Symmetry-adapted bases for ab initio structure and reaction theory

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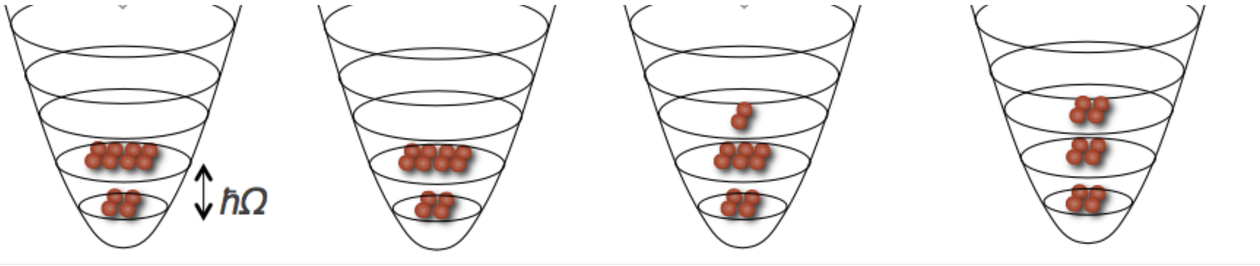
- **Symmetry-adapted no-core shell model (SA-NCSM)**



Based on NCSM:

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

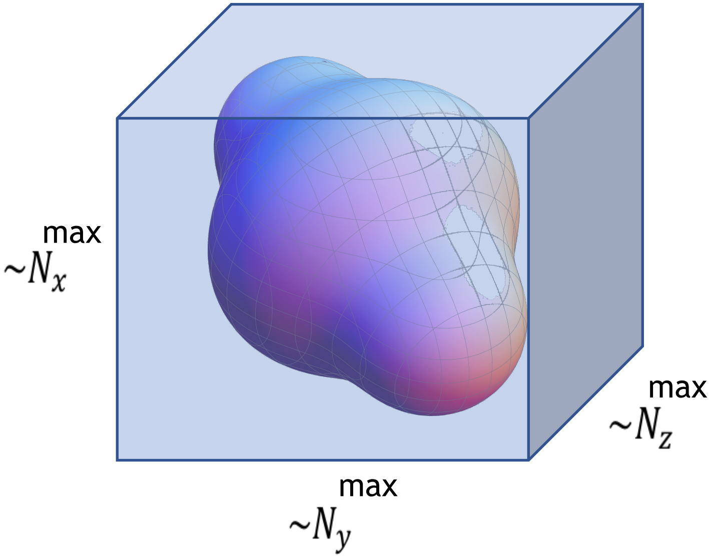
New features in SA-NCSM:

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: $|(\lambda\mu)KLM_L\rangle$

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

With spin: $\underbrace{|\alpha N(\lambda\mu)KL;(S_pS_n)S;JM\rangle}_{SU(3)\times SU(2)}$

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

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

Gives information about important deformed configurations

Spherical : (00)

Prolate : $(\lambda 0)$

Oblate: (0μ)

LSU code (LSU3shell): sourceforge.net/projects/lsu3shell

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?

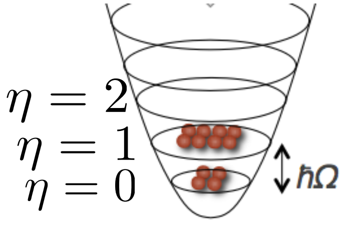
➢ Intuitive way: $|(\lambda\mu)KLS\rangle = \{a^\dagger_{(\eta_1,0)\sigma_1\tau_1} \otimes a^\dagger_{(\eta_2,0)\sigma_2\tau_2} \otimes \cdots \otimes a^\dagger_{(\eta_A,0)\sigma_A\tau_A}\}^{(\lambda\mu)KLS}|0\rangle$

spin isospin

Considering 2 particles:

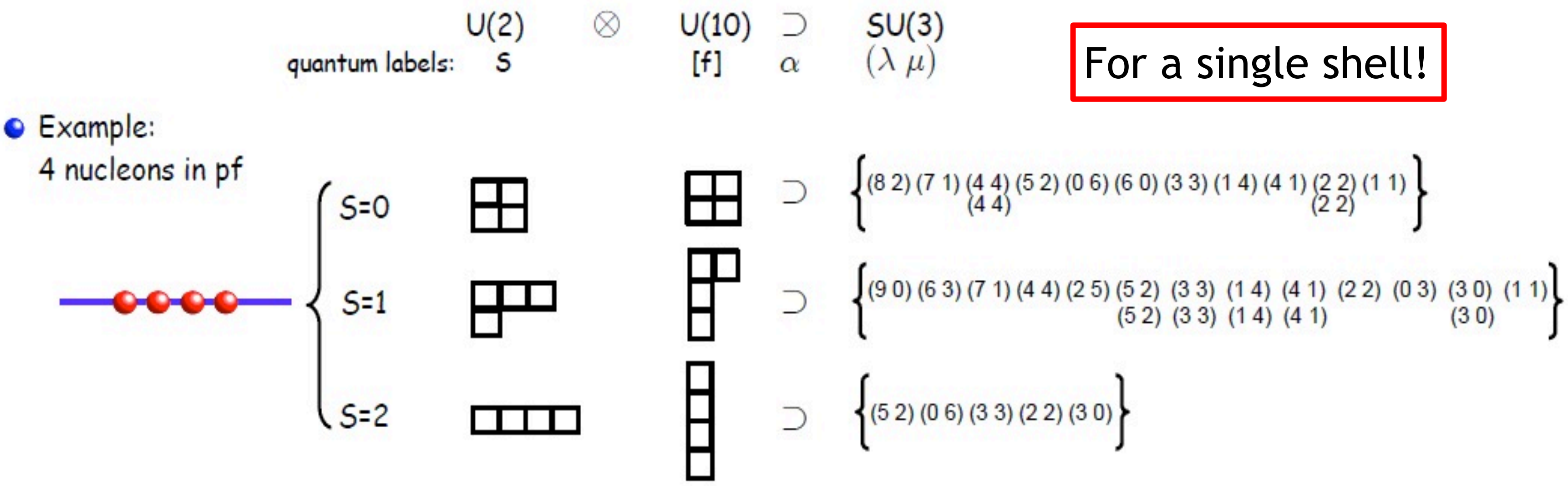
$$\{a^\dagger_{(\eta_1,0)\sigma_1\tau_1} \otimes a^\dagger_{(\eta_2,0)\sigma_2\tau_2}\}^{(\lambda\mu)KLST} = \sum_{\ell_1\ell_2} \underbrace{\langle(\eta_1,0)\ell_1;(\eta_2,0)\ell_2||(\lambda\mu)KL\rangle}_{\text{Reduced SU(3) CG}} \{a^\dagger_{\eta_1\ell_1\sigma_1\tau_1} \otimes a^\dagger_{\eta_2\ell_2\sigma_2\tau_2}\}^{LST}$$

Tedious... not used for many-particle system



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

For a single shell!



Draayer et al., "Representations of U(3) in U(N)", Comp. Phys. Commun. 56 (1989) 279

• SA-NCSM: SU(3)-scheme interaction

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

$n_r n_s$ (λ μ)

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

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

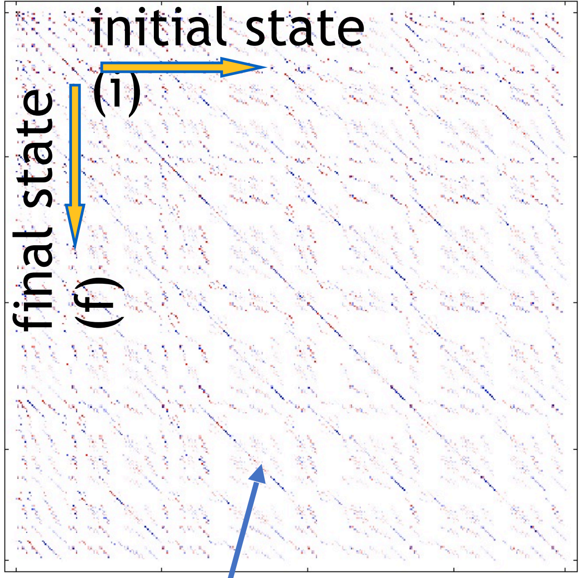
$$\Pi_{j_rj_sj_tj_u}\langle(\eta_t\,0)l_t;(\eta_u\,0)l_u\|(\omega\kappa L)_i\rangle\begin{Bmatrix} l_r & \frac{1}{2} & j_r \\ l_s & \frac{1}{2} & j_s \\ L_f & S_f & J \end{Bmatrix}\begin{Bmatrix} l_t & \frac{1}{2} & j_t \\ l_u & \frac{1}{2} & j_u \\ L_i & S_i & J \end{Bmatrix}V^{\Gamma}_{rstu},$$

jj-coupled NN

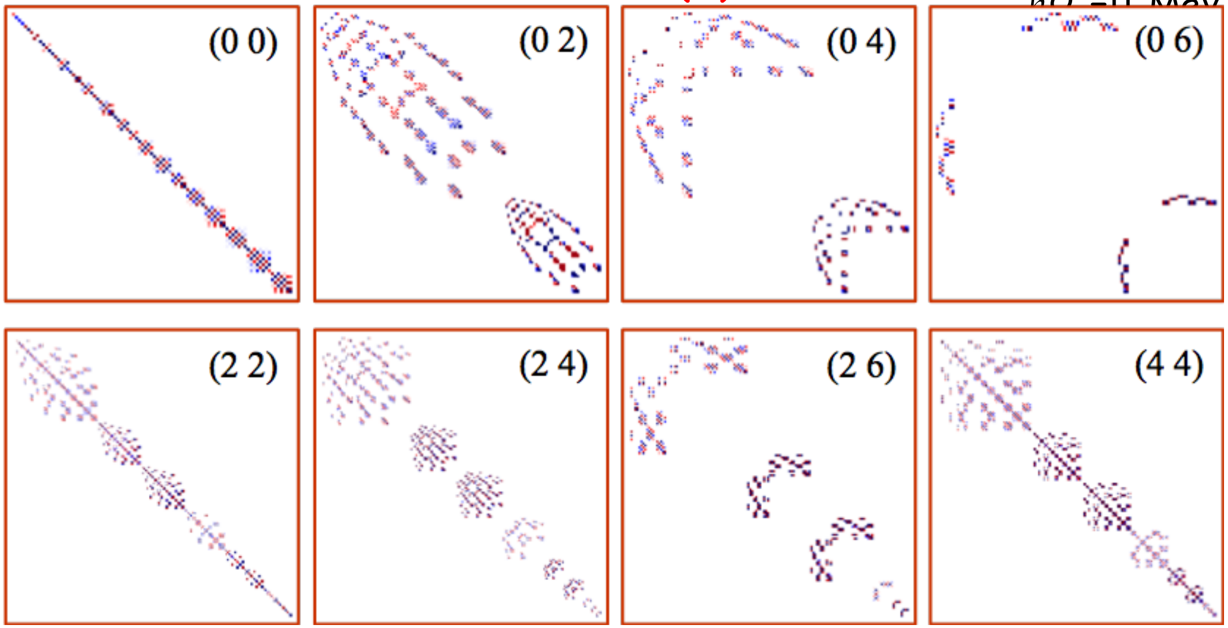
N3LO (N_{max}=6)

$\hbar\Omega$ =11 MeV

NN in SU(3) basis



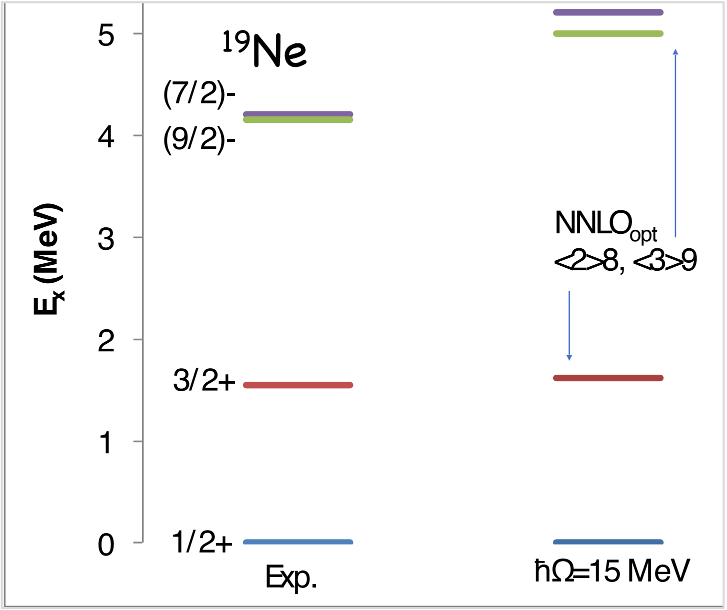
NN SU(3) Tensors

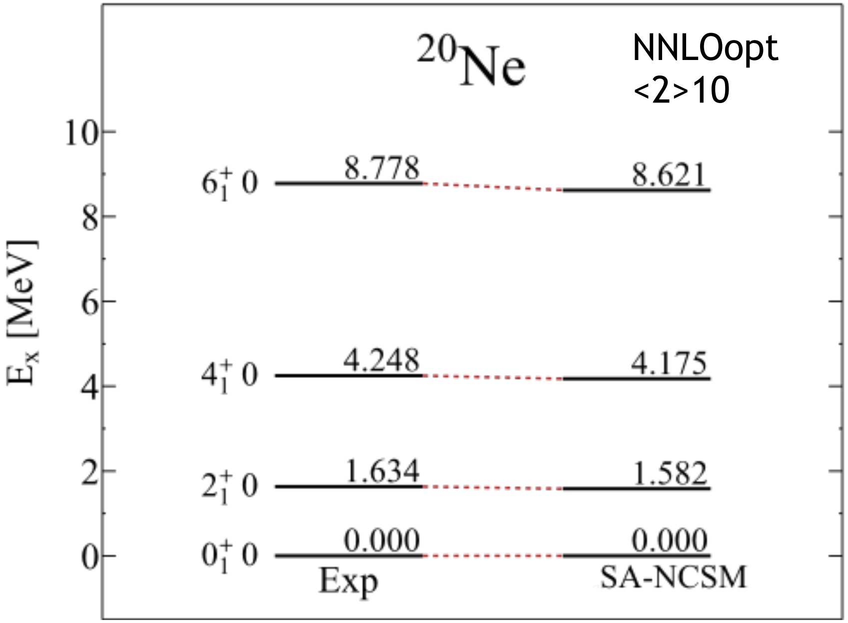


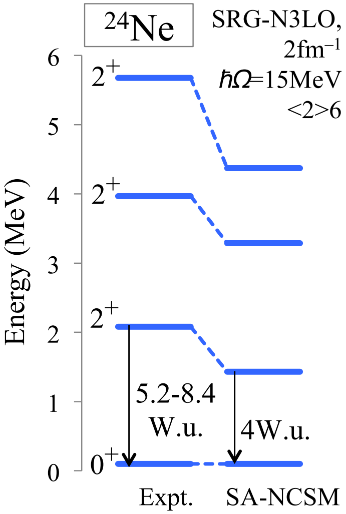
Equivalent to *m*-scheme

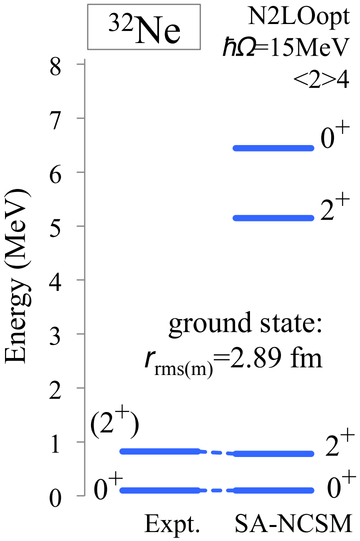
Matrices are smaller and sparser

SA-NCSM with SU(3) scheme: Examples









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

Complete model space: 1000 billion states

Robert Baker, PhD student, LSU

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

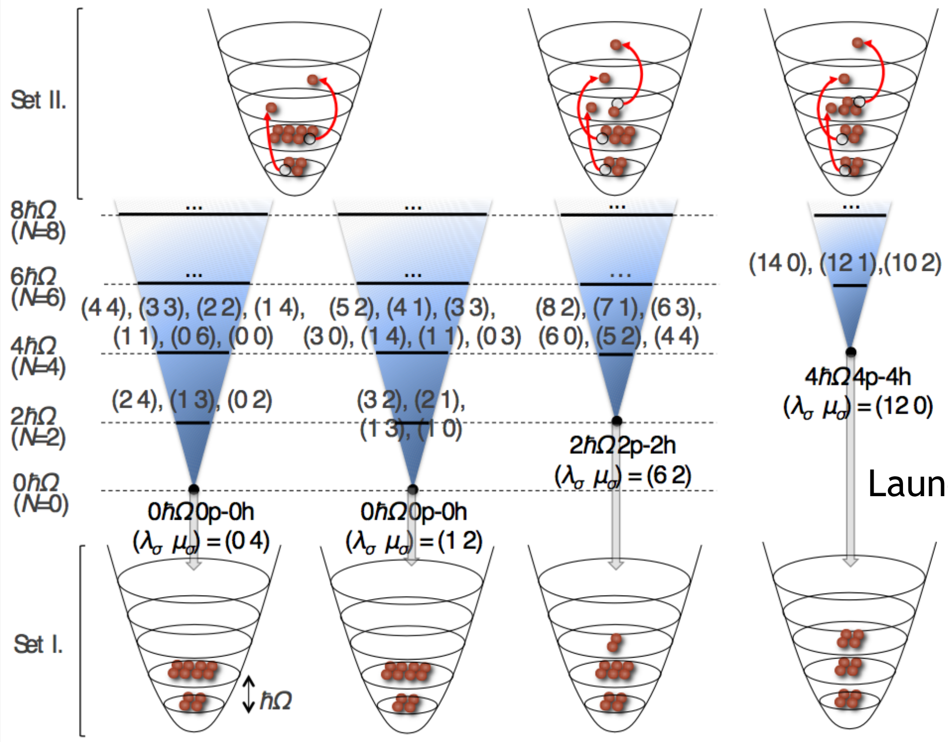
Symmetry-adapted:
SU(3), Sp(3,R)

Describes deformation Equilibrium shape

Symplectic Sp(3,R) basis: $|\sigma n\rho\omega\kappa L M_L\rangle$

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

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**

0p-0h equilibrium shape + SU(3) configurations up to N_{max}=12

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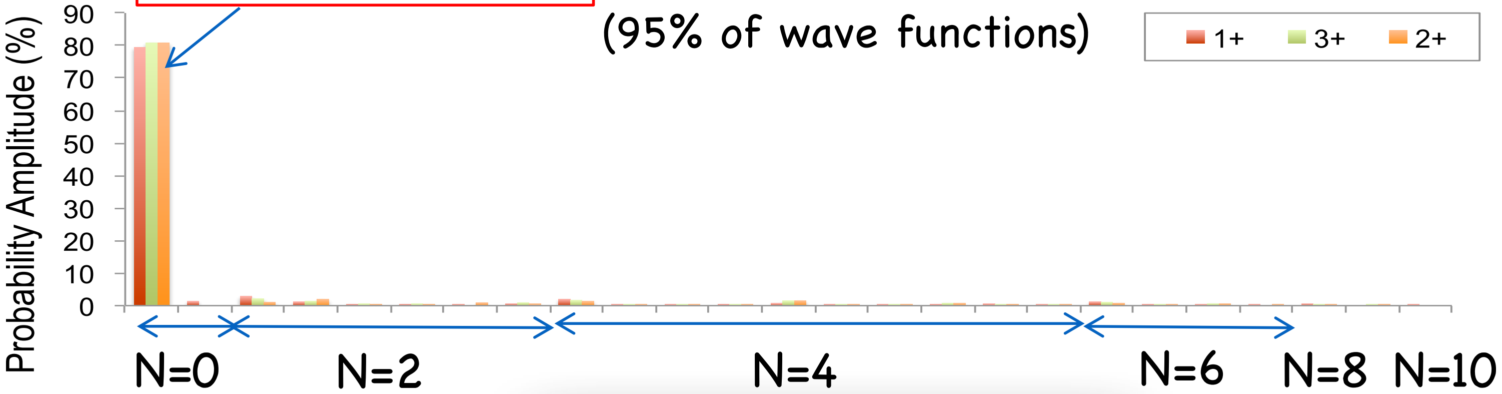
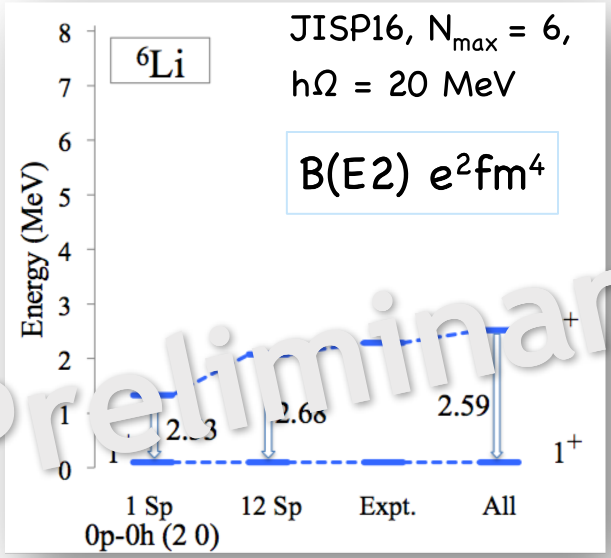


(95% of wave functions)

cf. Launey's talk



JISP16, N_{max} = 6, hΩ = 20 MeV

B(E2) e^2fm^4

Single Sp(3,R) irrep

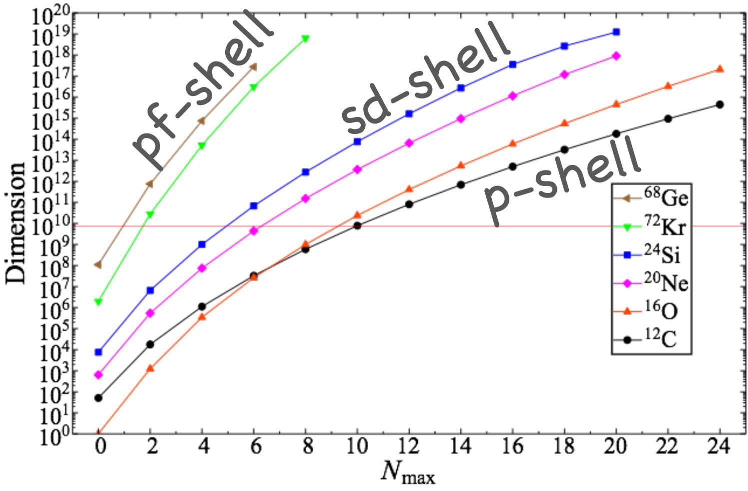
12 Sp(3,R) irreps

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 $Tn_1n_2n_1n_1$ -> Tn_2 x $Tn_1n_1n_1$
  - Important pieces of information … single-shell rme's

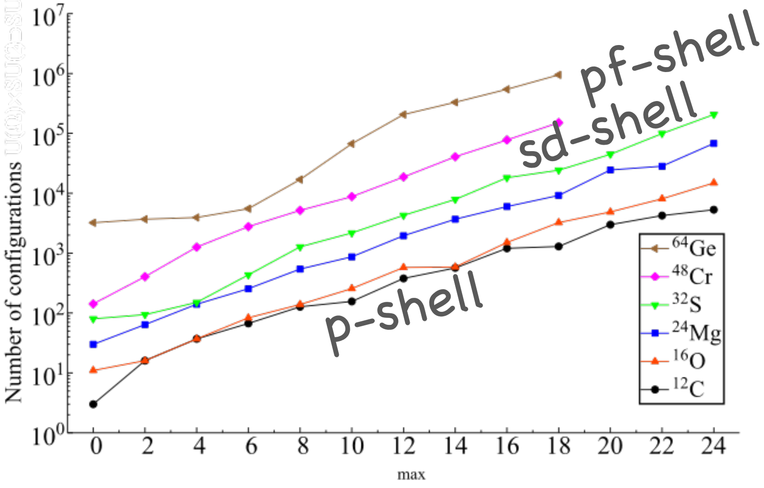
Important pieces of information (memory requirement)

NCSM



Current limit

SA-NCSM



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

- **Resonating Group Method**

Cluster wave function

$$\Psi = \mathcal{A}\{\overbrace{\sum_i c_i\phi_{1i}(\vec{\xi}_{1i})}^{\text{1-cluster}} + \overbrace{\sum_j \phi_{1j}(\vec{\xi}_{1j})\underbrace{\phi_{2j}(\vec{\xi}_{2j})}_{\text{intrinsic function}}\underbrace{g(\vec{r}_j)}_{\text{relative motion}}}^{\text{2-clusters}}$$

$$+ \underbrace{\sum_k \phi_{1k}(\vec{\xi}_{1k})\phi_{2k}(\vec{\xi}_{2k})\phi_{3k}(\vec{\xi}_{3k})g(\vec{r}_{1k},\vec{r}_{2k})}_{\text{3-clusters}} + \dots\}$$

For 2 clusters:

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

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

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

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

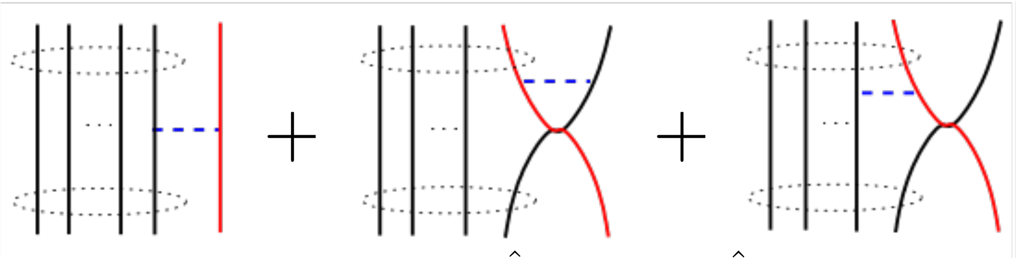
Y.C. Tang et al, Physics Report **47** (1978) 167

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: $$\sum_{\nu'} \int \left(H_{\nu\nu'}(r,r') - E N_{\nu\nu'}(r,r')\right) g_\nu(r) dr = 0 \longleftrightarrow \hat{H}\,|\Psi\rangle = E\,|\Psi\rangle$$

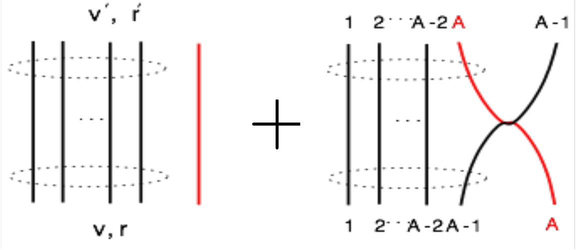
$$H_{\nu'\nu}(r',r) = \langle \Phi^{J^\pi T}_{\nu' r'} |\, \hat{\mathcal{A}} \hat{H} \hat{\mathcal{A}} \,| \Phi^{J^\pi T}_{\nu r}\rangle =$$



$V_{A-1,A}$ + $V_{A-1,A}\hat{P}_{A-1,A}$ + $\hat{P}_{A-1,A} V_{A-2,A-1}$

Antisymmetrizer:
Eigenvectors have SU(3) symmetry

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



$\delta_{\nu'\nu}\delta(r'-r)$ + $\hat{P}_{A,A-1}$

What we need:

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

Gives information on the structure of the ta

$$\langle \Phi^{J^\pi T}_{\nu' n'} |\, \hat{P}_{A,A-1} \,| \Phi^{J^\pi T}_{\nu n}\rangle = \frac{1}{A-1} \sum_{jj'J_o\tau_o} \Pi_{ss'jj'J_o\tau_o} (-1)^{I'_1+j'+J} (-1)_{T_1+\frac{1}{2}+T} \begin{Bmatrix} I_1 & \frac{1}{2} & s \\ \ell & J & j \end{Bmatrix} \begin{Bmatrix} I'_1 & \frac{1}{2} & s' \\ \ell' & J & j' \end{Bmatrix}$$

$$\times \begin{Bmatrix} I_1 & J_o & I'_1 \\ j' & J & j \end{Bmatrix} \begin{Bmatrix} T_1 & \tau_o & T'_1 \\ \frac{1}{2} & T & \frac{1}{2} \end{Bmatrix} \langle (A-1)\alpha'_1 I'_1 T'_1 |\,|| \{a^\dagger_{n\ell j \frac{1}{2}} \otimes a_{n'\ell' j' \frac{1}{2}}\}^{J_o\tau_o} ||\,| (A-1)\alpha_1 I_1 T_1\rangle$$

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

- **Resonating Group Method**

Non orthogonality is short range: $N_{\nu'\nu}(r',r) \longrightarrow \frac{\delta(r'-r)}{r'r}$ for $r',r >> 1$

Introduce an orthogonalized version of Hill-Wheeler equations:

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

Can be solved with R-matrix method

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

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

Translationally invariant equation using Talmi-Moshinsky transformation

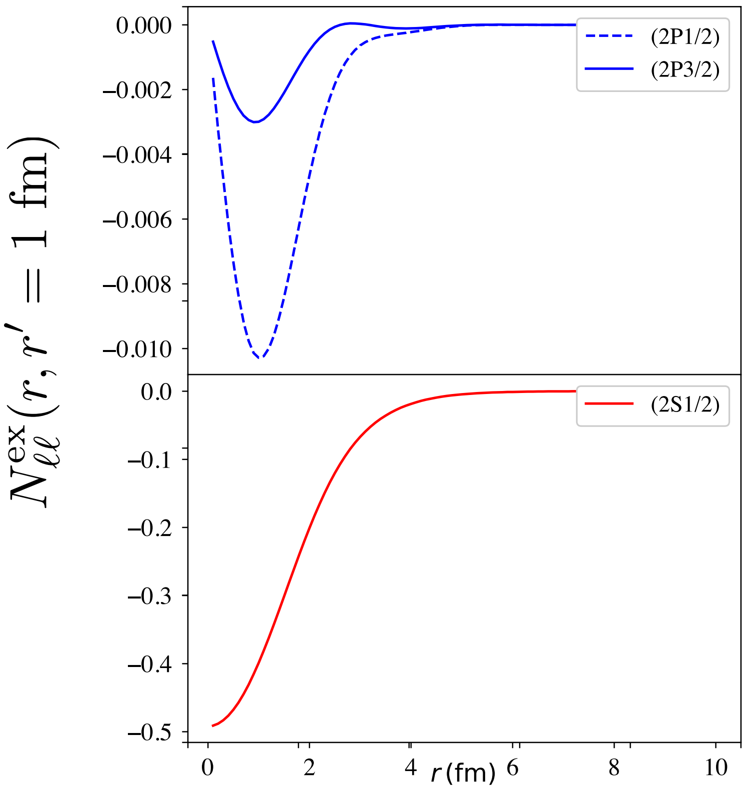
Calculation can become numerically challenging:
1. The inversion of the norm
2. The TM transformation

Some applications combining RGM + structure approach :
- ➢ NCSM+RGM
- ➢ NCSMC
- ➢ GSMCC
- ➢ SA-NCSM + RGM
- ➢ SA-NCSMC ?

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

$$\{a^\dagger_{n\ell j} \otimes a_{n'\ell' j'}\}^{JM} = \sum_{\rho_o(\lambda_o,\mu_o)K_oL_oS_o} (-1)^{n+n'-(\lambda_o+\mu_o)+j'-j-L_o} \Pi_{jj'L_oS_o} \langle(\lambda_o,\mu_o)K_oL_o;(n,0)0\ell|\,|(n',0)0\ell'\rangle_{\rho_o} \times \frac{\dim(\lambda_o,\mu_o)}{\dim(n,0)} \begin{Bmatrix} \ell & \ell' & L_o \\ \frac{1}{2} & \frac{1}{2} & S_o \\ j & j' & J_o \end{Bmatrix} \{a^\dagger_{(n,0)\frac{1}{2}} \otimes a_{(0,n)\frac{1}{2}}\}^{\rho_o(\lambda_o,\mu_o)K_oL_oS_o}$$

SU(2) SD OBDMEs

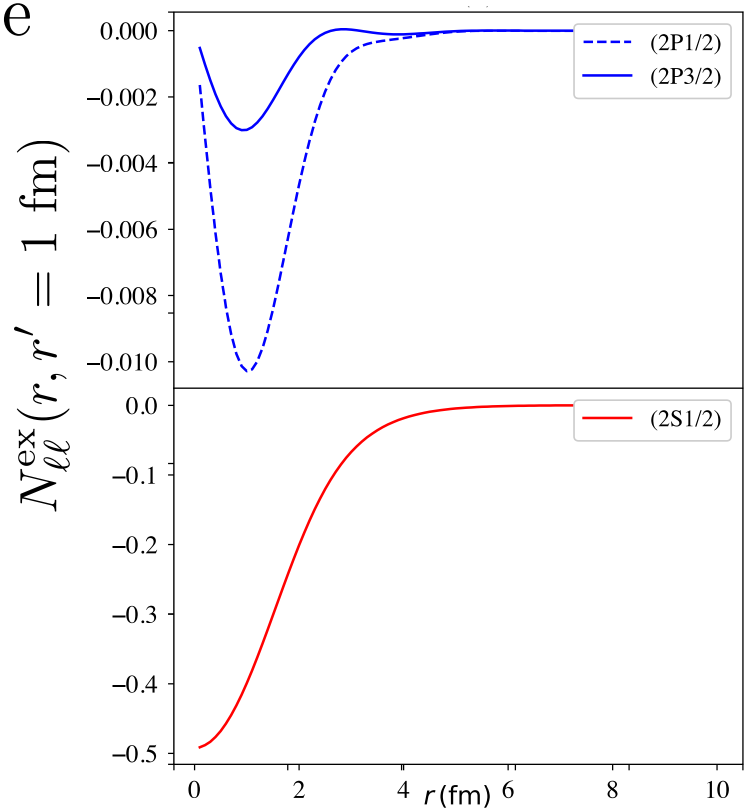


$n + {}^4\text{He}$

N3LO

$N_{\rm max}$ =12

SU(3) SD OBDMEs



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

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

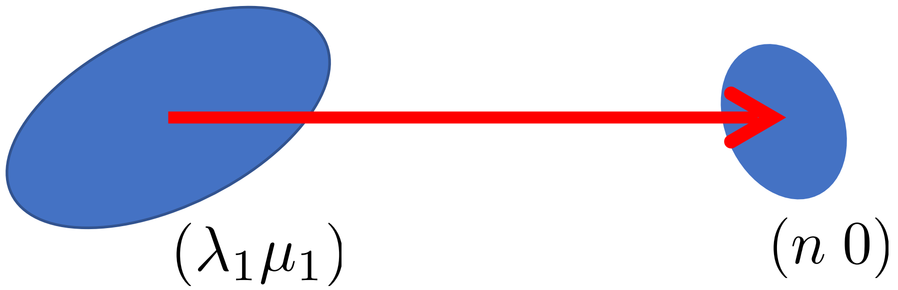
Relation to partial-wave channels *l* [or SU(2)]: $|\Phi^{JMTM_T}_{\nu n}\rangle = \sum_{\rho(\lambda,\mu)KLSi} \dots |\Phi^{\rho(\lambda\mu)KLSJMTM_T}_{\gamma_i n}\rangle$

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

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

Expansion in terms of composite shapes

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



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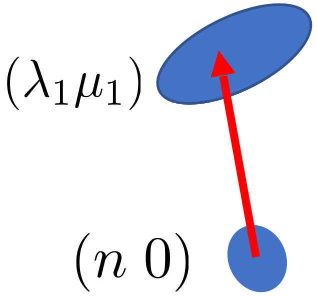

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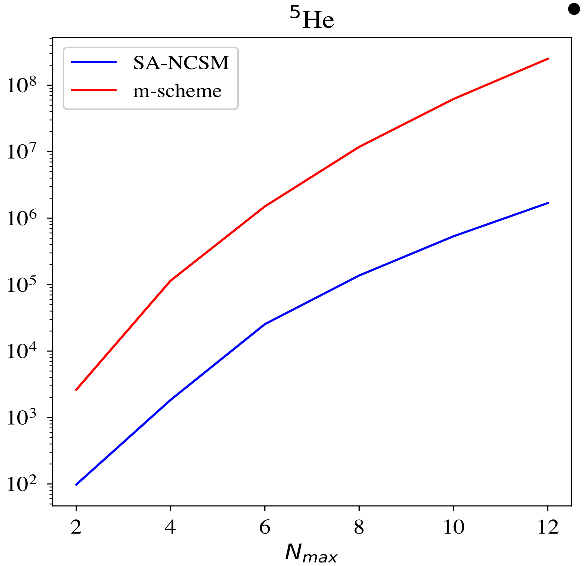
Expansion in terms of composite shapes

SU(3)-scheme

$$\langle\Phi^{\rho'(\lambda',\mu')K'(L'S')JMTM_T}_{\gamma' n'}|\,\hat{P}_{A,A-1}|\Phi^{\rho(\lambda,\mu)K(LS)JMTM_T}_{\gamma n}\rangle \propto \delta_{\rho'\rho}\delta_{(\lambda',\mu')(\lambda,\mu)}\delta_{KK'}\delta_{LL'}\delta_{SS'}$$

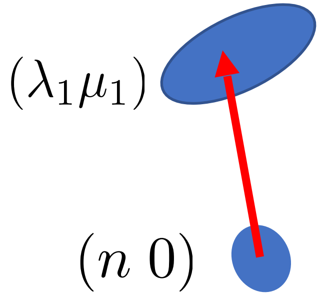
$$\times \sum_{\rho_o(\lambda_o,\mu_o)S_o\tau_o} \ldots \langle\alpha'_1(\lambda'_1,\mu'_1)S'_1T'_1|||\{a^\dagger_{(n,0)\frac{1}{2}\frac{1}{2}} \otimes \tilde{\tilde{a}}_{(0,\tilde{n}')\frac{1}{2}\frac{1}{2}}\}^{\rho_o(\lambda_o,\mu_o)S_o\tau_o}|||\alpha_1(\lambda_1,\mu_1)S_1T_1\rangle$$



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

Hecht and Suzuki

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



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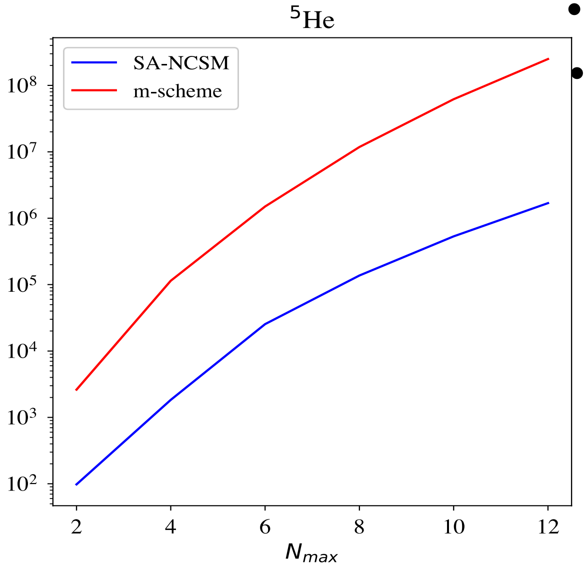
$$\times \sum_{\rho_o(\lambda_o,\mu_o)S_o\tau_o} \ldots \langle \alpha'_1(\lambda'_1,\mu'_1)S'_1T'_1| || \{a^\dagger_{(n,0)\frac{1}{2}\frac{1}{2}} \otimes \tilde{\tilde{a}}_{(0,\tilde{n}')\frac{1}{2}\frac{1}{2}}\}^{\rho_o(\lambda_o,\mu_o)S_o\tau_o} || \, |\alpha_1(\lambda_1,\mu_1)S_1T_1\rangle$$



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

$$\frac{1}{[\bar{N}^Q_{(\lambda\mu)}]^2} = \frac{1}{[N^Q_{(\lambda\mu)}]^2}\left(\frac{A-4}{A}\right)^Q$$

$$+ \sum_{\substack{Q_2=1\\ Q_1+Q_2=Q}} \frac{Q!}{Q_1!Q_2!}\left(\frac{A-4}{A}\right)^{Q_1}\left(\frac{4}{A}\right)^{Q_2} \sum_{(\lambda'\mu')} \frac{1}{[N^{Q_1}_{(\lambda'\mu')}]^2} U^2((\lambda_c\mu_c)(Q_10)(\lambda\mu)(Q_20);(\lambda'\mu')(Q0)).$$

Hecht and Suzuki

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

Target wave function:

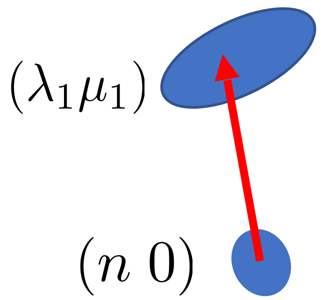
$$|I_1\rangle = \sum_i C_i |\alpha_1, (\lambda_1\mu_1), K_1, L_1, S_1, I_1\rangle_i$$

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

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

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

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

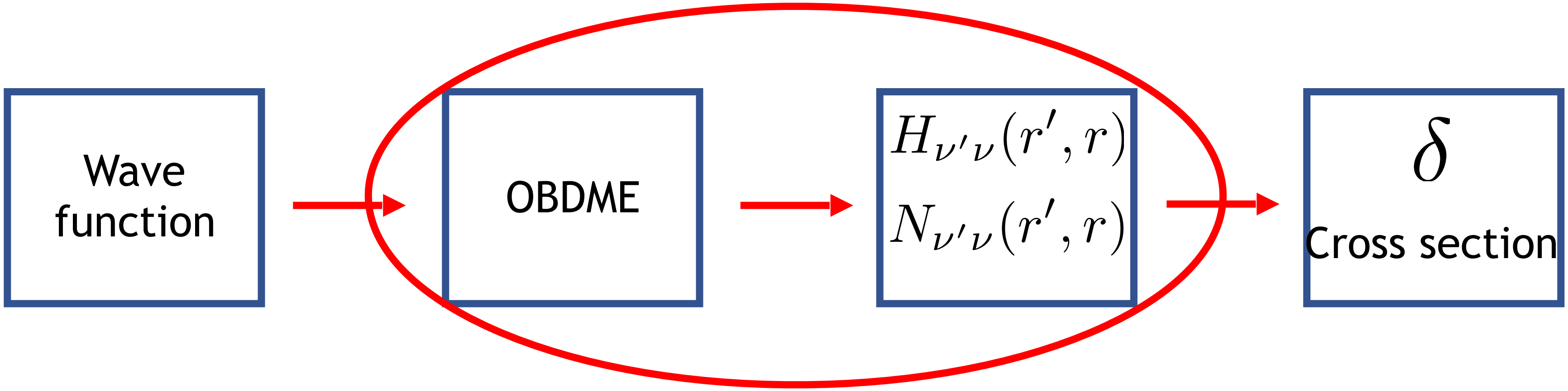


Expansion in terms of composite shapes

SU(3)-scheme

$$\langle\Phi^{\rho'(\lambda',\mu')K'(L'S')JMTM_T}_{\gamma' n'}|\,\hat{P}_{A,A-1}|\Phi^{\rho(\lambda,\mu)K(LS)JMTM_T}_{\gamma n}\rangle \propto \delta_{\rho'\rho}\delta_{(\lambda',\mu')(\lambda,\mu)}\delta_{KK'}\delta_{LL'}\delta_{SS'}$$

$$\times \sum_{\rho_o(\lambda_o,\mu_o)S_o\tau_o} \dots \langle\alpha'_1(\lambda'_1,\mu'_1)S'_1T'_1|\,||\{a^\dagger_{(n,0)\frac{1}{2}\frac{1}{2}} \otimes \tilde{\tilde{a}}_{(0,\tilde{n}')\frac{1}{2}\frac{1}{2}}\}^{\rho_o(\lambda_o,\mu_o)S_o\tau_o}||\,|\alpha_1(\lambda_1,\mu_1)S_1T_1\rangle$$



Wave function

OBDME

$H_{\nu'\nu}(r',r)$

$N_{\nu'\nu}(r',r)$

δ

Cross section

• 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}Al(p,γ)^{24}Si (important for X-ray burst nucleosynthesis)