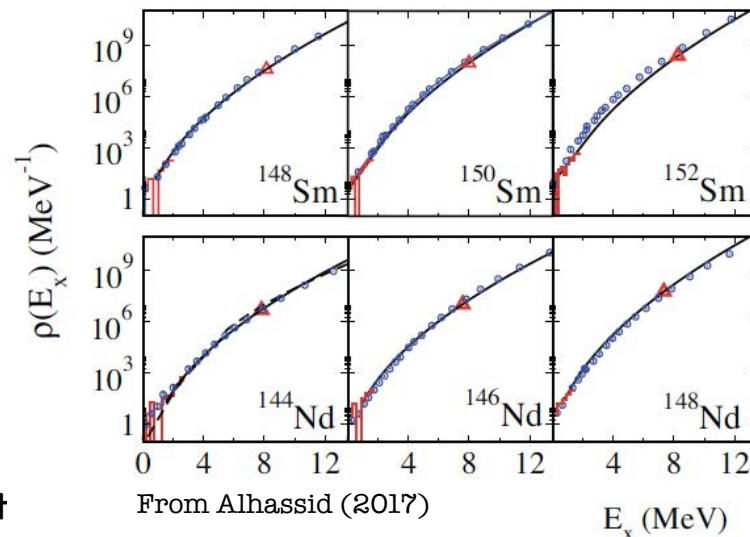
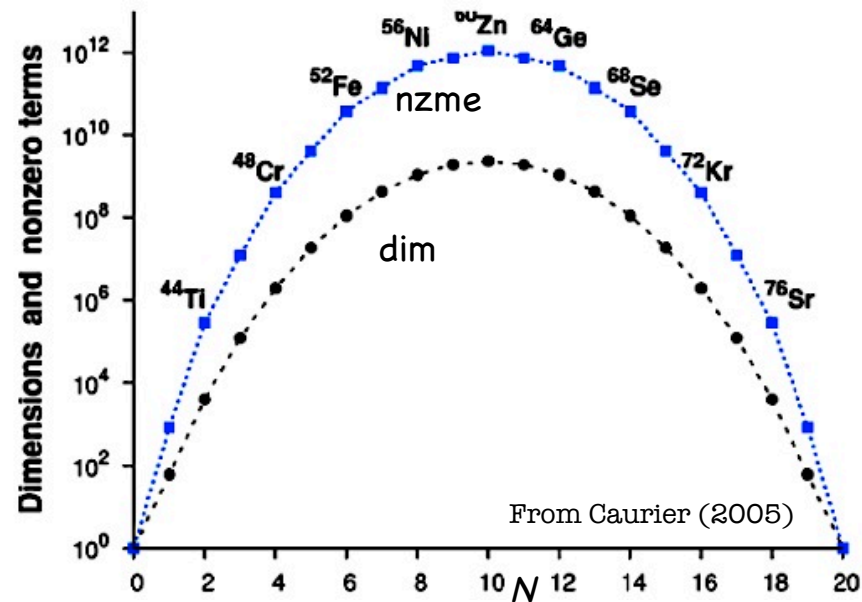


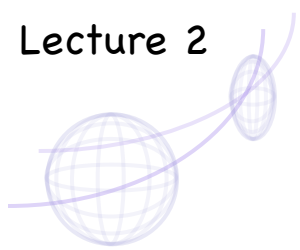
Current limits of model space sizes:

- ❖ Diagonalization: ~10<sup>9</sup>
- ❖ Monte Carlo: ~10<sup>15</sup>

Publicly available codes:

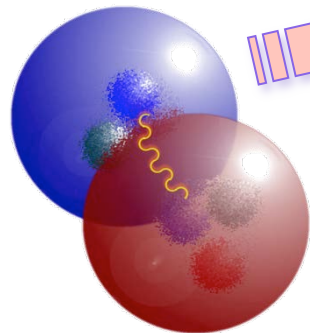
- Oxbash (MSU): [arXiv:nucl-th/9406020](https://arxiv.org/abs/nucl-th/9406020)
- Antoine (Strasbourg): [www.iphc.cnrs.fr/nutheo/code\\_ant](http://www.iphc.cnrs.fr/nutheo/code_ant)





# Ab initio models

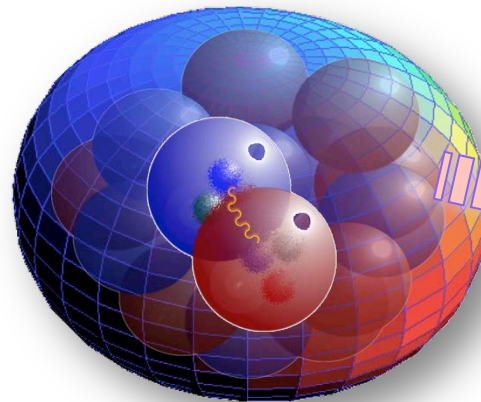
Nuclear force



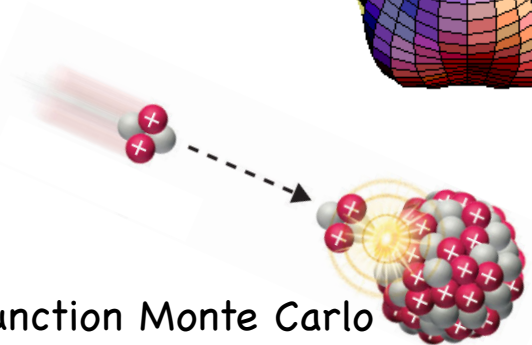
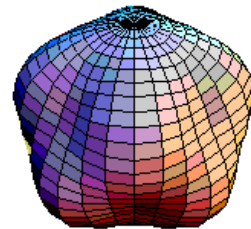
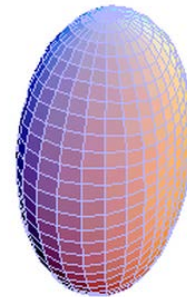
NN, 3N, ...

- ✧ Hyperspherical Harmonics
- ✧ No-core Shell Model
- ✧ NCSM/Resonating Group Method
- ✧ Symmetry-adapted NCSM
- ✧ Importance Truncation NCSM
- ✧ Monte Carlo NCSM

Many-body Approach



Nuclear properties:  
structure & reactions



- ✧ Green's function Monte Carlo
- ✧ Lattice Effective Field Theory
  - ✧ Coupled-cluster method
  - ✧ In-Medium SRG
- ✧ Gorkov-Green's function
- ✧ Many-body perturbation theory

I will give a few examples...

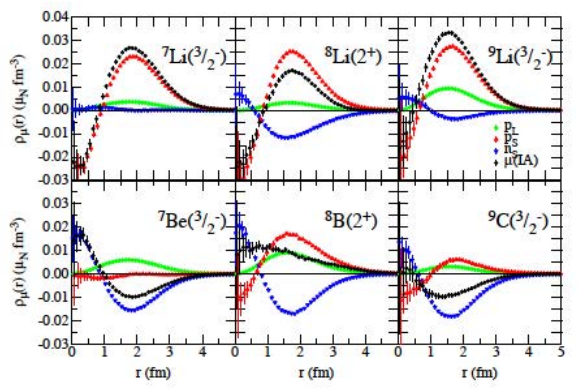
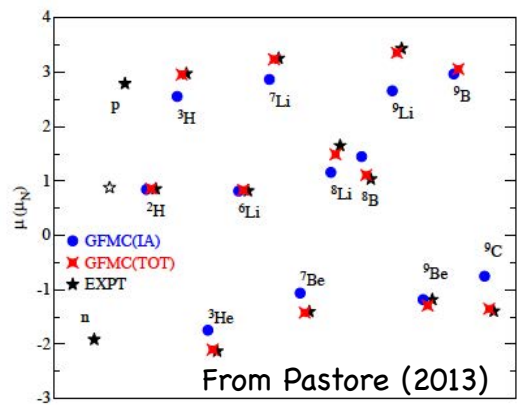
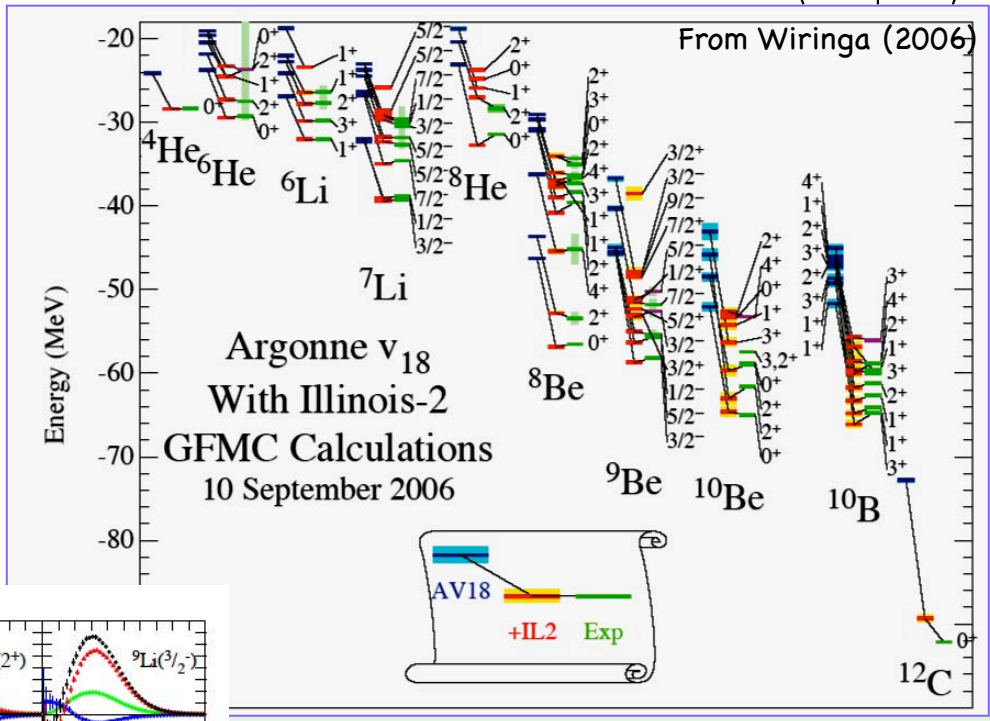
# Ab initio Variational and Green's Function Monte Carlo

- Variational Monte Carlo  $\Psi_T$ :
  - contains variational parameters adjusted via energy minimization,  $E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$
  - excellent approximation
- GFMC propagates the VMC  $\Psi_T$  to imaginary time

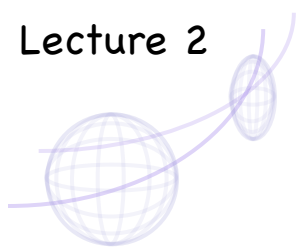
$$|\Psi(\tau)\rangle = e^{-(H-E_0)\tau} \Psi_T \xrightarrow{\tau \rightarrow \infty} |\Psi_0\rangle$$

(filters out excited-state contamination to leave lowest state of given  $J^\pi ; T$ )

Virtually exact method  
 Limited to local interactions  
 Light nuclei





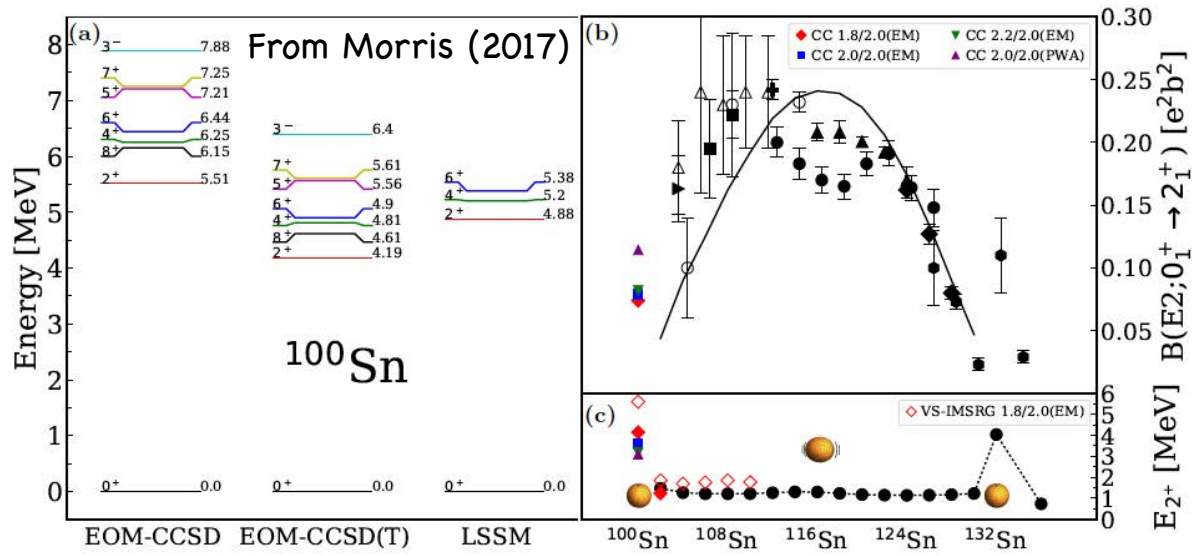
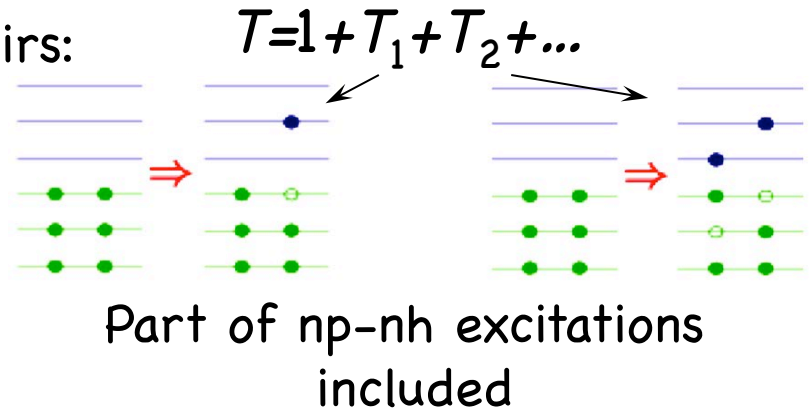


# Ab initio Coupled-cluster Theory

➤ Ansatz:  $|\Psi\rangle = e^T |\Phi\rangle \quad E = \langle \Phi | e^{-T} H e^T | \Phi \rangle$

➤ Expansion in number of particle-hole pairs:

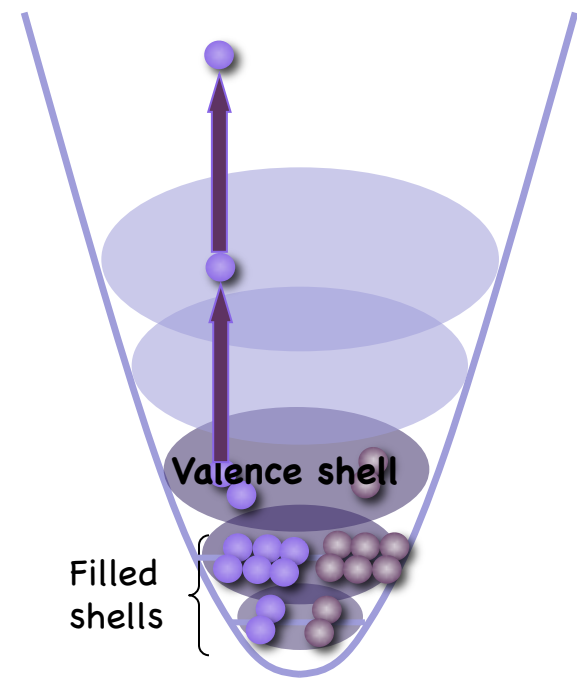
Scales gently with increasing  $A$   
 -> first calculations of  $^{100}\text{Sn}$ !  
 Limited near closed-shell nuclei  
 Missing correlations



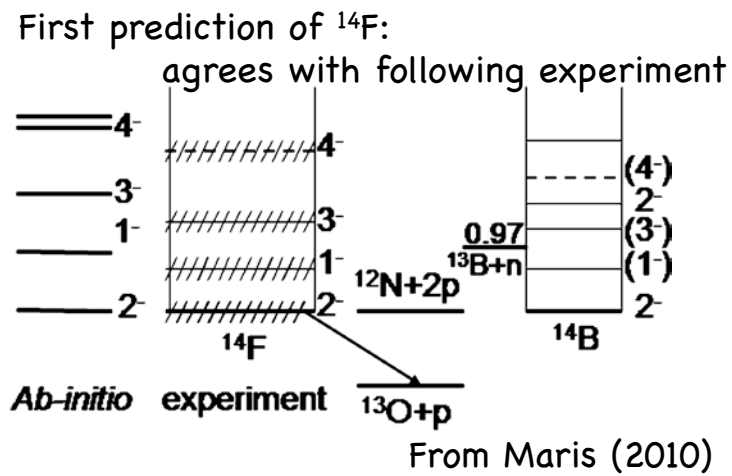
# Ab Initio No-Core Shell Model

- Harmonic-oscillator single-particle basis
- Construct many-body basis states (Slater determinants)
- Express Hamiltonian in this basis (huge matrix)
- Find low-lying states (eigenfunctions)

Convergence to exact solutions with increasing model space  
 Limited to light nuclei  
 No restrictions on interaction/nucleus



Solve Schrödinger equation in infinite space

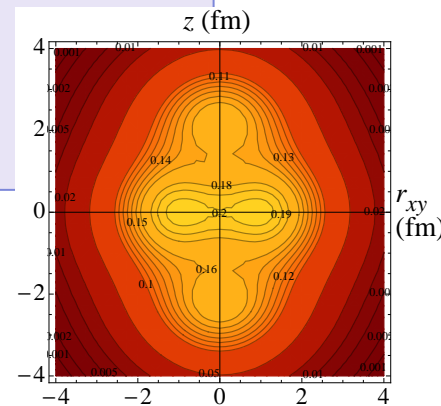
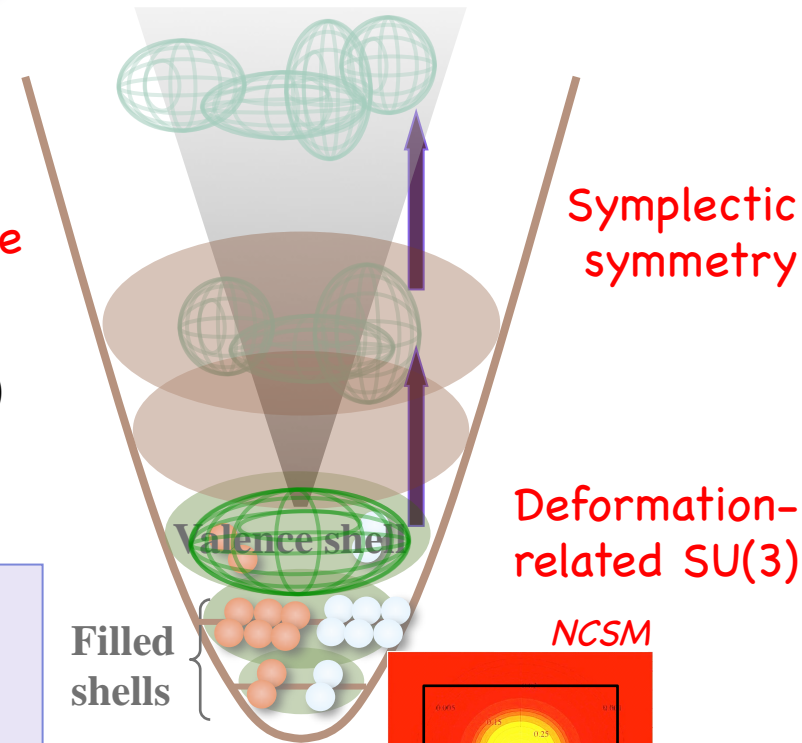
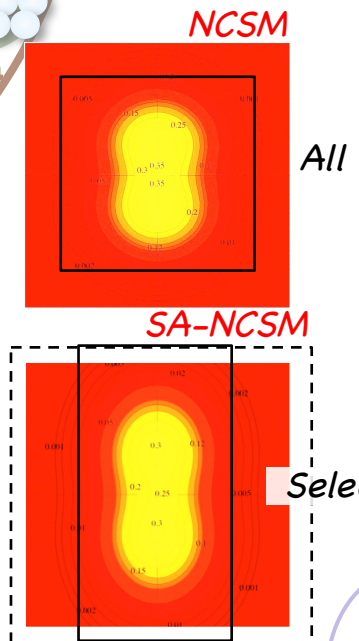
$$H\Psi(1,2,\dots,A) = E\Psi(1,2,\dots,A)$$




# Ab Initio Symmetry-adapted (SA) NCSM

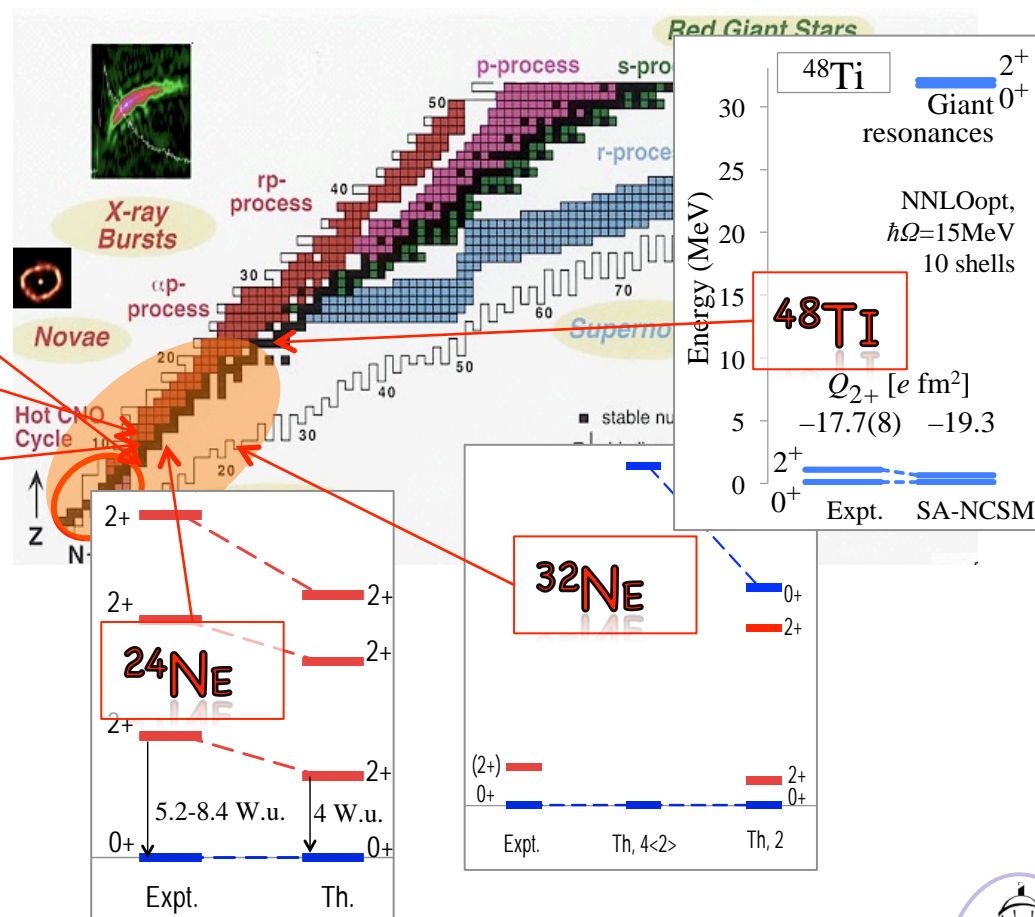
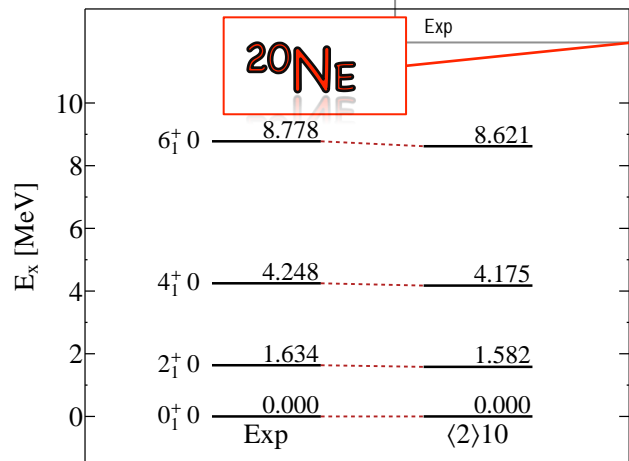
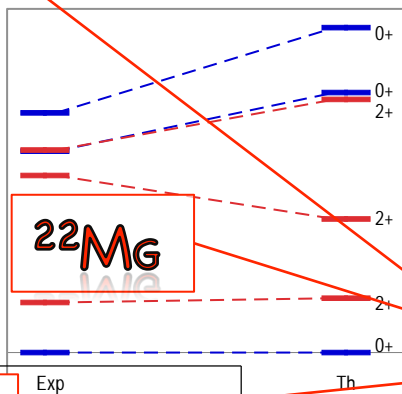
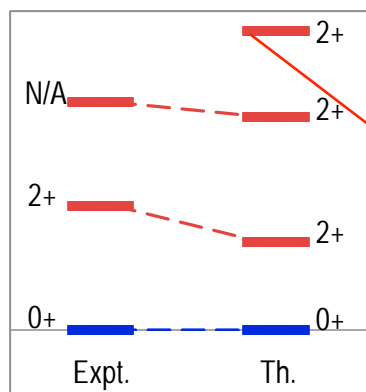
- Harmonic-oscillator single-particle basis
- Construct many-body basis states - **all possible shapes**
- Take physically relevant shapes
- Express Hamiltonian in this basis (huge matrix)
- Find low-lying states (eigenfunctions)

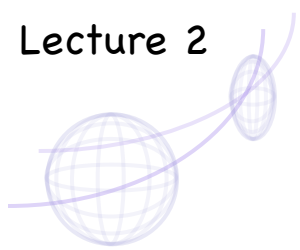
Up to Ca region ( $A < 50$ , so far)  
 Accounts for collective correlations & clustering  
 Convergence to exact solutions with increasing model space  
 CPU-bound calculations  
 Selected model spaces may be too restrictive

Ab initio modeling of  $^{20}\text{Ne}$ 

Code available at:  
<https://sourceforge.net/projects/lsu3shell/>

# Ab Initio Symmetry-adapted (SA) NCSM





# Ab initio Lattice EFT

- Nucleon and pion fields on lattice
- Use Auxiliary Field Method:
  - Replace contact interaction by interaction of each nucleon with a background field (particles decouple and interact only with the auxiliary field)

**LATTICE EFT**

lattice

Effective Field Theory

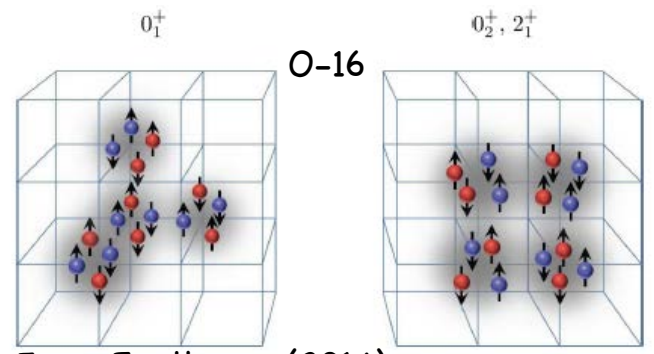
Courtesy D. Lee From D. Lee (2017)

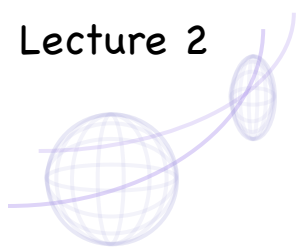
$$\exp \left[ -\frac{C}{2} (N^\dagger N)^2 \right] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds \exp \left[ -\frac{1}{2} s^2 + \sqrt{-C} s (N^\dagger N) \right]$$

↖ 2-body
↗ 1-body



Scales gently with increasing  $A$   
 Descriptions of clustering  
 Lattice spacing may be too large





# Symmetries (Exact & Approximate)

*Symmetry*



Emergent symmetries within nuclei

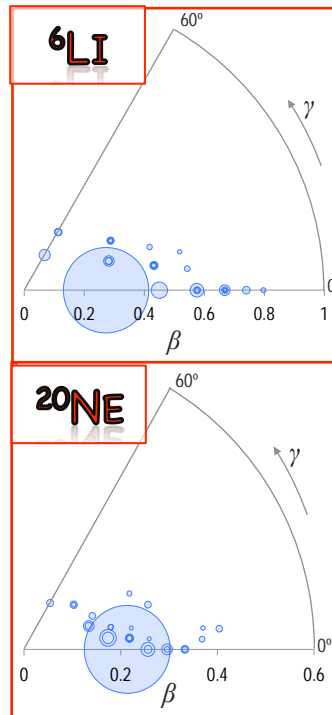
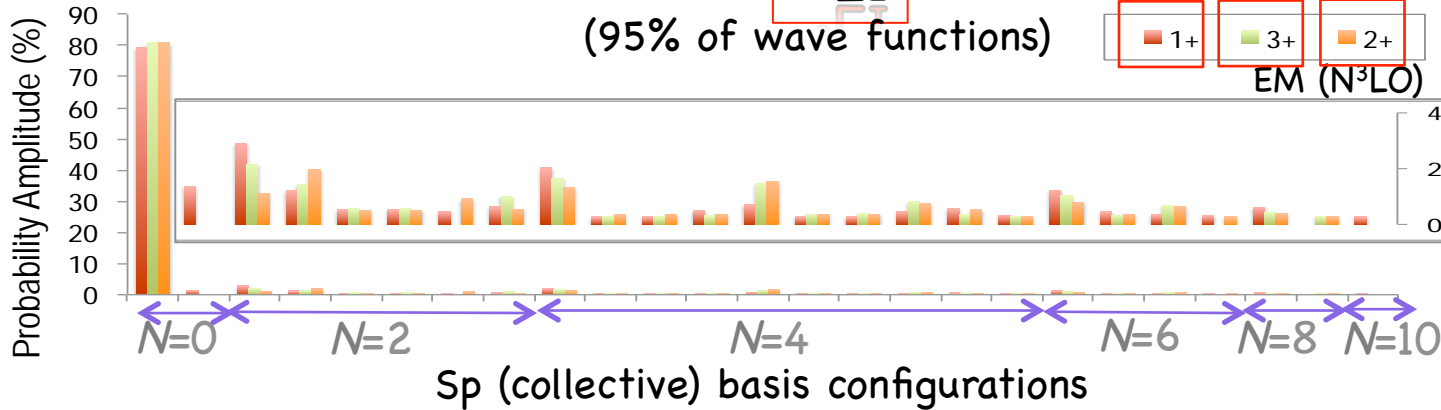
# Preference of Nature

Use Symmetry-adapted no-core shell model (SA-NCSM)

**<sup>6</sup>Li**

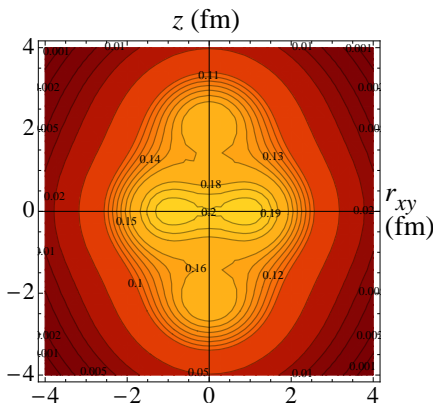
(95% of wave functions)

EM (N<sup>3</sup>LO)  
 1+ 3+ 2+



<sup>6</sup>Li, 14 shells

- #  $J=1,2,3$  states..... $2 \times 10^7$
- # Sp configurations.....528
- # Sp configurations with  $P > 0.2\%$ .....**25**

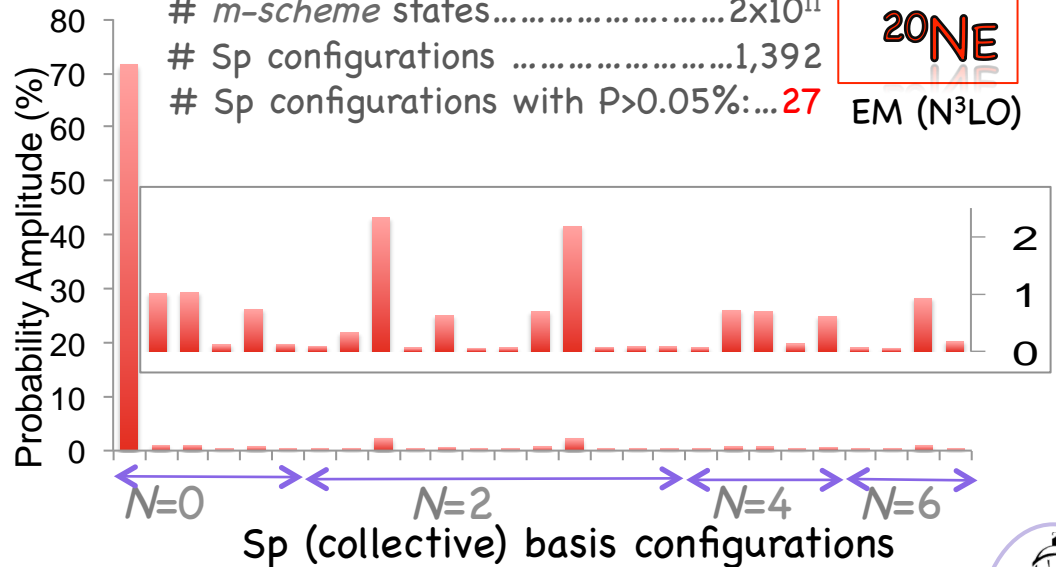


<sup>20</sup>Ne, 11 shells

- #  $m$ -scheme states..... $2 \times 10^{11}$
- # Sp configurations .....1,392
- # Sp configurations with  $P > 0.05\%$ :...**27**

**<sup>20</sup>Ne**

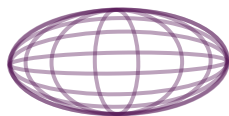
EM (N<sup>3</sup>LO)



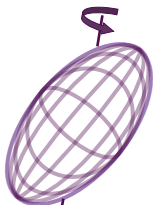


# What physics can we learn from Sp basis?

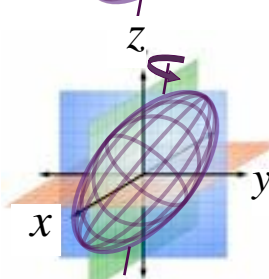
Sp (collective) basis configuration:



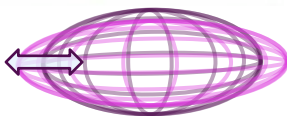
**one** equilibrium deformation ("shape")



rotations



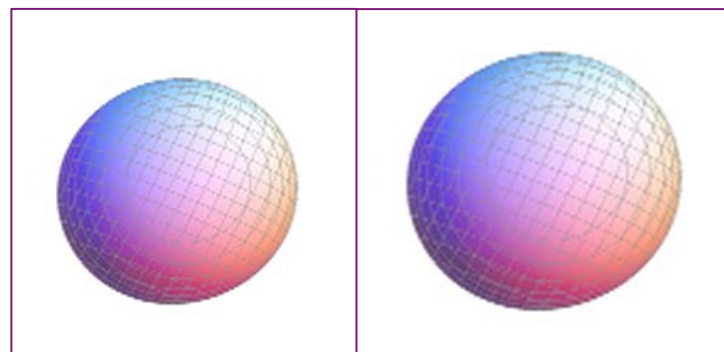
space orientation



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

All states preserve the equilibrium shape...

Symmetry?



# Symplectic Sp(3,R) Symmetry!

## Formal definition

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

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

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

that **preserve the canonical commutation relation**

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

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

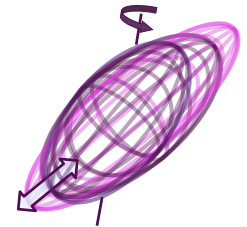
$$S_{ij} = \sum_n (x_{ni} p_{nj} + p_{ni} x_{nj}),$$

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

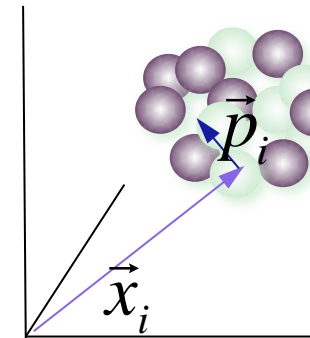
$$K_{ij} = \sum_n p_{ni} p_{nj},$$

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

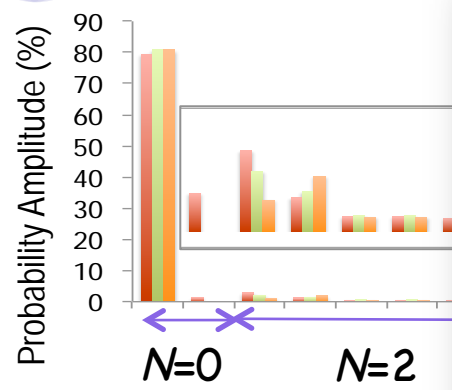
SU(3)  
in a HO shell  
(Elliott, 1958)



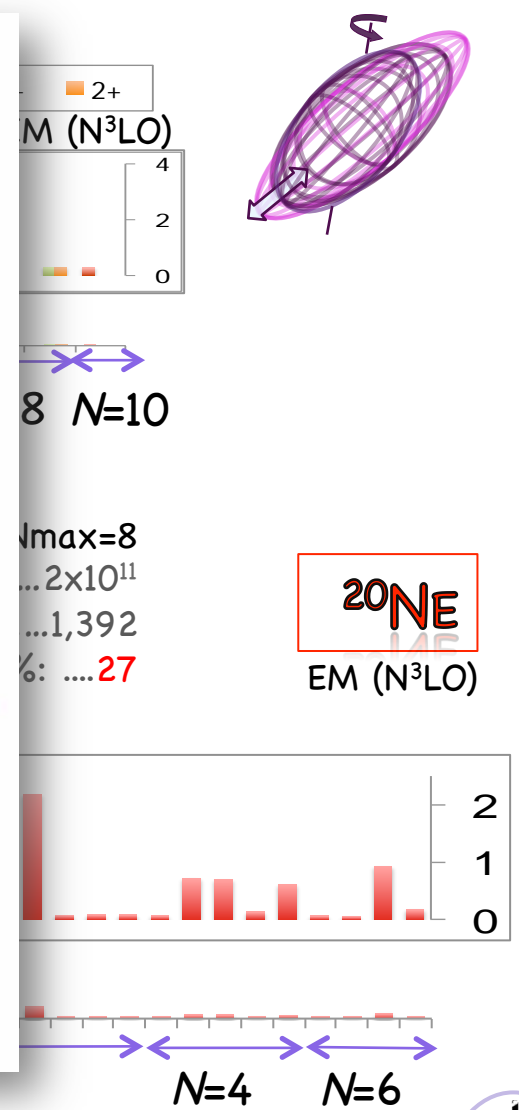
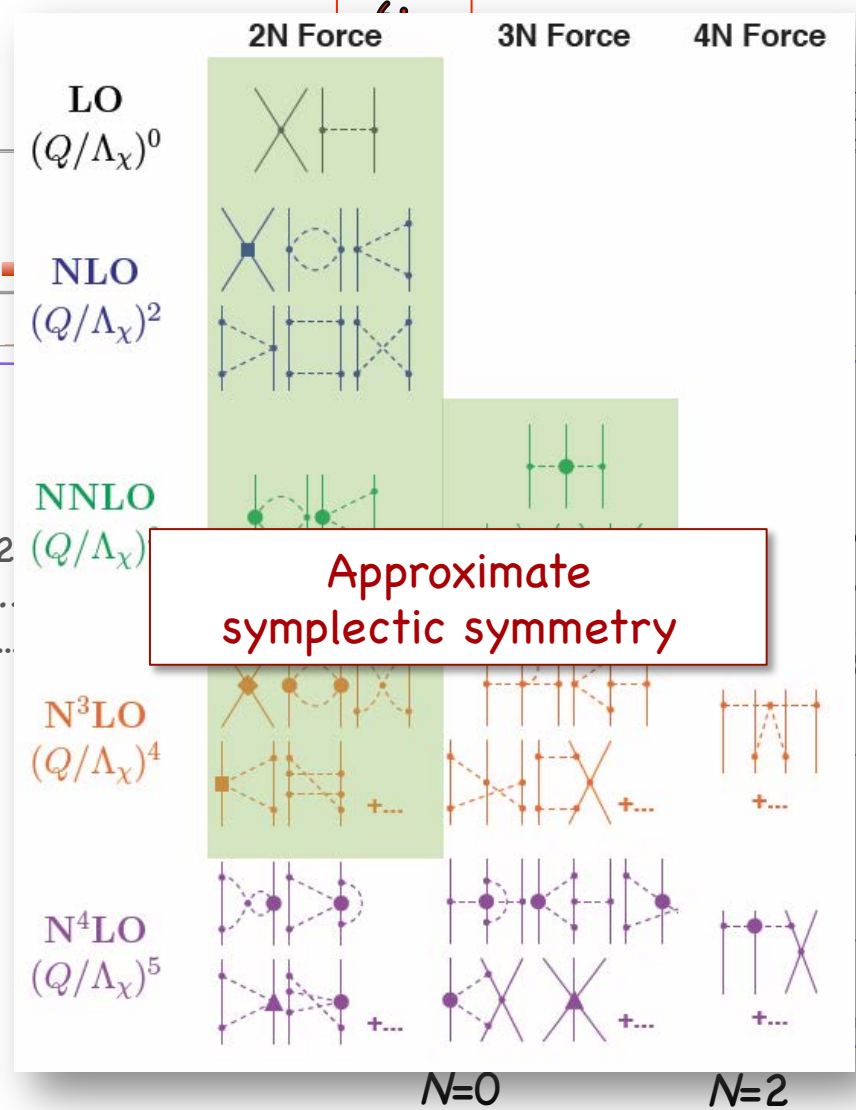
Nucleus with A nucleons



# Approximate Symmetry in Nuclei

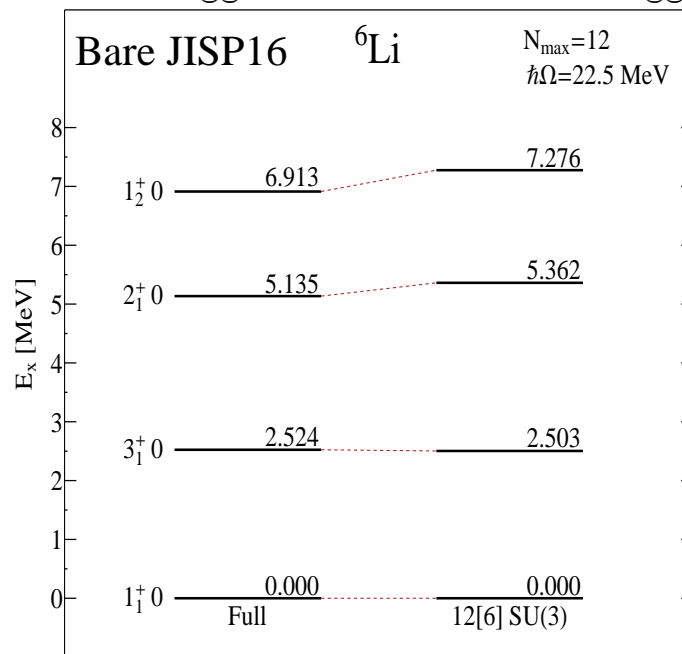
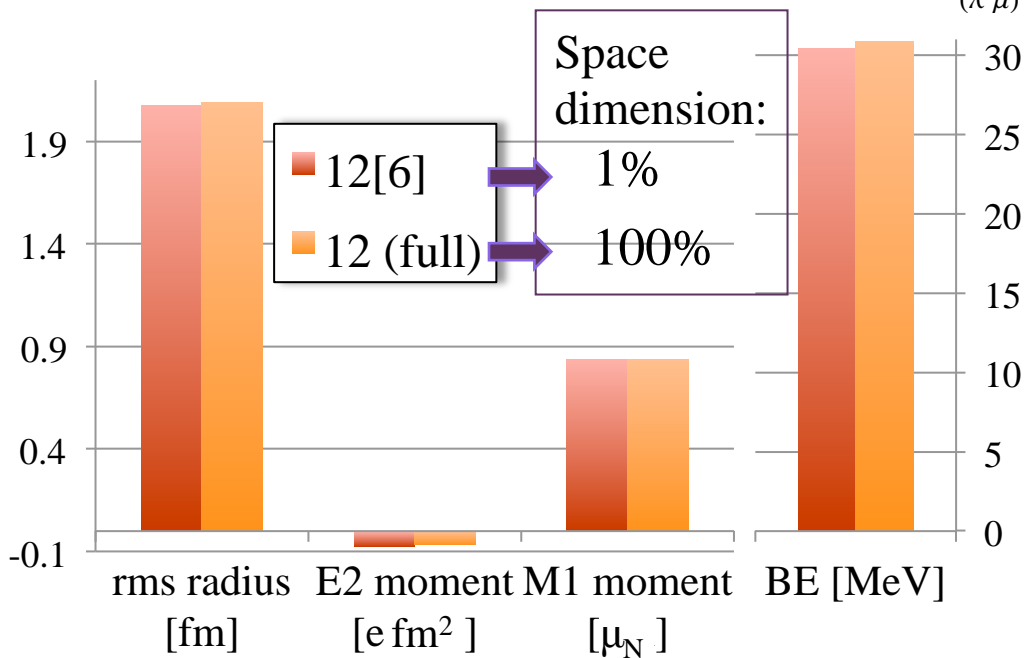
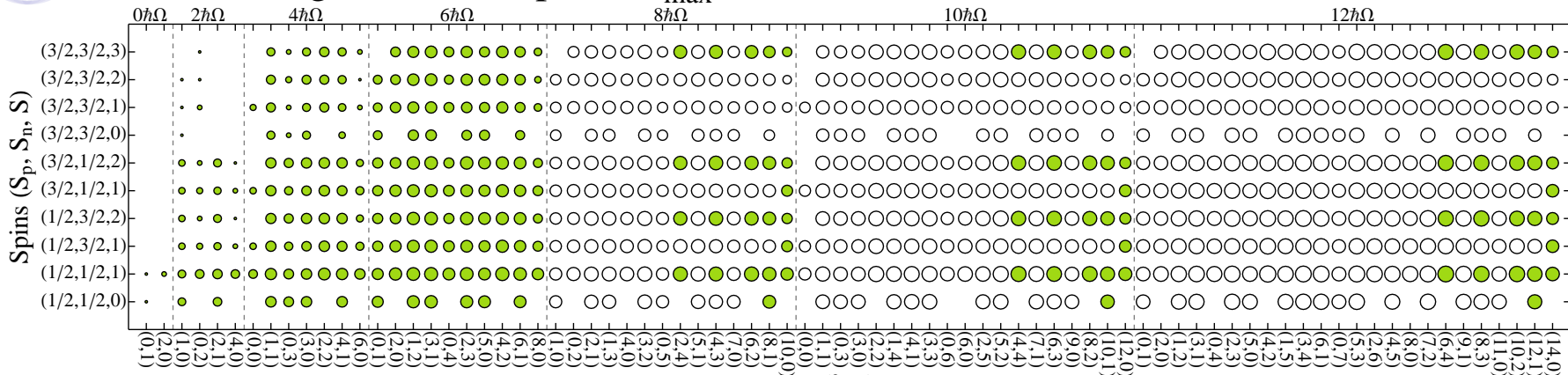


- ${}^6\text{Li}$ ,  $N_{\text{max}}=12$
- #  $J=1,2,3$  states.....2
- #  $\text{Sp}(3,\text{R})$  irreps.....2
- #  $\text{Sp}(3,\text{R})$  with  $P>0.2\%$ .....

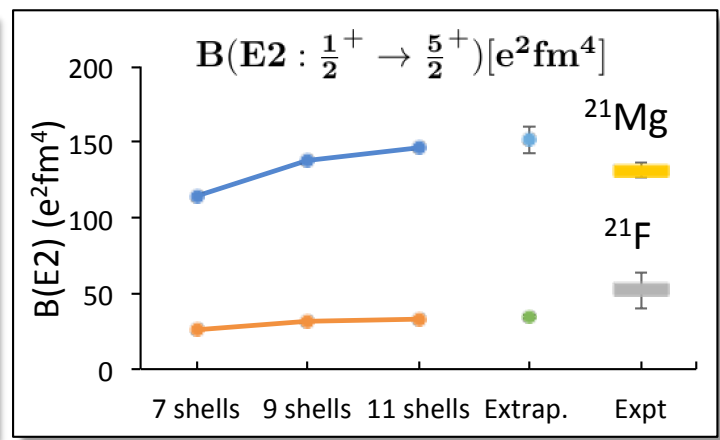
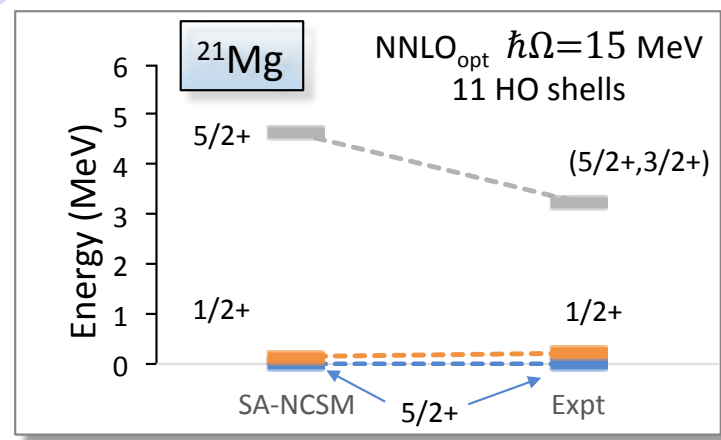


# Efficacy of SA-NCSM: Li-6

Winnowing the model space:  $N_{\max}=12[6]$  (full up to  $6\hbar\Omega$ ; selected configurations in  $8-12\hbar\Omega$ )



# Collectivity in intermediate-mass nuclei



## Ne & Mg isotopes

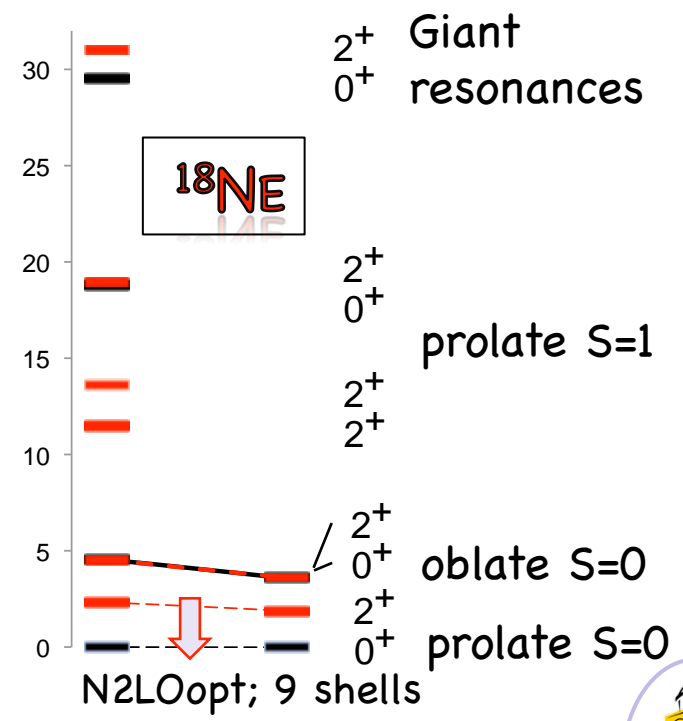
<sup>18</sup>Ne, B(E2: 2<sup>+</sup>→0<sup>+</sup>)

-----

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

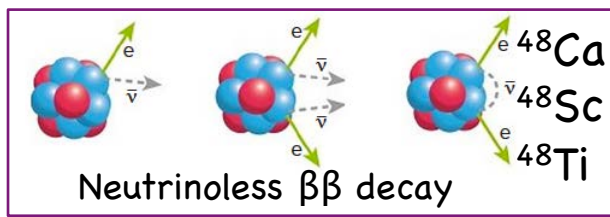
9 shells ..... 1.13 W.u.

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





# Structure of Ca-48 and Ti-48



8 shells, N2LOopt  
 $0^+$

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

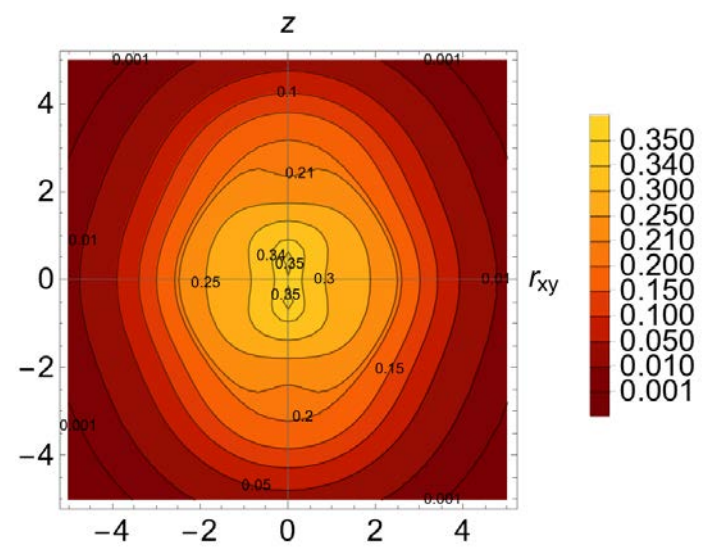
$2^+$   
SA-NCSM (selected): .....3,055,554  
Complete model space: ...14,522,234,982

8 shells, N2LOopt  
 $0^+$

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

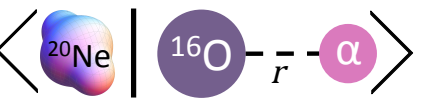
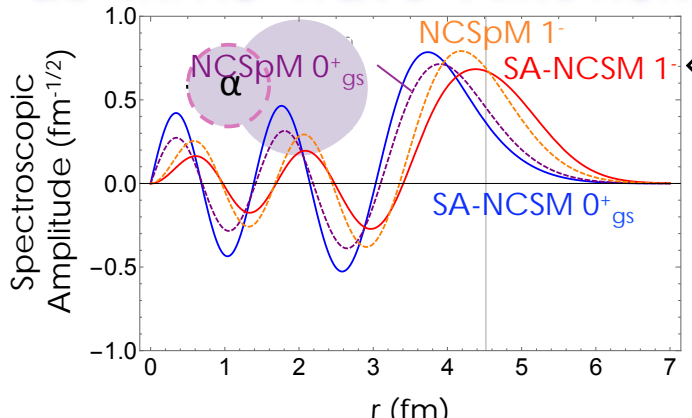
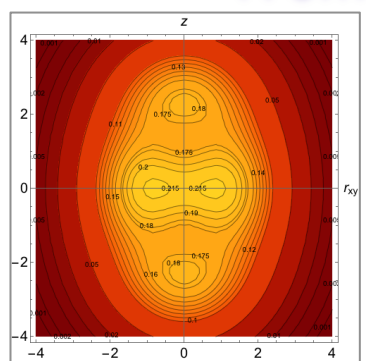
$2^+$   
SA-NCSM (selected): .....1,178,834  
Complete model space: ...113,920,316,658

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

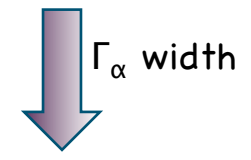
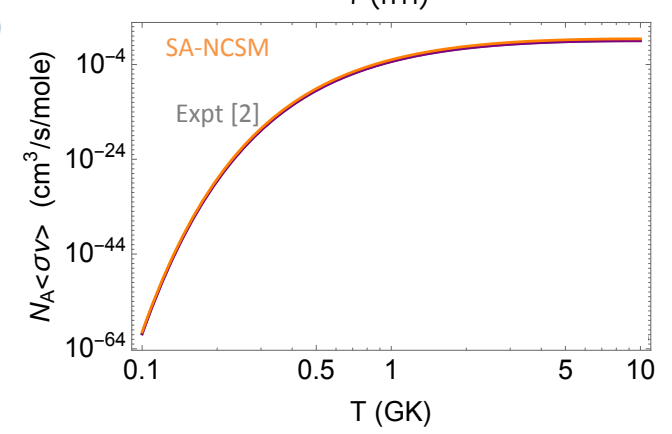
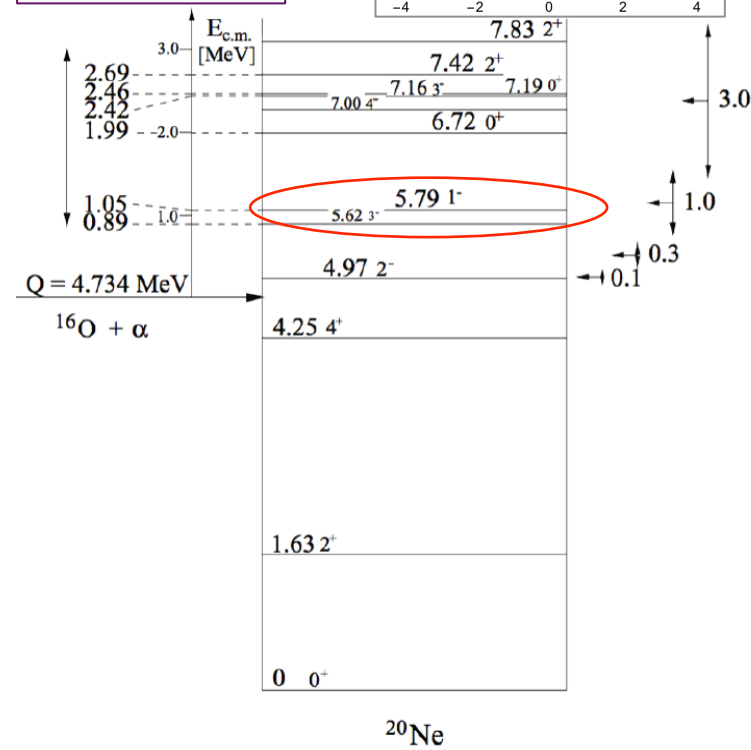
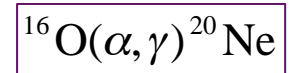




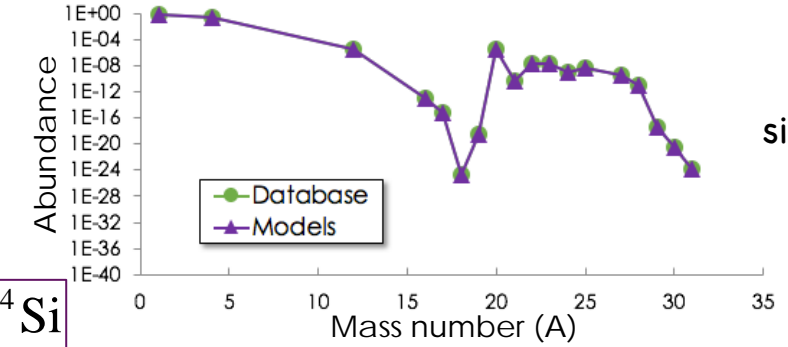
# XRB nucleosynthesis abundances from *ab initio* wave functions



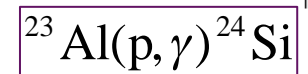
Wave functions from *ab initio* SA-NCSM with N2LOopt



Reaction rates

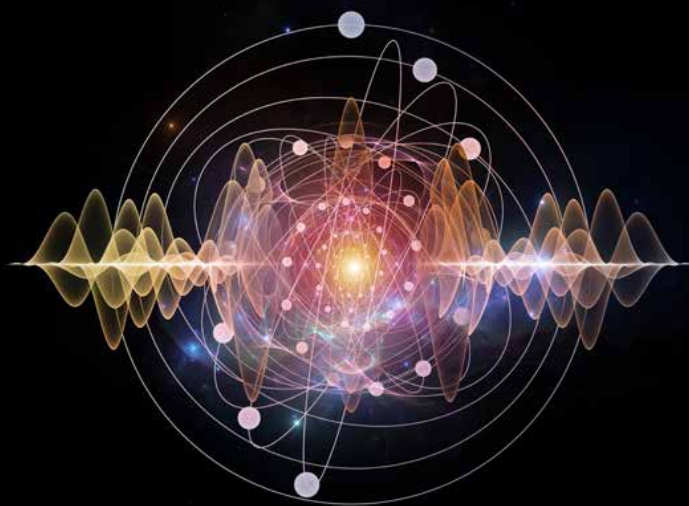


Nucleosynthesis simulations (Xnet): XRB abundance pattern



# EMERGENT PHENOMENA IN ATOMIC NUCLEI FROM LARGE-SCALE MODELING

A Symmetry-Guided Perspective



Kristina D Launey

 World Scientific

Nuclear Collectivity – Experimental perspective  
(John L Wood)

Configuration–interaction models  
(Calvin W Johnson)

Symplectic rotor model  
(David J Rowe)

Electron Scattering in the Symplectic Shell Model  
(Jutta E Escher)

Lattice QCD  
(Thomas Luu and Andrea Shindler)

Ab Initio Lattice Effective Field Theory  
(Dean Lee)

Correlated Gaussian Approach and Clustering  
(Yasuyuki Suzuki and Wataru Horiuchi)

Symmetry-Adapted No-Core Shell Model  
(Jerry P Draayer, Tomas Dytrych and KD Launey)

Auxiliary-Field Quantum Monte Carlo Methods  
(Yoram Alhassid)

Lie Density Functional Theory  
(George Rosensteel)

Exactly Solvable Pairing  
(Feng Pan, Xin Guan & Jerry P Draayer)