

Symmetry-adapted bases for ab initio structure and reaction theory

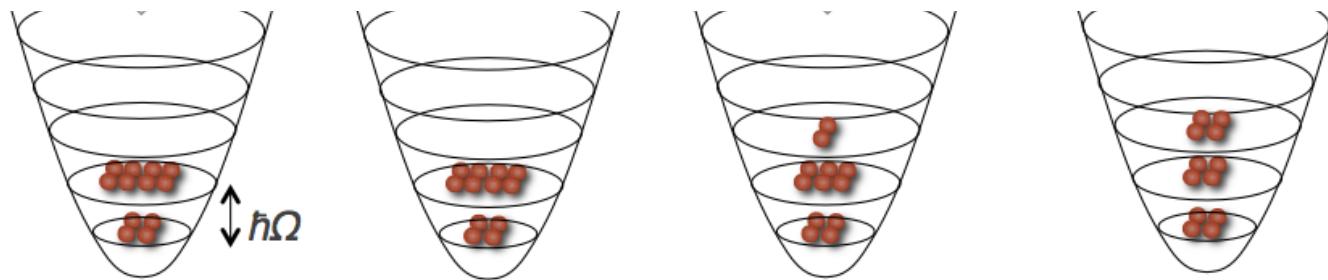
Alexis Mercenne, Kristina Launey, Tomas Dytrych, Jerry Draayer

*Department of Physics & Astronomy, Louisiana State University, Baton Rouge, LA,
70803*

Jutta Escher

Lawrence Livermore National Laboratory, Livermore, California 94550, USA

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



Based on NCSM:

- Spherical harmonic oscillator basis
- Distributions of nucleons over shells
- *Ab initio* (no restrictions for interactions ...NN, NNN, non-local,...)

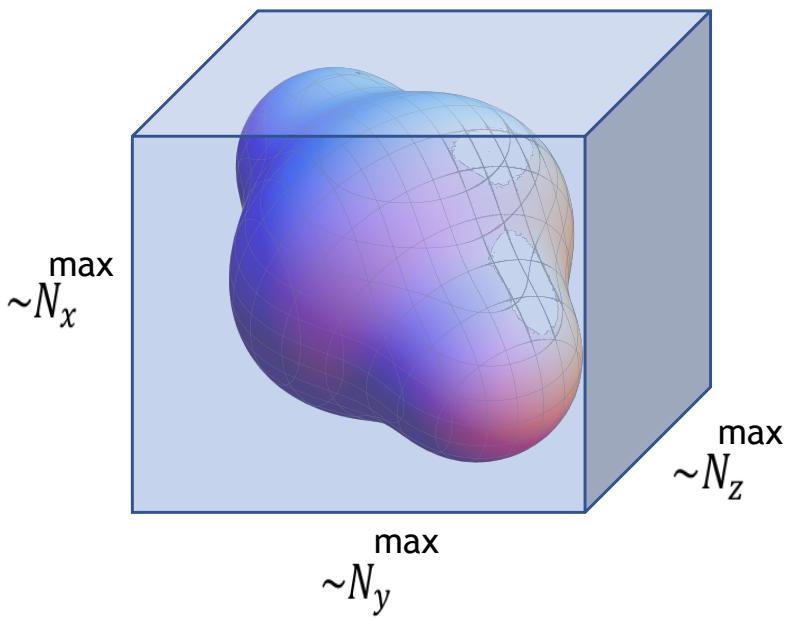
New features in SA-NCSM:

NCSM with symmetry-adapted (SA) basis (reorganization of model space):
SU(3)-coupled basis states or Sp(3,R)-coupled basis states

Model space selection (truncation) - physically relevant + exact center-of-mass factorization!

Equal to NCSM in complete- N_{\max} model space

- **SA-NCSM: SU(3)-scheme basis**



Total HO quanta: $N = N_x + N_y + N_z$
 NCSM: N_{max} determines the size of model space
 SA-NCSM: keeps track of N_x , N_y , N_z
 $\lambda = N_z - N_x$; $\mu = N_x - N_y$

SU(3) basis states: $|(\lambda\mu)KLM_L\rangle$

$$SU(3)_{(\lambda,\mu)} \stackrel{K}{\supset} SO(3)_L \supset SO(2)_{M_L}$$

With spin: $|\alpha N(\lambda\mu)KL; (S_p S_n)S; JM\rangle$
 $SU(3) \times SU(2)$

SU(3) basis states: unitary transformation from m-scheme

$$|\Psi^{JM}\rangle = \sum_i C_i |\alpha N(\lambda\mu)KL; (S_p S_n)S; JM\rangle_i$$



Gives information about important deformed configurations

Spherical : (00)

Prolate : ($\lambda 0$)

Oblate: (0μ)

LSU code (LSU3shell): sourceforge.net/projects/lisu3shell

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

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

- **SA-NCSM: SU(3)-scheme basis**

How is the SU(3)-scheme basis constructed?

> Intuitive way: $|\langle \lambda\mu \rangle KLS\rangle = \{a_{(\eta_1,0)\sigma_1\tau_1}^\dagger \otimes a_{(\eta_2,0)\sigma_2\tau_2}^\dagger \otimes \cdots \otimes a_{(\eta_A,0)\sigma_A\tau_A}^\dagger\}^{(\lambda\mu)KLS} |0\rangle$

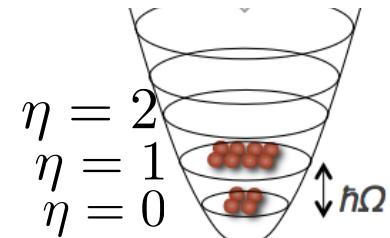
Considering 2 particles:

spin **isospin**

$$\{a_{(\eta_1,0)\sigma_1\tau_1}^\dagger \otimes a_{(\eta_2,0)\sigma_2\tau_2}^\dagger\}^{(\lambda\mu)KLST} = \sum_{\ell_1\ell_2} \langle (\eta_1,0)\ell_1; (\eta_2,0)\ell_2 | |(\lambda\mu)KL\rangle \{a_{\eta_1\ell_1\sigma_1\tau_1}^\dagger \otimes a_{\eta_2\ell_2\sigma_2\tau_2}^\dagger\}^{LST}$$

Tedious... not used for many-particle system

Reduced SU(3) CG



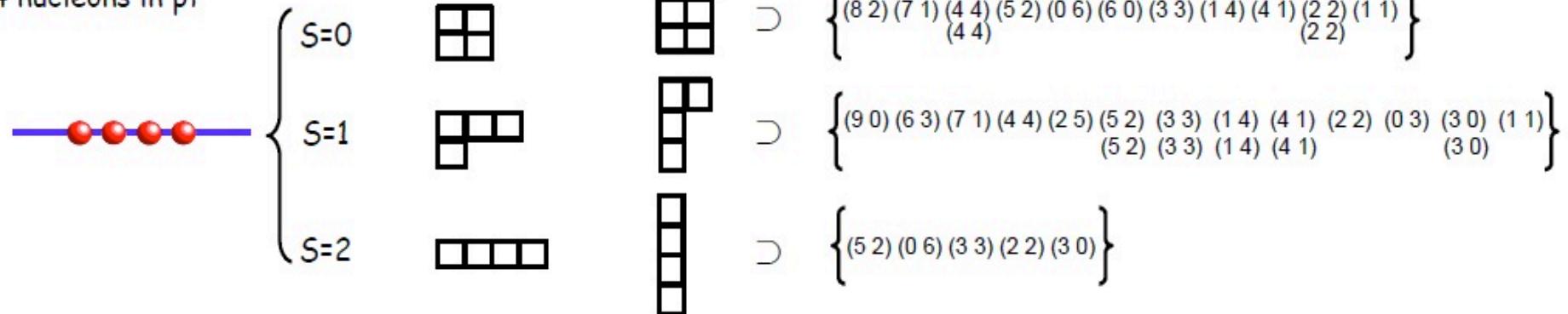
➤ For fast basis construction, use of Gel'fand patterns

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

For a single shell!

● Example:

4 nucleons in pf



• SA-NCSM: SU(3)-scheme interaction

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

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

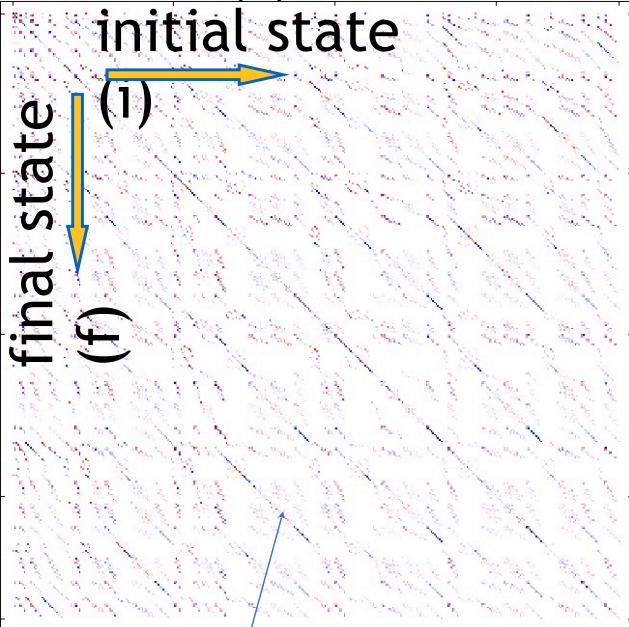
$n_r n_s (\lambda \mu)$

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

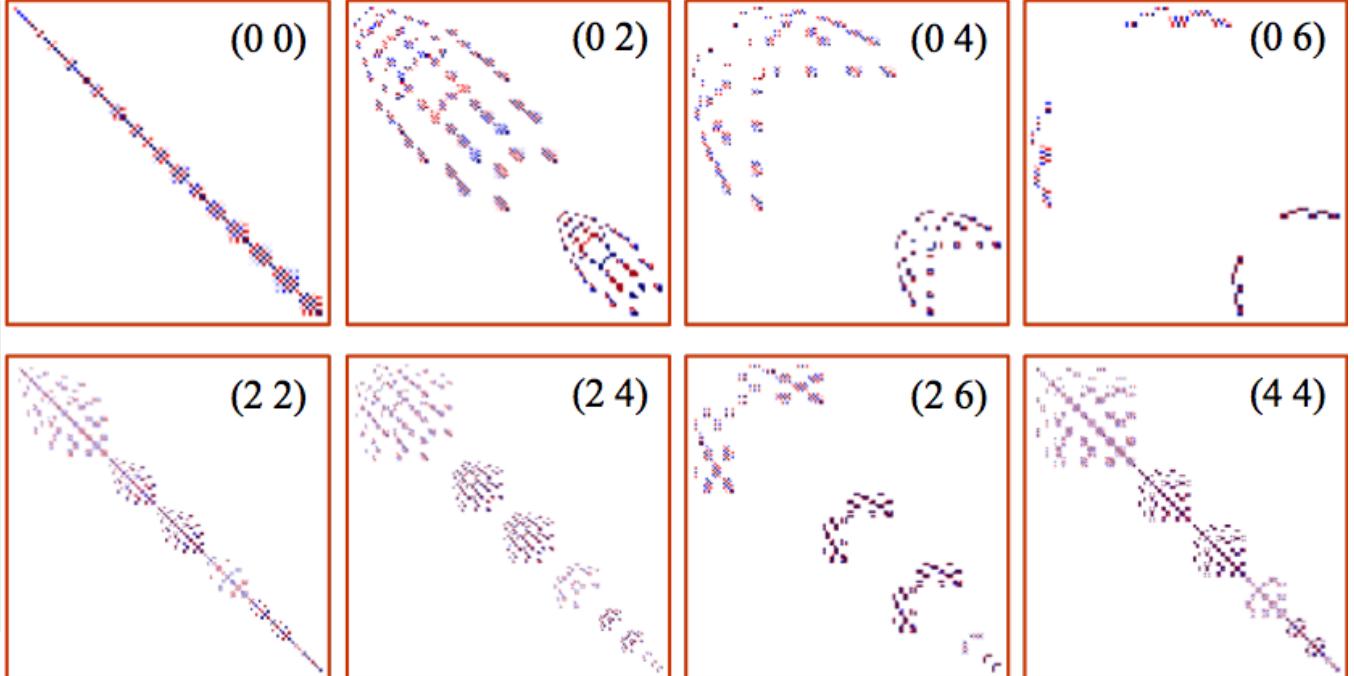
$$\Pi_{j_r j_s j_t j_u} \langle (\eta_t 0) l_t; (\eta_u 0) l_u \| (\omega \kappa L)_i \rangle \begin{Bmatrix} l_r & \frac{1}{2} & j_r \\ l_s & \frac{1}{2} & j_s \\ L_f & S_f & J \end{Bmatrix} \begin{Bmatrix} l_t & \frac{1}{2} & j_t \\ l_u & \frac{1}{2} & j_u \\ L_i & S_i & J \end{Bmatrix} V_{rstu}^{\Gamma}$$

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

NN in SU(3) basis

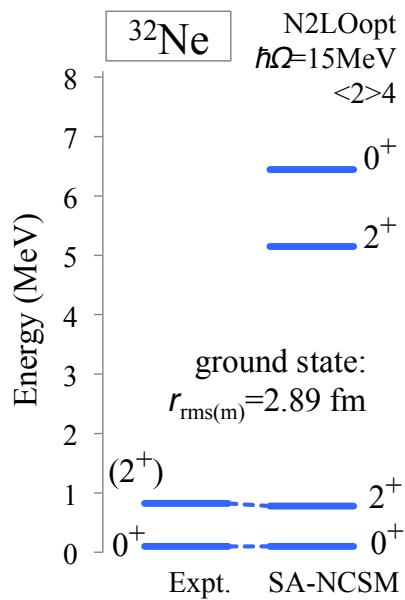
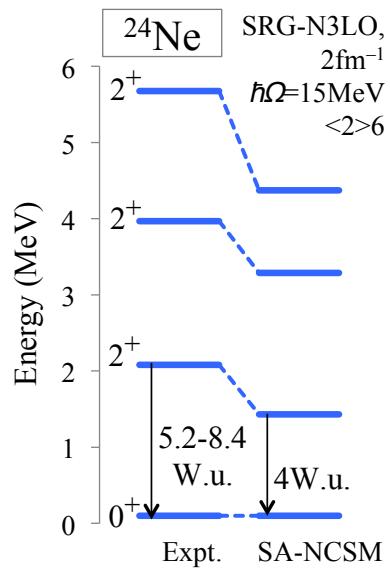
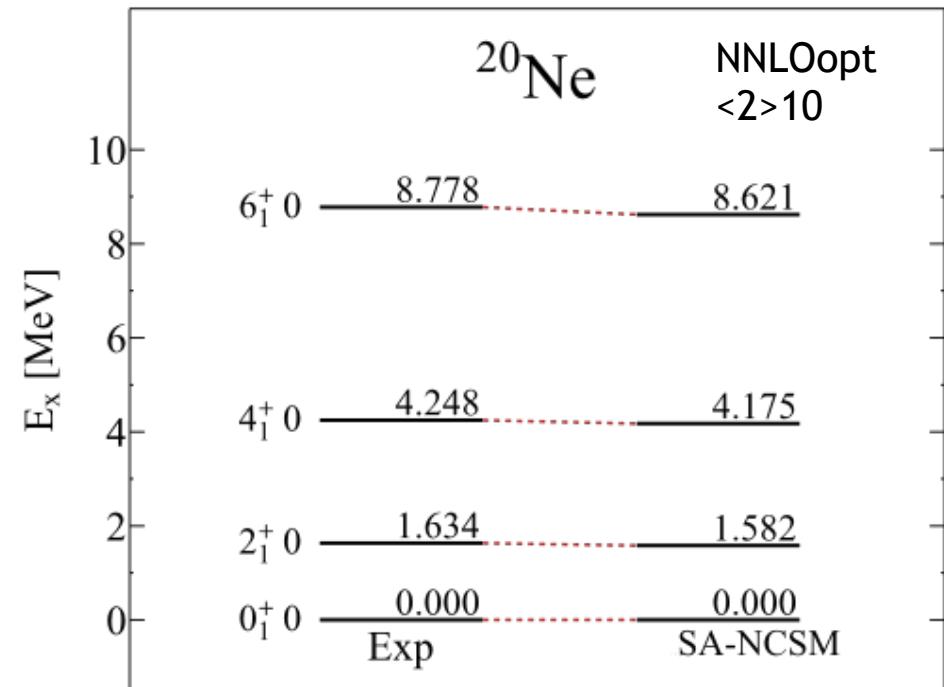
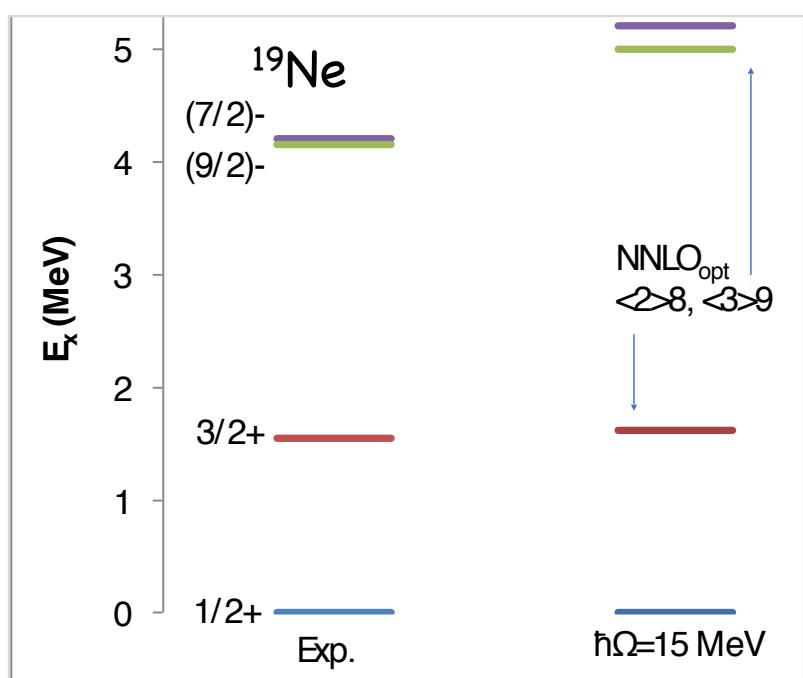


Equivalent to m -scheme



Matrices are smaller and sparser

- SA-NCSM with SU(3) scheme: Examples



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

Complete model space: 1000 billion states

- SA-NCSM: $Sp(3,R)$ -scheme basis

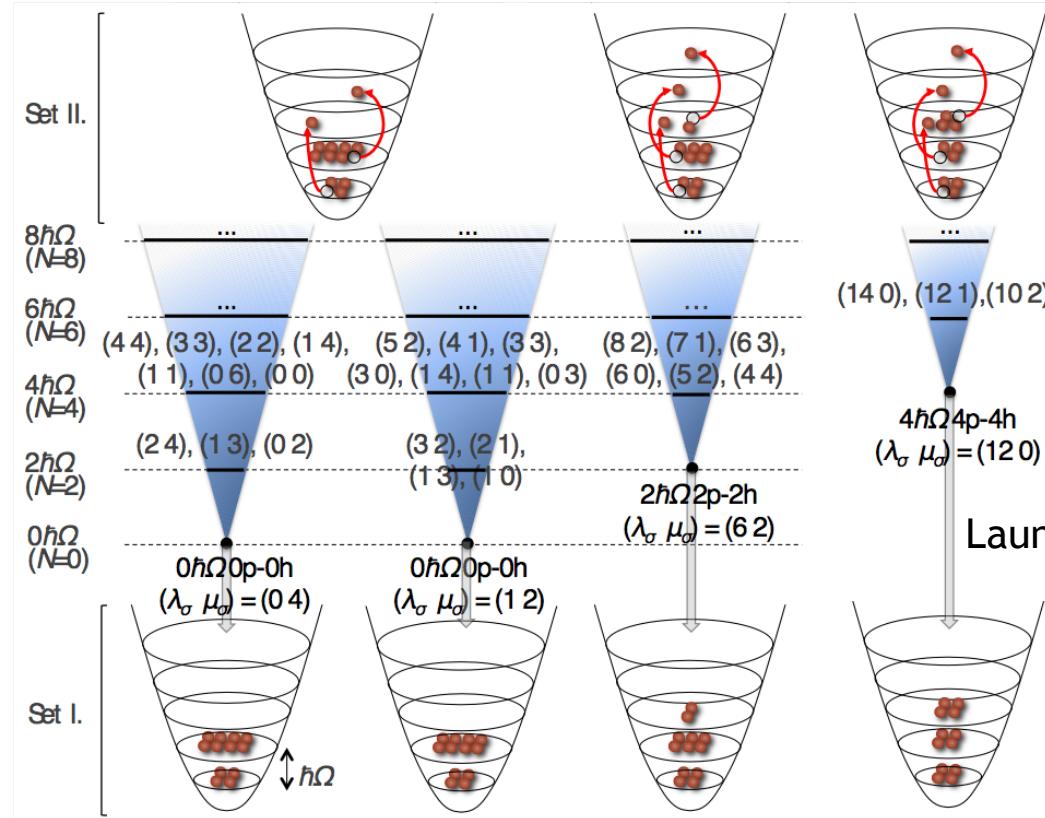
Symmetry-adapted:
 $SU(3)$, $Sp(3,R)$

Describes deformation Equilibrium shape

Symplectic $Sp(3,R)$ basis: $\sigma n \rho \omega \kappa LM_L$

$$Sp(3, \mathbb{R}) \underset{\sigma}{\supset} U(3) \underset{n\rho}{\supset} SO(3) \underset{\omega}{\supset} SO(2) \underset{\kappa}{\supset} L \underset{M_L}{\supset}$$

Find eigenvectors/eigenvalues of the second-order
 $Sp(3,R)$ Casimir invariant for each $SU(3)$ irrep

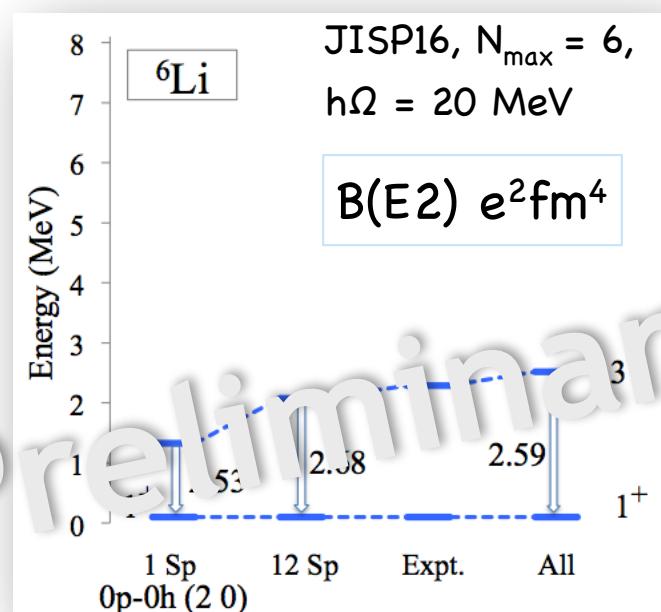
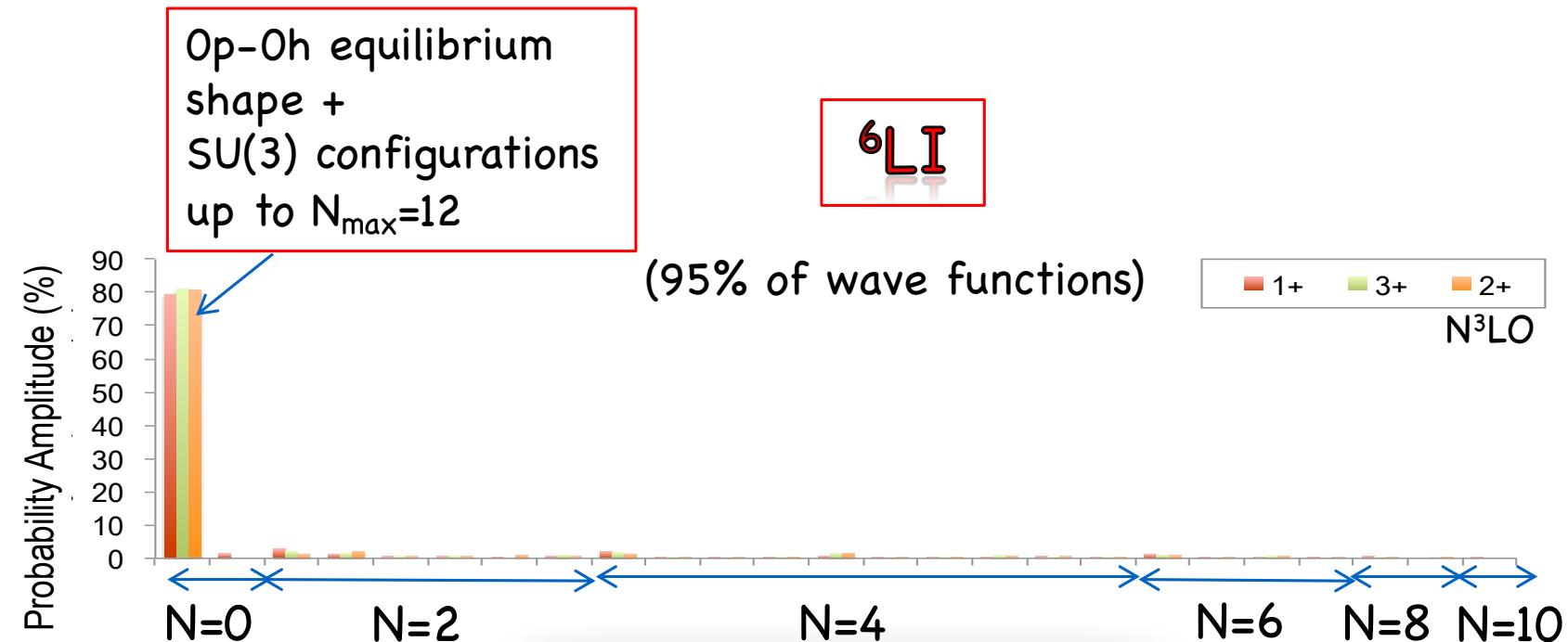


Reorganization of model space:
“bin” $SU(3)$ basis states into
 $Sp(3,R)$ symplectic irreps

Unitary transformation from
 $SU(3)$ scheme

Launey, Dytrych, Draayer, Prog. Part. Nucl. Phys. 89 (2016)
101

- SA-NCSM with Sp(3,R) scheme: Examples



cf. Launey's talk

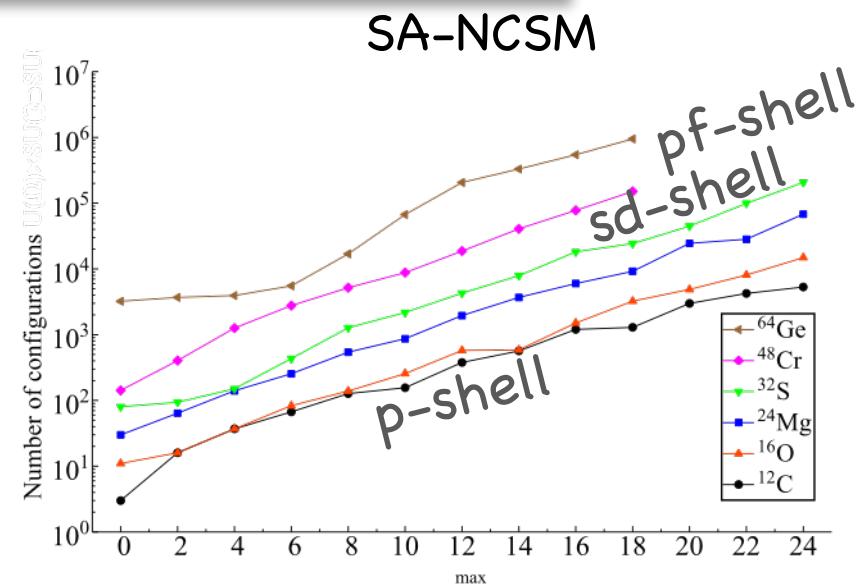
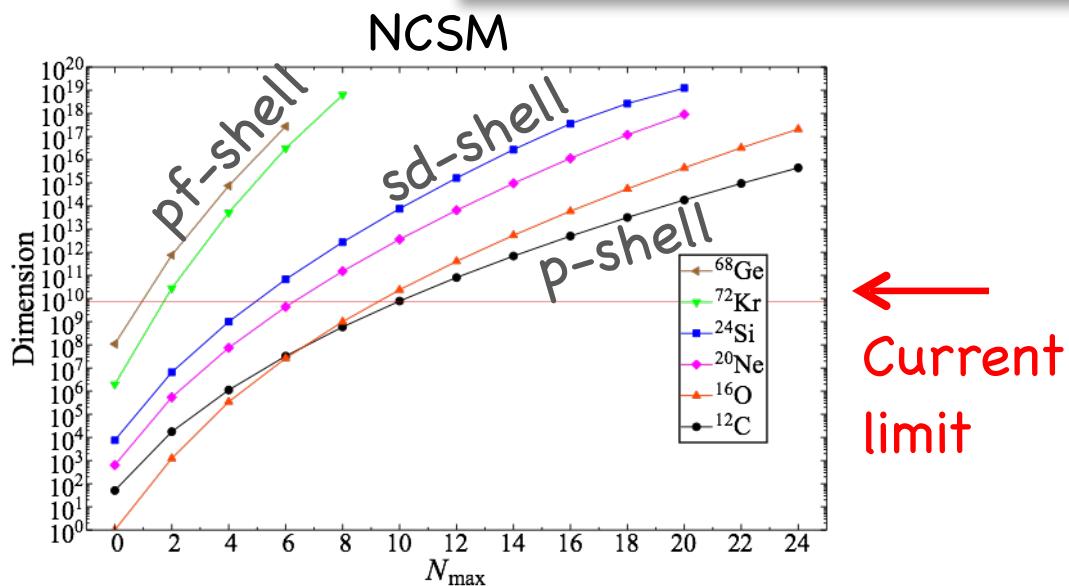
Single Sp(3,R) irrep

12 Sp(3,R) irreps

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)



- Sp(3,R)-coupled basis – fast construction (in selected spaces)
- Hamiltonian – matrices of small dimension; eigenvectors solved on a laptop

- Resonating Group Method

intrinsic function relative motion

1-cluster

2-clusters

3-clusters

$$\text{Cluster wave function } \Psi = \mathcal{A} \left\{ \sum c_i \phi_{1i}(\vec{\xi}_{1i}) + \sum \phi_{1j}(\vec{\xi}_{1j}) \phi_{2j}(\vec{\xi}_{2j}) g(\vec{r}_j) \right. \\ \left. + \sum_k^i \phi_{1k}(\vec{\xi}_{1k}) \phi_{2k}(\vec{\xi}_{2k}) \phi_{3k}(\vec{\xi}_{3k}) g(\vec{r}_{1k}, \vec{r}_{2k}) + \dots \right\}$$

For 2 clusters:

$|\Phi_{\nu r}^{J^\pi T}\rangle$

$\nu \equiv \{(A-a)\alpha_1 I_1^{\pi_1} T_1; a\alpha_2 I_2^{\pi_2} T_2; \ell s\}$

$$|\Psi^{J^\pi T}\rangle = \sum_{\nu} \int r^2 \frac{g_{\nu}(r)}{r} \hat{\mathcal{A}} \left[(|(A-a)\alpha_1 I_1^{\pi_1} T_1\rangle \otimes |a\alpha_2 I_2^{\pi_2} T_2\rangle)^{(sT)} \otimes Y_{\ell}(\hat{r}_{A,A-a}) \right]^{J^\pi T} \frac{\delta(r - r_{A,A-a})}{rr_{A,A-a}} dr$$

↑

Unknown

$$\vec{r}_{A,A-a} = r_{A,A-a} \hat{r}_{A,A-a} = \frac{1}{A-a} \sum_{i=1}^{A-a} \vec{r}_i - \frac{1}{a} \sum_{j=A-a+1}^A \vec{r}_j$$

- Antisymmetrizer does not act on r
- Set of basis vectors which are not orthogonal between each other
- Very relevant to unify structure and reaction

Y.C. Tang et al, Physics Report **47** (1978) 167

S. Quaglioni and P. Navratil Phys. Rev. C **79**, 044606 (2009)

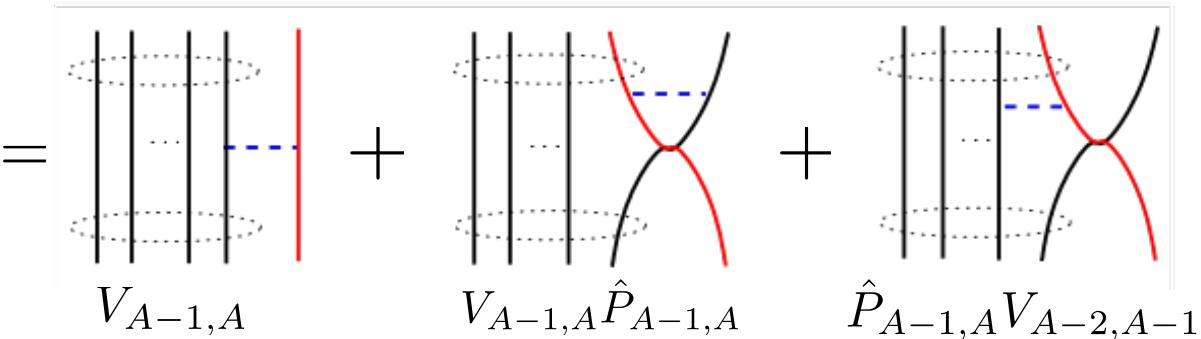
- **Resonating Group Method**

$$\nu \equiv \{(A - a)\alpha_1 I_1^{\pi_1} T_1; a\alpha_2 I_2^{\pi_2} T_2; \ell s\}$$

Hill-Wheeler equations: $\sum_{\nu'} \int (H_{\nu\nu'}(r, r') - EN_{\nu\nu'}(r, r')) g_{\nu}(r) dr = 0 \longleftrightarrow \hat{H} |\Psi\rangle = E |\Psi\rangle$

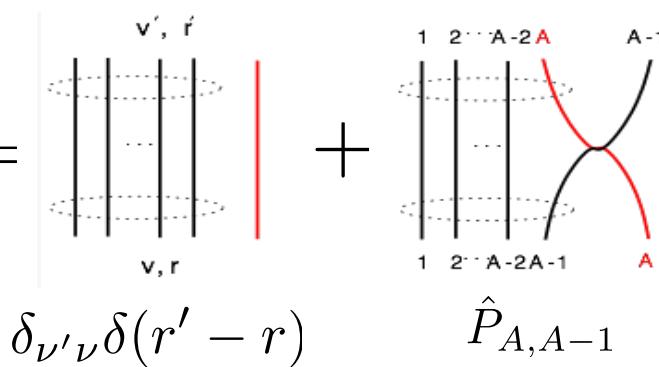
$$H_{\nu'\nu}(r', r) = \langle \Phi_{\nu'r'}^{J^\pi T} | \hat{\mathcal{A}} \hat{H} \hat{\mathcal{A}} | \Phi_{\nu r}^{J^\pi T} \rangle$$

Antisymmetrizer:



Eigenvectors have SU(3) symmetry

$$N_{\nu'\nu}(r', r) = \langle \Phi_{\nu'r'}^{J^\pi T} | \hat{\mathcal{A}} \hat{\mathcal{A}} | \Phi_{\nu r}^{J^\pi T} \rangle =$$



What we need:

- Interaction
- 1-body and 2-body density matrices (OBDME, TBDME)

Gives information on the structure of the target

$$\langle \Phi_{\nu'n'}^{J^\pi T} | \hat{P}_{A,A-1} | \Phi_{\nu n}^{J^\pi T} \rangle = \frac{1}{A-1} \sum_{jj'J_o\tau_o} \Pi_{ss'jj'J_o\tau_o} (-1)^{I'_1+j'+J} (-1)_{T_1+\frac{1}{2}+T} \left\{ \begin{array}{c} I_1 \\ \ell \\ j \end{array} \right\} \left\{ \begin{array}{c} \frac{1}{2} \\ J \\ j \end{array} \right\} \times \left\{ \begin{array}{c} I'_1 \\ \ell' \\ j' \end{array} \right\} \left\{ \begin{array}{c} \frac{1}{2} \\ J \\ j' \end{array} \right\} \langle (A-1)\alpha'_1 I'_1 T'_1 | | \{a_{n\ell j \frac{1}{2}}^\dagger \otimes a_{n'\ell' j' \frac{1}{2}}\}^{J_o \tau_o} | | (A-1)\alpha_1 I_1 T_1 \rangle$$

Figs. from S. Quaglioni and P. Navratil Phys. Rev. C 79, 044606 (2009)

- Resonating Group Method

Non orthogonality is short range $\mathcal{V}_{\nu'\nu}(r', r) \rightarrow \frac{\delta(r' - r)}{r'r}$ for $r', r \gg 1$

Introduce an orthogonalized version of Hill-Wheeler equations:

$$\sum_{\nu} \int dr r^2 \left[\mathcal{H}_{\nu'\nu}(r', r) - E \delta_{\nu'\nu} \frac{(r' - r)}{r'r} \right] \frac{\chi_{\nu}(r)}{r} = 0$$

$\mathcal{H} = N^{-\frac{1}{2}} H N^{-\frac{1}{2}}$

$$\frac{\chi_{\nu}(r)}{r} = \langle \Phi_{\nu r} | N^{\frac{1}{2}} | \Psi \rangle$$

Can be solved with R-matrix method

Translationally invariant equation using Talmi-Moshinsky transformation

Calculation can become numerically challenging:

1. The inversion of the norm
2. The TM transformation

Some applications combining RGM + structure approach :

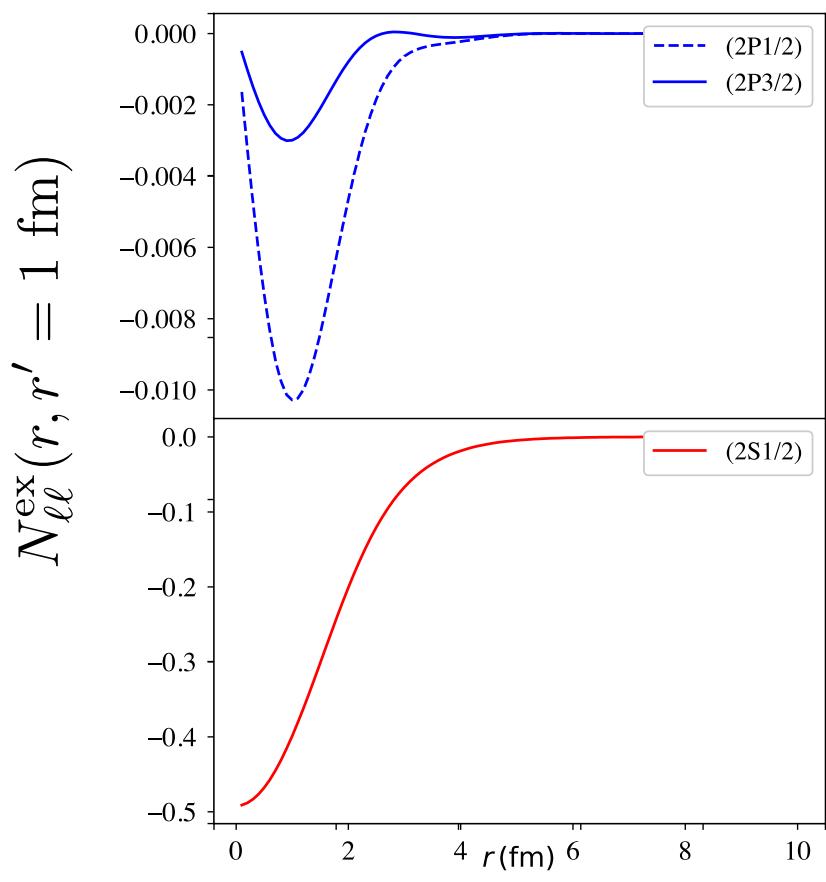
- NCSM+RGM
- NCSMC
- GSMCC
- SA-NCSM + RGM
- SA-NCSMC ?

- Resonating Group Method with SU(3)-scheme basis (benchmarks)

$$\{a_{n\ell j}^\dagger \otimes a_{n'\ell' j'}\}^{JM} = \sum_{\rho_o(\lambda_o, \mu_o) K_o L_o S_o} (-1)^{n+n'-(\lambda_o+\mu_o)+j'-j-L_o} \Pi_{jj'L_oS_o} \langle (\lambda_o, \mu_o) K_o L_o; (n, 0) 0\ell | | (n', 0) 0\ell' \rangle_{\rho_o}$$

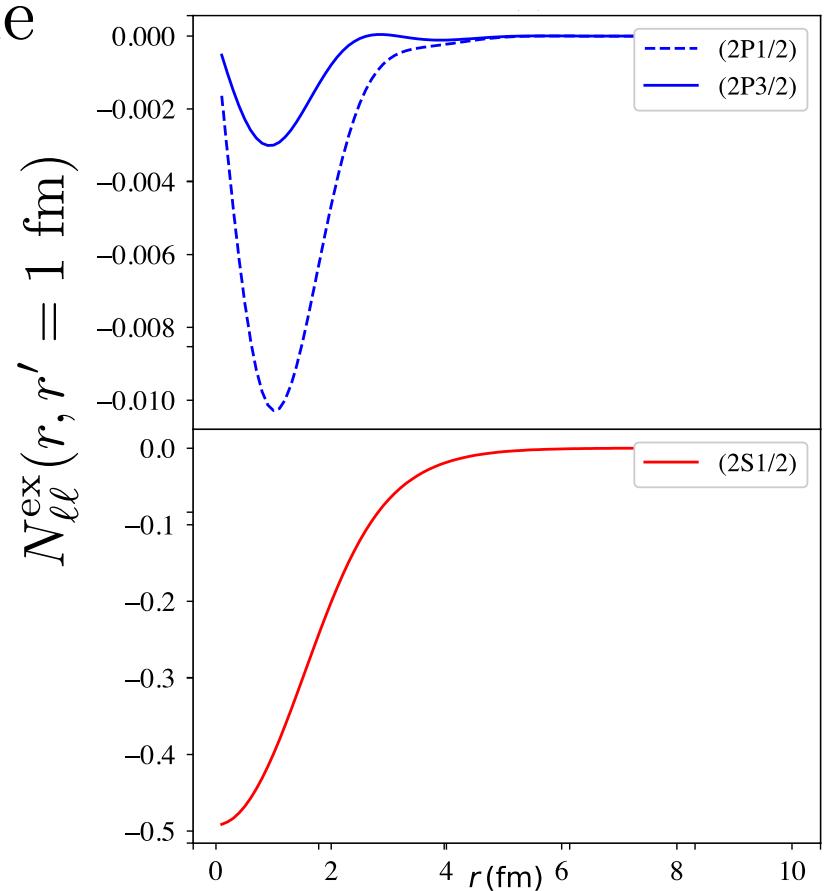
$$\times \frac{\dim(\lambda_o, \mu_o)}{\dim(n, 0)} \left\{ \begin{array}{ccc} \ell & \ell' & L_o \\ \frac{1}{2} & \frac{1}{2} & S_o \\ j & j' & J_o \end{array} \right\} \{a_{(n,0)\frac{1}{2}}^\dagger \otimes a_{(0,n)\frac{1}{2}}\}^{\rho_o(\lambda_o, \mu_o) K_o L_o S_o}$$

SU(2) SD OBDMEs



$n + {}^4\text{He}$
N3LO
 $N_{\max} = 12$

SU(3) SD OBDMEs



- Resonating Group Method with SU(3)-scheme basis

Target wave function:

$$|I_1\rangle = \sum_i C_i |\alpha_1, (\lambda_1\mu_1), K_1, L_1, S_1, I_1\rangle_i$$

Relation to partial-wave channels l [or SU(2)]:

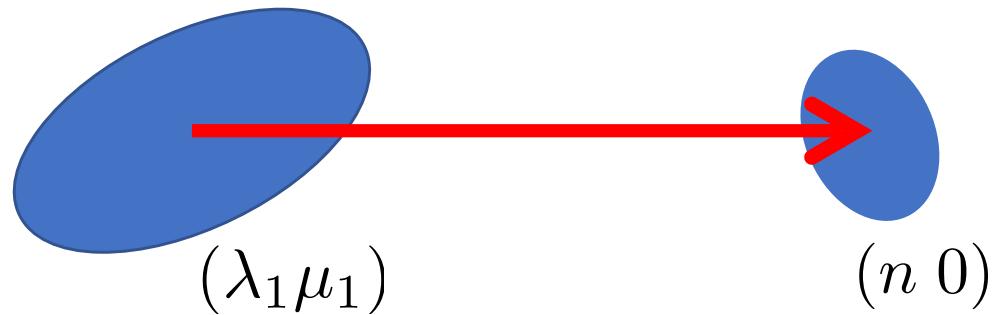
$$|\Phi_{\nu n}^{JMTM_T}\rangle = \sum_{\rho(\lambda,\mu)KLSi} \dots |\Phi_{\gamma_i n}^{\rho(\lambda\mu)KLSJMTM_T}\rangle$$

$$\nu \equiv \{(A-1)I_1T_1; a\frac{1}{2}\frac{1}{2}; \ell s\}$$

$$\gamma \equiv \{(A-1)\alpha_1(\lambda_1, \mu_1)S_1I_1; a\frac{1}{2}\frac{1}{2}\}$$

Expansion in terms of composite shapes

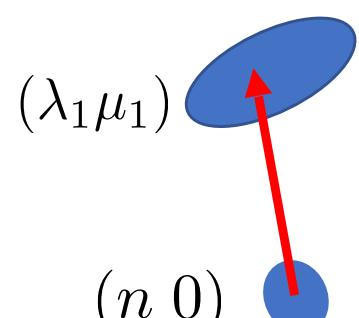
$$|\Phi_{\gamma n}^{\rho(\lambda\mu)KLSJMTM_T}\rangle = \{|\alpha(\lambda_1\mu_1)S_1T_1\rangle \otimes |(n\ 0)\frac{1}{2}\frac{1}{2}\rangle\}$$



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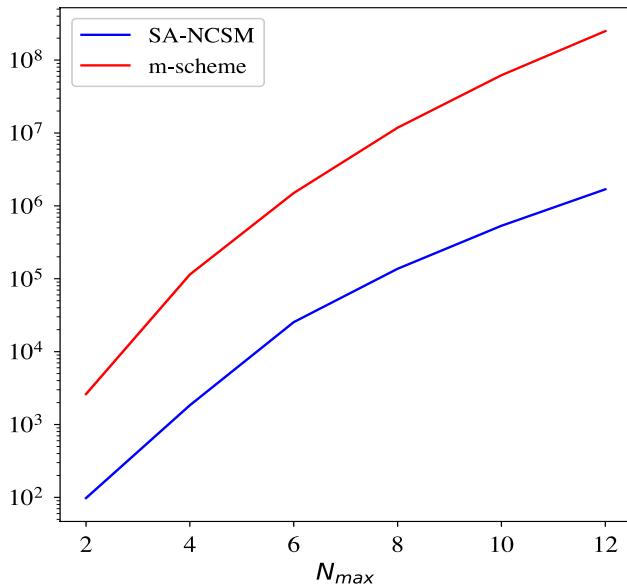
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SU(3)-scheme

Expansion in terms of composite shapes

$$\langle \Phi_{\gamma' n'}^{\rho'(\lambda', \mu') K'(L'S')} JMTM_T | \hat{P}_{A, A-1} | \Phi_{\gamma n}^{\rho(\lambda, \mu) K(LS) JMTM_T} \rangle \propto \delta_{\rho' \rho} \delta_{(\lambda', \mu')(\lambda, \mu)} \delta_{KK'} \delta_{LL'} \delta_{SS'} \\ \times \sum_{\rho_o(\lambda_o, \mu_o) S_o \tau_o} \dots \langle \alpha'_1(\lambda'_1, \mu'_1) S'_1 T'_1 | | \{a_{(n, 0) \frac{1}{2} \frac{1}{2}}^\dagger \otimes \tilde{a}_{(0, \tilde{n}') \frac{1}{2} \frac{1}{2}}\}^{\rho_o(\lambda_o, \mu_o) S_o \tau_o} | | \alpha_1(\lambda_1, \mu_1) S_1 T_1 \rangle$$

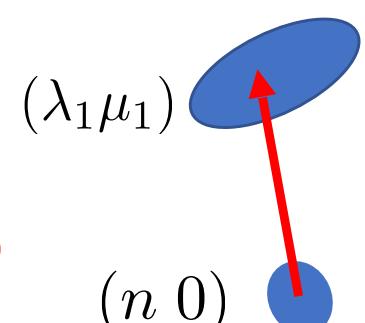
• Norm kernel is diagonal in the SU(3) basis



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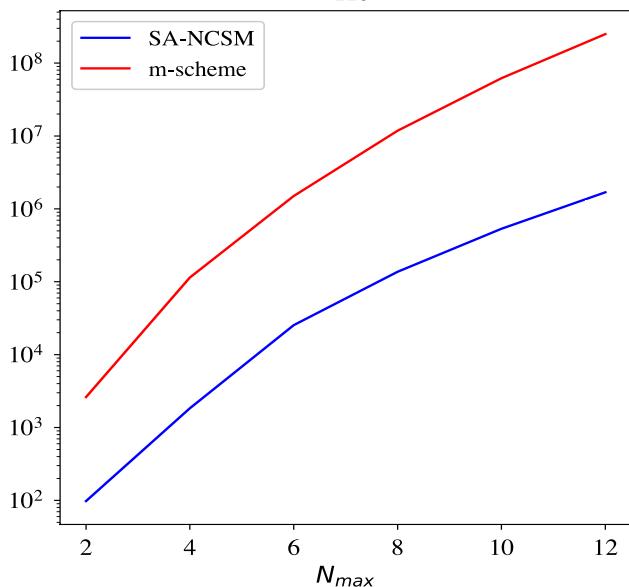
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SU(3)-scheme

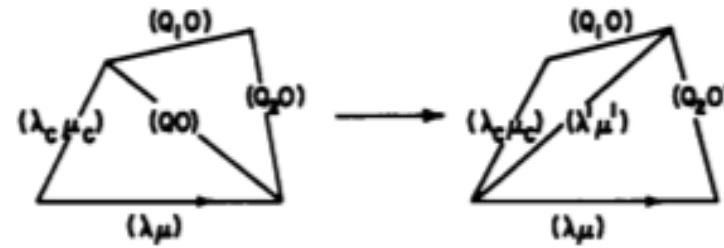
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$$\times \sum_{\rho_o(\lambda_o, \mu_o) S_o \tau_o} \dots \langle \alpha'_1(\lambda'_1, \mu'_1) S'_1 T'_1 | | | \{ a_{(n, 0) \frac{1}{2} \frac{1}{2}}^\dagger \otimes \tilde{a}_{(0, \tilde{n}') \frac{1}{2} \frac{1}{2}} \}^{\rho_o(\lambda_o, \mu_o) S_o \tau_o} | | | \alpha_1(\lambda_1, \mu_1) S_1 T_1 \rangle$$



- Norm kernel is diagonal in the SU(3) basis
- Transformation $|\lambda_{\text{lab}} \mu_{\text{lab}}\rangle \rightarrow |\lambda_{\text{rel}} \mu_{\text{rel}}\rangle$ based on $U(A) \times U(3)$

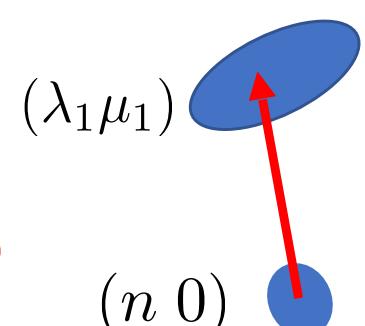


Hecht and Suzuki

- Resonating Group Method with SU(3)-scheme basis

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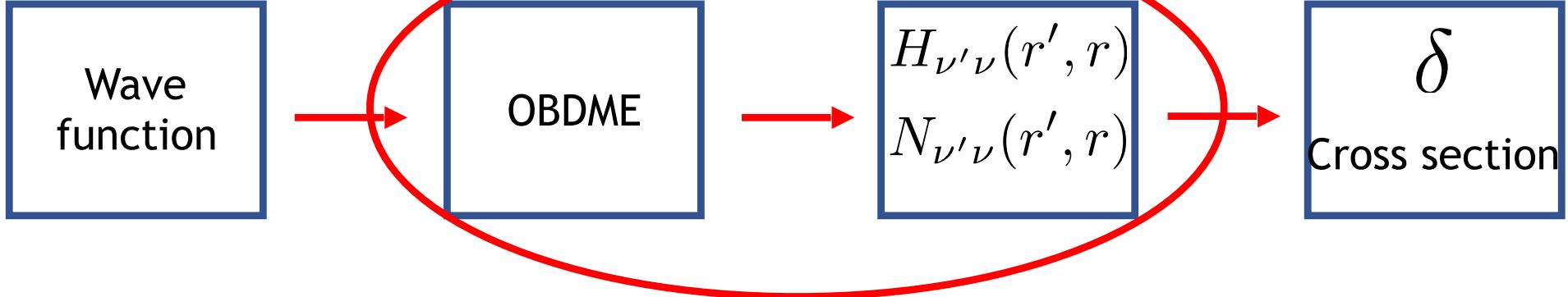
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SU(3)-scheme

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- Conclusion

- Taking advantage of SA-NCSM in the RGM to reach heavier nuclei
- Current work: SU(3) symmetry; next: use of Sp(3,R)
- Reactions of interest:
 - n + alpha (benchmark)
 - Ne isotopes (intermediate mass)
 - Ca isotopes (medium mass)
 - $^{23}\text{Al}(\text{p},\gamma)^{24}\text{Si}$ (important for X-ray burst nucleosynthesis)