



***Microscopic Studies Of Alpha Clustering
Using Configuration Interaction Approach***

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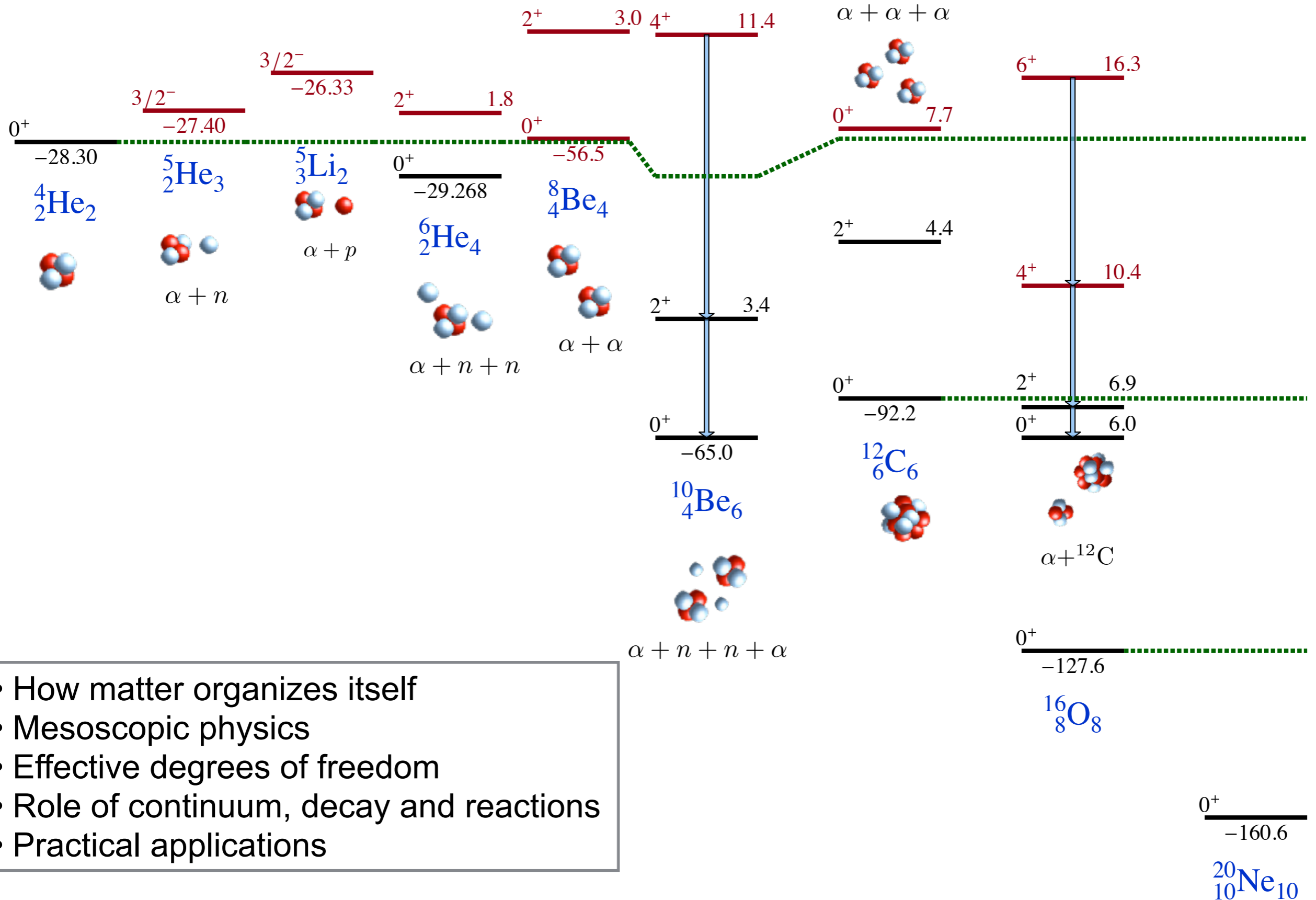
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Clustering in light nuclei



- How matter organizes itself
- Mesoscopic physics
- Effective degrees of freedom
- Role of continuum, decay and reactions
- Practical applications

Configuration interaction approach (shell model)

A powerful tool in studies of nuclear many-body problems

- Well-established many-body technique
- Excellent predictive power
- New computational techniques broaden applicability to nearly all nuclei
- Extensions to continuum and reaction physics.
- **Clustering**

The Nuclear Shell Model

The Hamiltonian

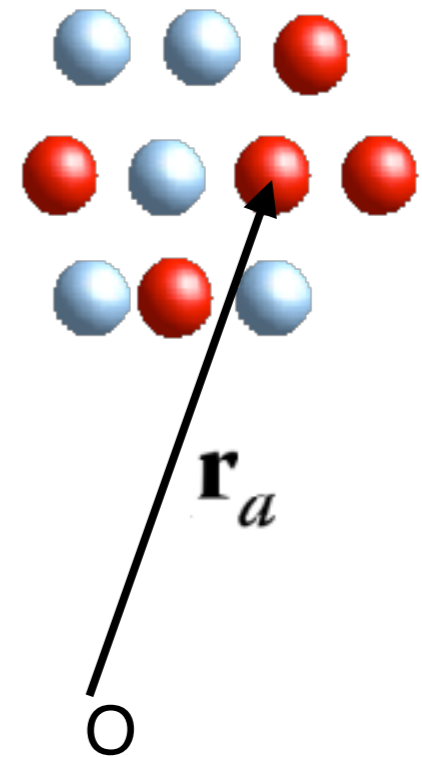
$$H = \sum_a \frac{\mathbf{p}_a^2}{2M} + \frac{1}{2} \sum_{a \neq b} U_{ab}$$

Translational invariance tells us

$$H = \frac{\mathbf{P}^2}{2MA} + H_{\text{int}} \quad \mathbf{P} = \sum_a \mathbf{p}_a$$

$$H_{\text{int}} = \frac{1}{2A} \sum_{a,b} \frac{(\mathbf{p}_a - \mathbf{p}_b)^2}{2M} + \frac{1}{2} \sum_{a \neq b} U_{ab}$$

$$\Psi = e^{i\mathbf{P}\mathbf{R}} \Psi'$$



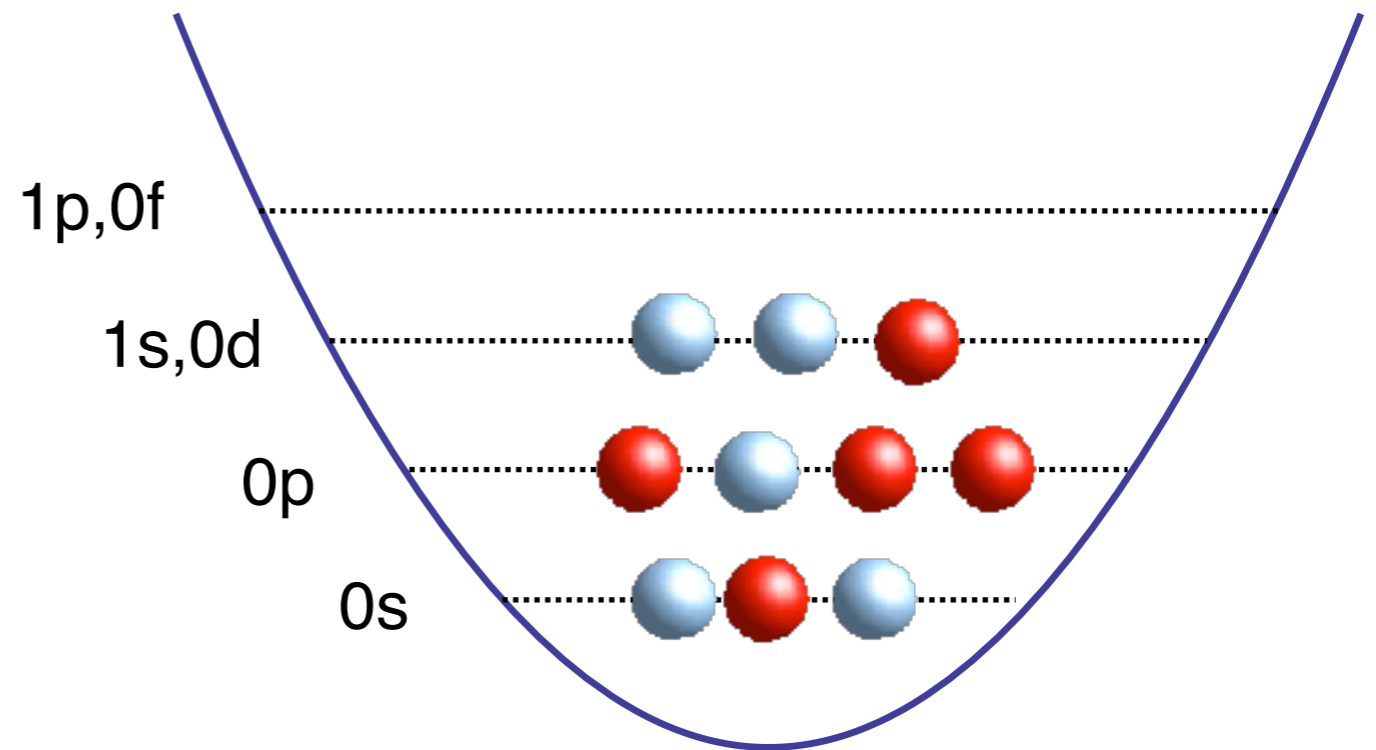
The Nuclear Shell Model

$$H = \frac{\mathbf{p}^2}{2MA} + H_{\text{int}}; \quad H(\omega_0) = H + \frac{AM\omega_0^2}{2}\mathbf{R}^2 = H_{\text{cm}}(\omega_0) + H_{\text{int}}$$

$$H_{\text{cm}}(\omega_0) = \frac{\mathbf{p}^2}{2MA} + \frac{AM\omega_0^2}{2}\mathbf{R}^2 \quad \Psi_{n\ell m} = \phi_{n\ell m}(\mathbf{R}) \Psi'$$

$$E(\omega_0) = \hbar\omega_0(N_{\text{cm}} + 3/2) + E'$$

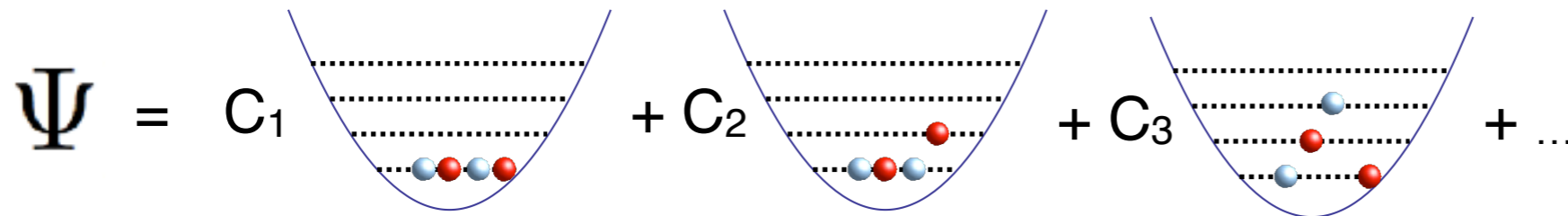
$$N_{\text{cm}} = 2n + \ell$$



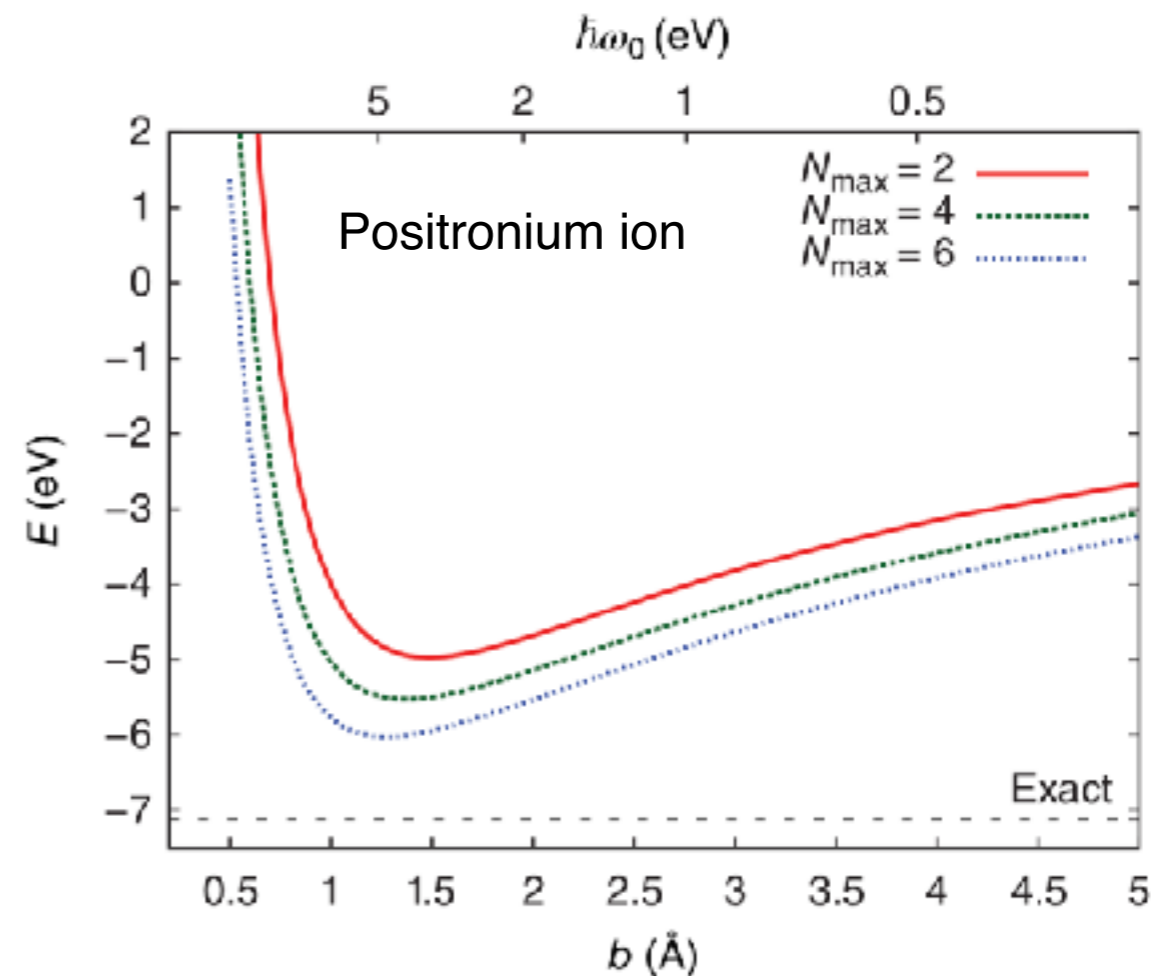
Configuration interactions (variational principle)

Configurations (Slater determinants or more)

$$|\Psi(\mathbf{r}_a, \mathbf{r}_b)\rangle = \hat{\Psi}|0\rangle = \sum_{i,j} C_{ij} a_i^\dagger a_j^\dagger |0\rangle \quad \langle \mathbf{r}_a, \mathbf{r}_b | a_i^\dagger a_j^\dagger |0\rangle = \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_i(\mathbf{r}_a) & \phi_i(\mathbf{r}_b) \\ \phi_j(\mathbf{r}_a) & \phi_j(\mathbf{r}_b) \end{vmatrix}$$



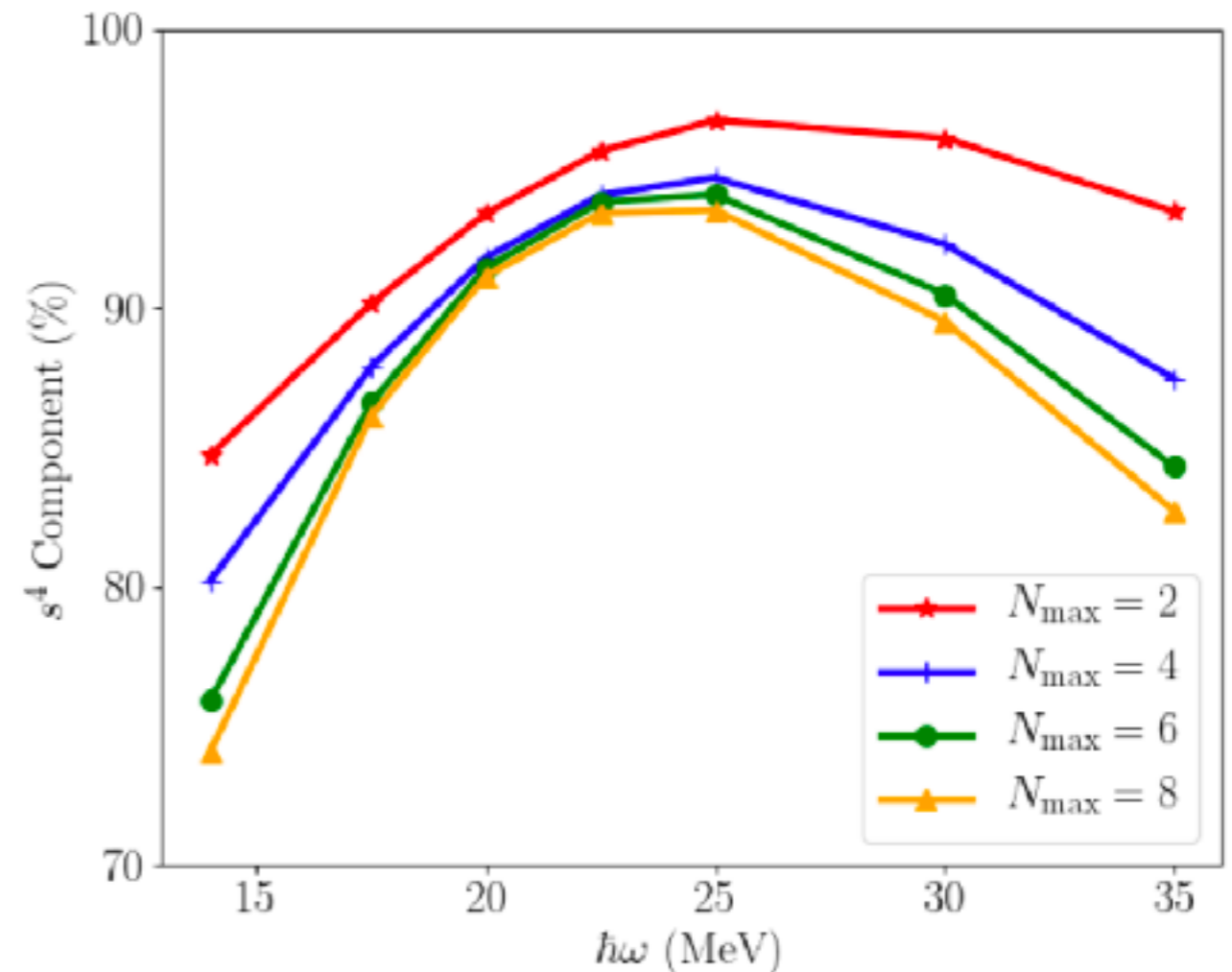
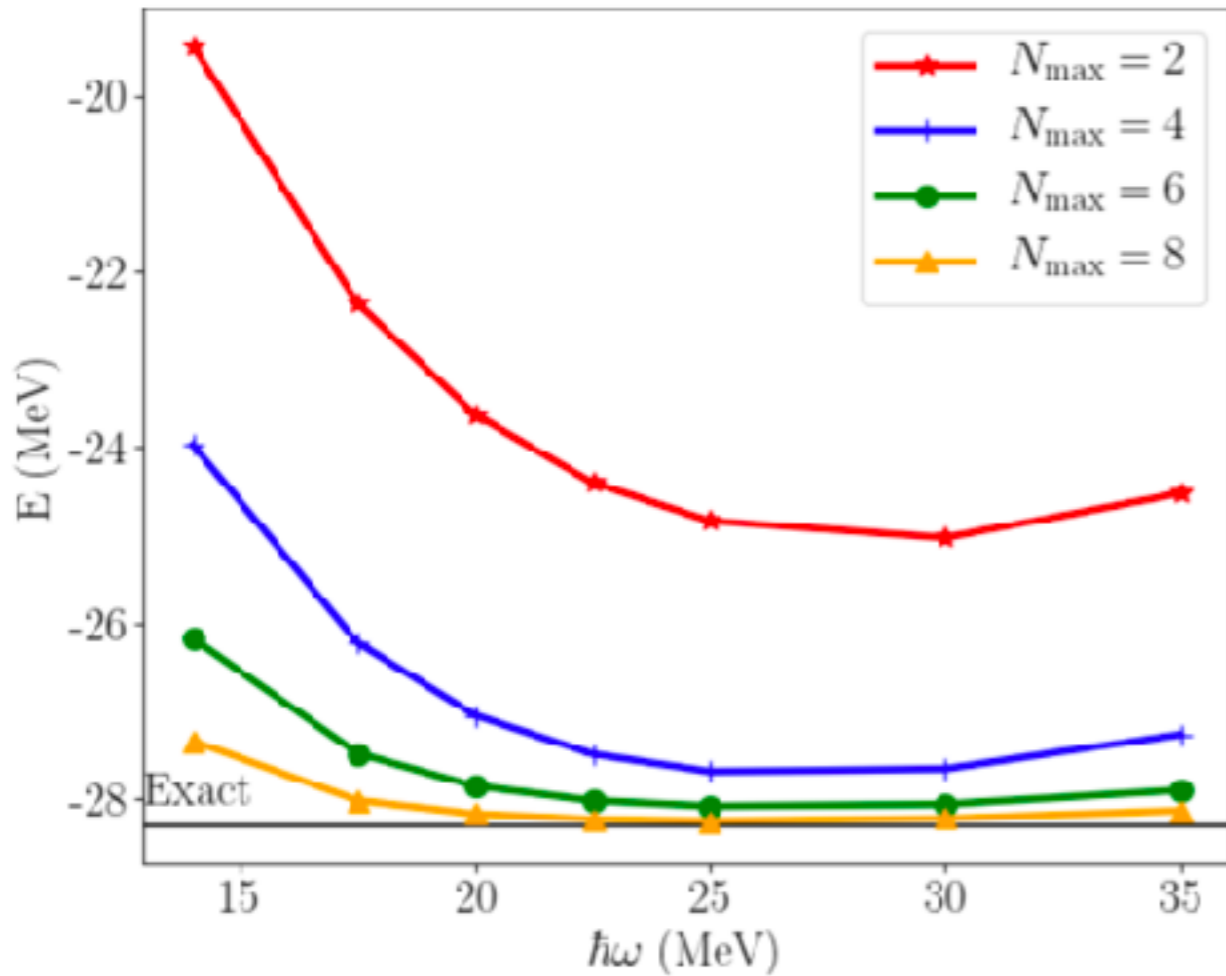
Second quantization
 Full antisymmetry
 Fast numeric strategies
 Selection of basis and truncation



Configuration interactions (variational principle)

$$\Psi = C_1 \left[\begin{array}{c} \text{Diagram 1: 4 particles in ground state} \end{array} \right] + C_2 \left[\begin{array}{c} \text{Diagram 2: 3 particles in ground state, 1 in first excited state} \end{array} \right] + C_3 \left[\begin{array}{c} \text{Diagram 3: 2 particles in ground state, 2 in first excited state} \end{array} \right] + \dots$$

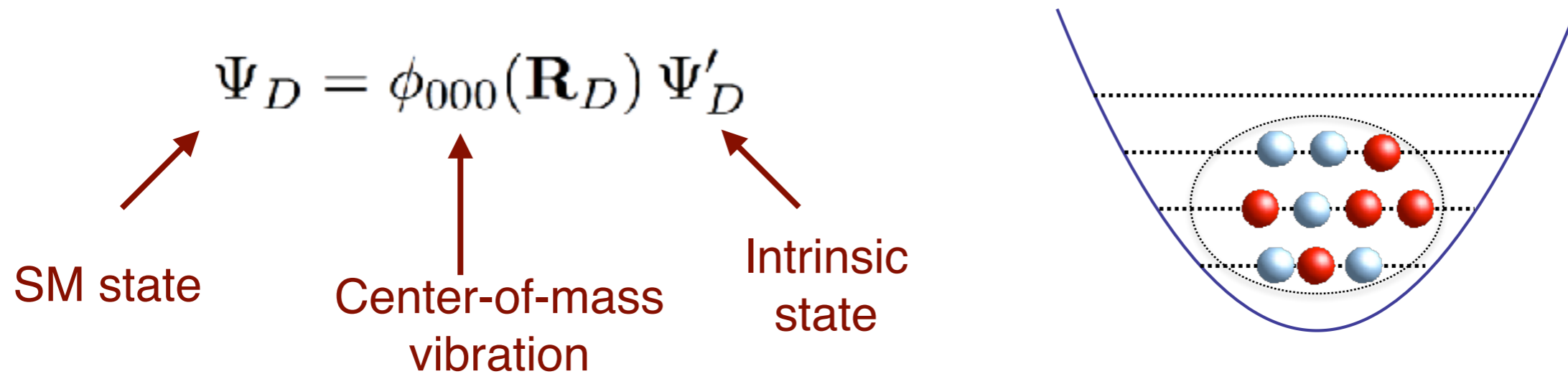
Alpha particle in no-core shell model



JISP-16 interaction

Translational invariance and Center of Mass (CM)

Shell model, Glockner-Lawson procedure



Controlling CM with operator \mathbf{R}

$$D_\mu = \sqrt{\frac{4\pi}{3}} R_\mu$$

$$R_\mu = \sqrt{\frac{\hbar}{2Am\omega}} (\mathcal{B}_\mu^\dagger + \mathcal{B}_\mu)$$

Control only
CM quanta

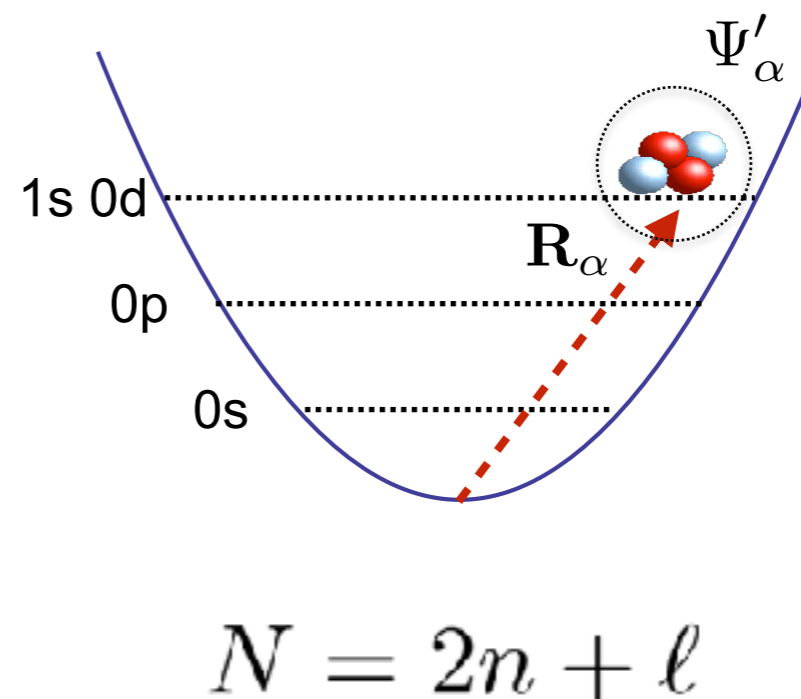
Center-of-Mass boosts

$$\Psi_{n\ell m} = \phi_{n\ell m}(\mathbf{R}) \Psi'$$

\mathcal{B}^\dagger and \mathcal{B} CM quanta creation and annihilation (vectors)

$$\Psi_{n+1\ell m} \propto \mathcal{B}^\dagger \cdot \mathcal{B}^\dagger \Psi_{n\ell m}$$

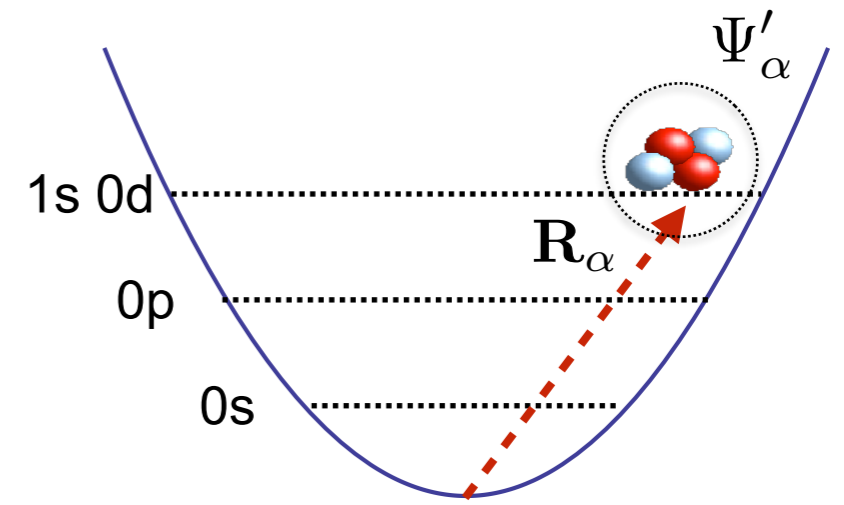
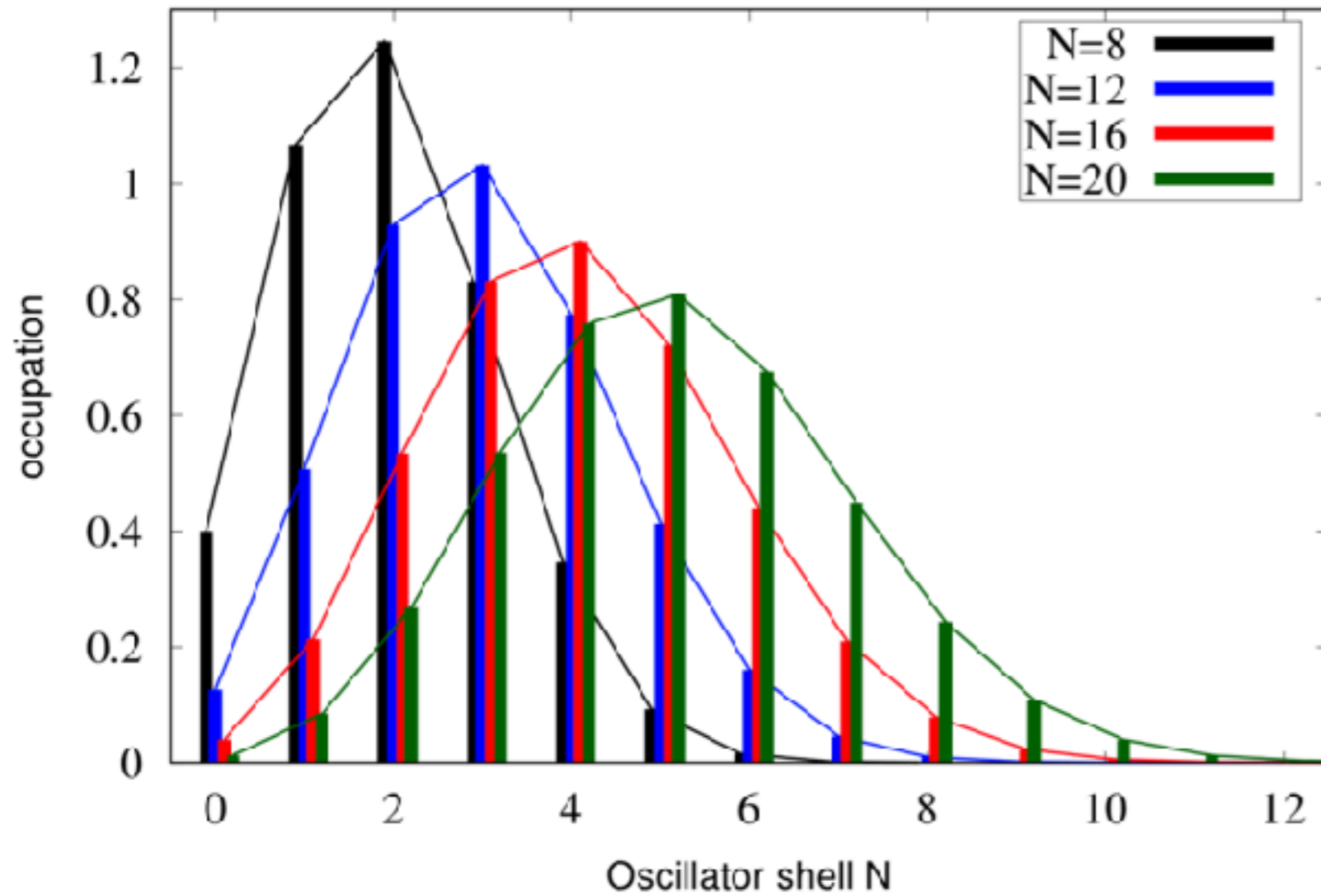
$\mathcal{B}^\dagger \times \mathcal{B}$ CM angular momentum operator



Select configuration content of NCSM wave functions for ${}^4\text{He}$ with $\hbar\Omega = 20$ MeV boosted by 8 quanta ($L = 0$).

Configuration	$N_{\max} = 0$	$N_{\max} = 4$
$(sd)^4$	0.038	0.035
$(p)(sd)^2(pf)$	0.308	0.282
$(p)^2(pf)^2$	0.103	0.094
$(p)^2(sd)(sdg)$	0.154	0.141
$(p)(sd)(sdg)(pfh)$	0.000	0.005
$(p)(sd)(pf)(sdg)$	0.000	0.009

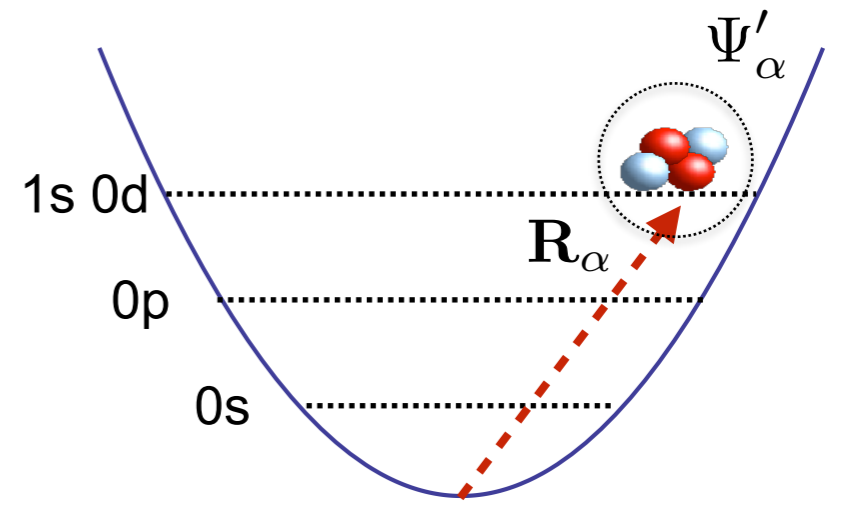
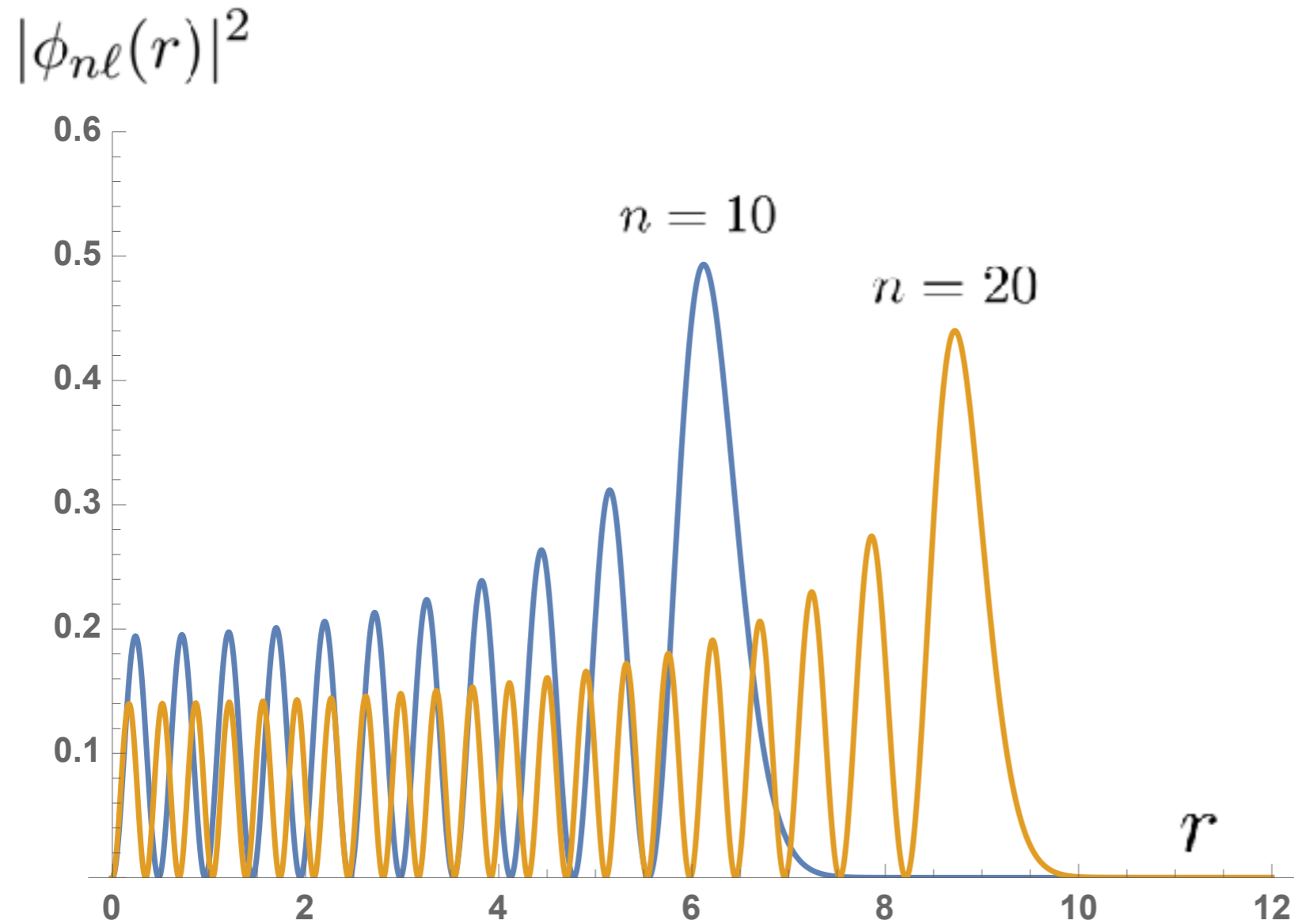
CM-boosted configuration from shell model perspective



CM-boosted configuration from shell model perspective

$$\langle \mathbf{R}^2 \rangle = \frac{\hbar}{M\omega_0} (N_{\text{cm}} + 3/2)$$

$$|\phi_{nl}(r)|^2 \sim \frac{1}{\sqrt{\langle \mathbf{R}^2 \rangle - r^2}}$$



Configuration Interaction

State, equivalent to operator (polymorphism)

$$|\Psi\rangle \equiv \hat{\Psi}^\dagger |0\rangle = \sum_{\{1,2,3,\dots,A\}} \langle 1,2,\dots,A|\Psi\rangle \hat{a}_1^\dagger \hat{a}_2^\dagger \dots \hat{a}_A^\dagger |0\rangle$$

$$|\Psi_\alpha\rangle = \Psi_\alpha^\dagger | \rangle = \sum_{\{m\}} X_m^\alpha a_{m_1}^\dagger a_{m_2}^\dagger a_{m_3}^\dagger a_{m_4}^\dagger | \rangle$$

$$|\Psi_D\rangle = \Psi_D^\dagger | \rangle = \sum_{\{m\}} X_m^D a_{m_1}^\dagger a_{m_2}^\dagger \dots a_{m_{A_D}}^\dagger | \rangle$$

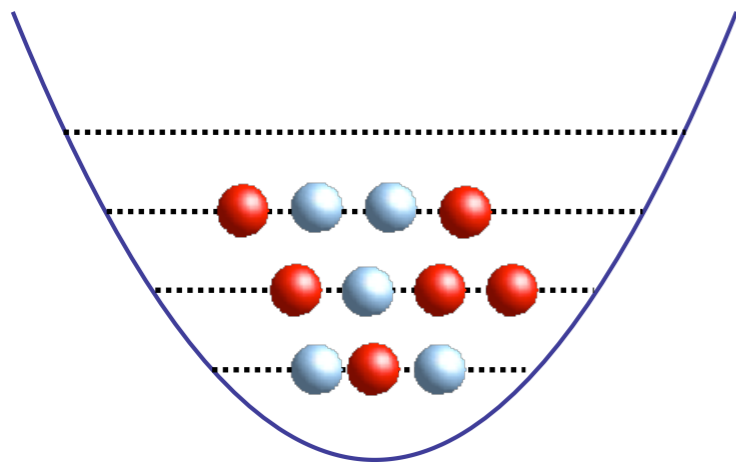
Anti-symmetrized channel wave function components are generated by acting with state creation operator and forward ordering.

$$|\Psi_C\rangle = \Psi_\alpha^\dagger \Psi_D^\dagger | \rangle$$

Configuration interaction approach and clustering

Traditional shell model configuration m-scheme

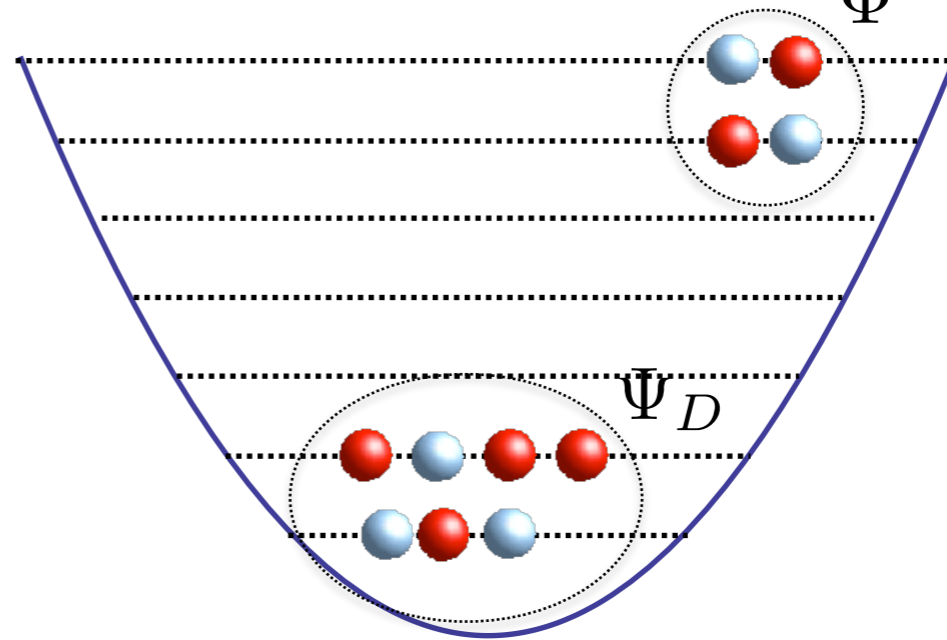
$$|\Psi\rangle = \Psi^\dagger |0\rangle \sim a_1^\dagger a_2^\dagger \dots a_A^\dagger |0\rangle$$



$|\Psi\rangle$

Cluster configuration

$$|\text{channel}\rangle \sim |\Phi\Psi_D\rangle \equiv \Phi^\dagger \Psi_D^\dagger |0\rangle$$

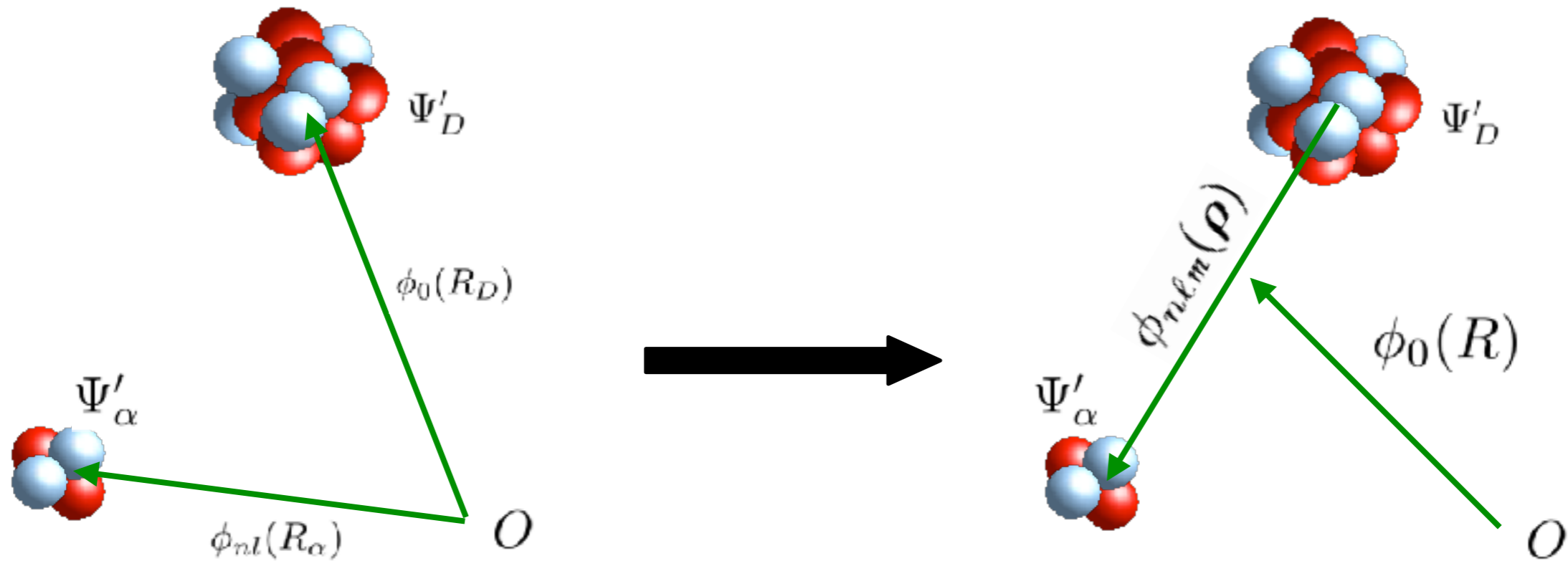


$\Phi^\dagger |\Psi_D\rangle$

+

+

Recoil Recoupling

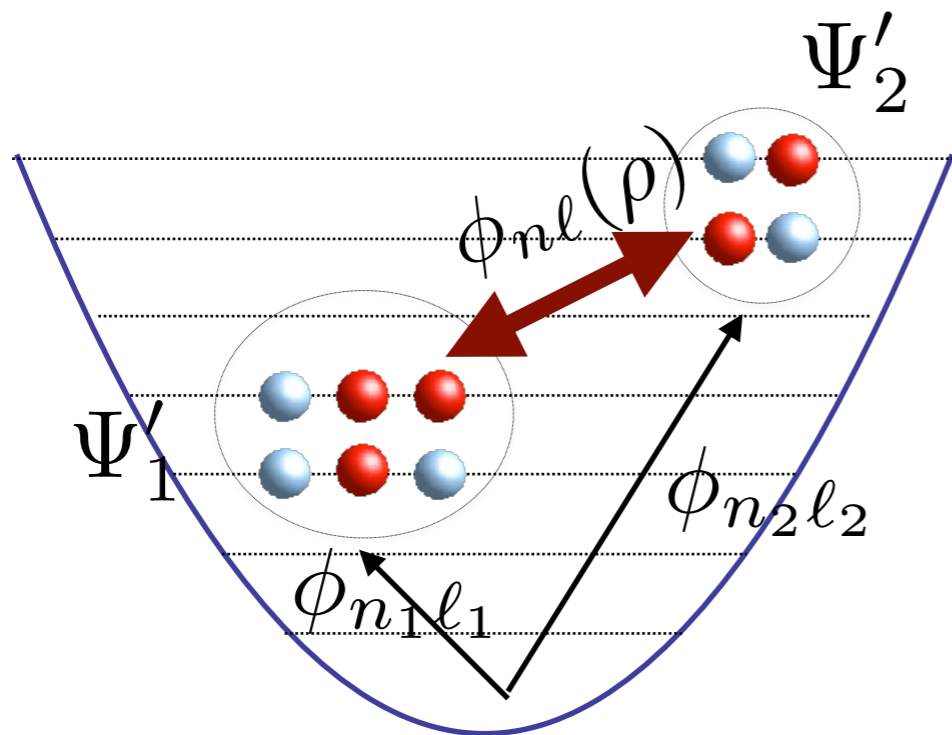


- Recoupling is done with Talmi-Moshinsky brackets

$$\Phi_{nlm} = \mathcal{A} \left\{ \phi_{000}(\mathbf{R}) \phi_{nlm}(\boldsymbol{\rho}) \Psi'^{(1)} \Psi'^{(2)} \right\}$$

Clustering reaction basis channel

(basis states for clustering)



$$\Psi = \phi_{000}(\mathbf{R}) \Psi'$$

Boost

$$\Psi_{nlm} = \phi_{nlm}(\mathbf{R}) \Psi'$$

CM-Recouple

$$\Phi_{nlm} = \mathcal{A} \left\{ \phi_{000}(\mathbf{R}) \phi_{nlm}(\boldsymbol{\rho}) \Psi'^{(1)} \Psi'^{(2)} \right\}$$

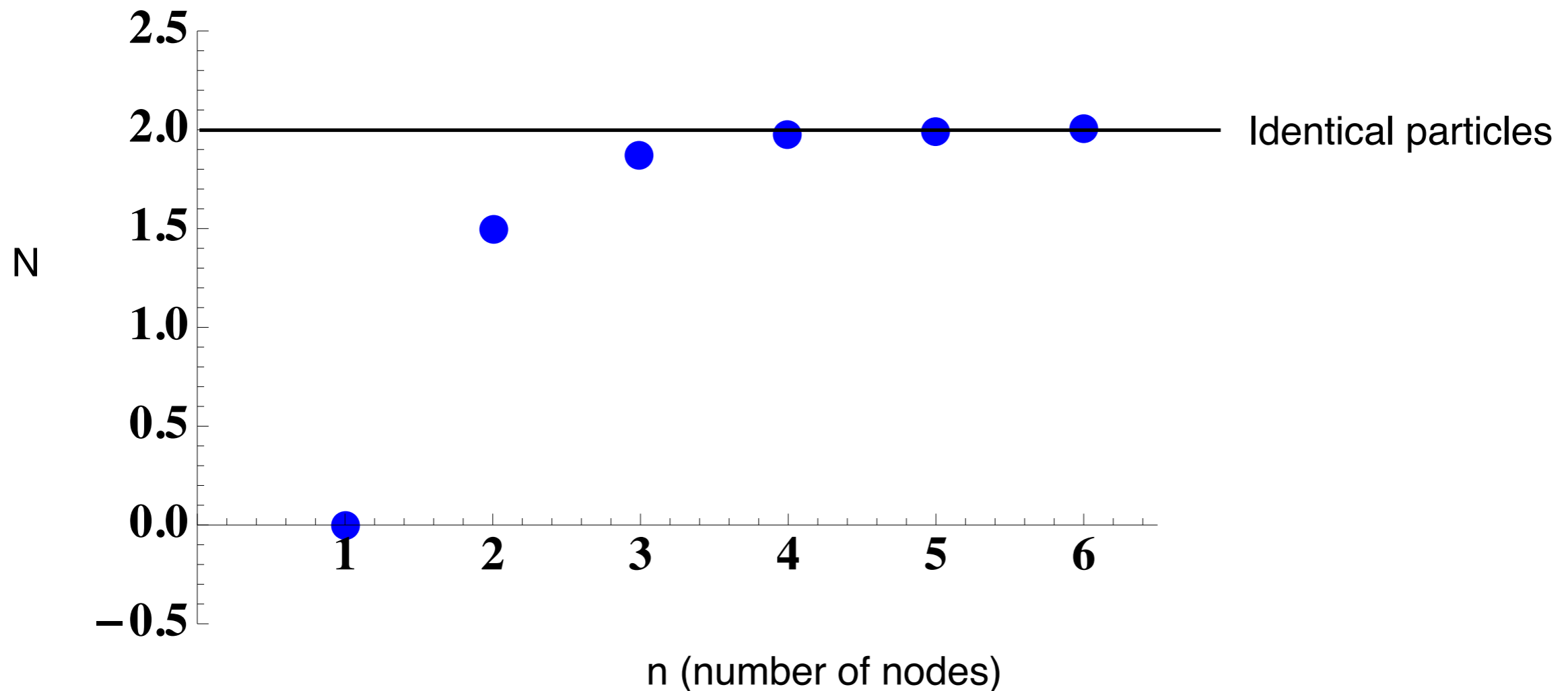
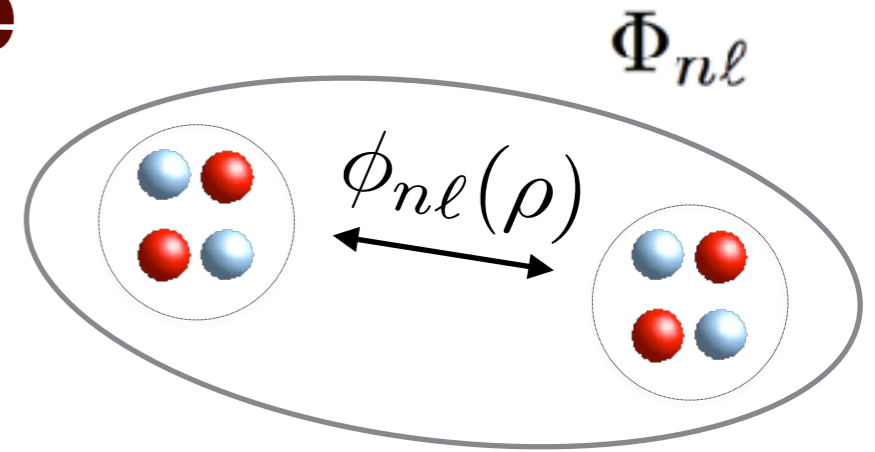
$$\Phi_{n\ell}^\dagger = \sum_{\substack{n_1 \ell_1 \\ n_2 \ell_2}} \mathcal{M}_{n_1 \ell_1 n_2 \ell_2}^{n\ell 00; \ell} \left[\Psi_{n_1 \ell_1 m_1}^\dagger \times \Psi_{n_2 \ell_2 m_2}^\dagger \right]_\ell$$

Resonating group method ^8Be

$$\mathcal{F}_\ell(\rho) = \sum_n \chi_n \Phi_{n\ell}$$

$$\sum_n \mathcal{H}_{nn}^{(\ell)} \chi_n = E \sum_n \mathcal{N}_{nn}^{(\ell)} \chi_n$$

$$\mathcal{H}_{nn}^{(\ell)} = \langle \Phi_{n\ell} | H | \Phi_{n\ell} \rangle \quad \mathcal{N}_{nn}^{(\ell)} = \langle \Phi_{n\ell} | \Phi_{n\ell} \rangle$$

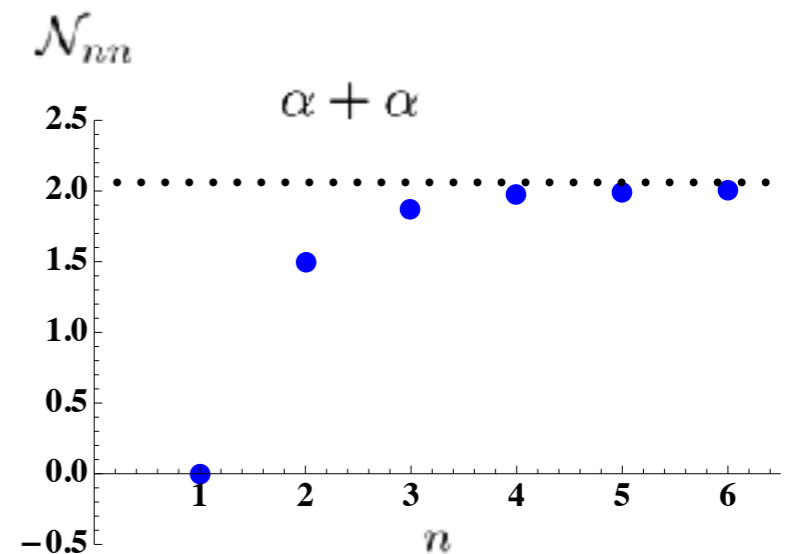
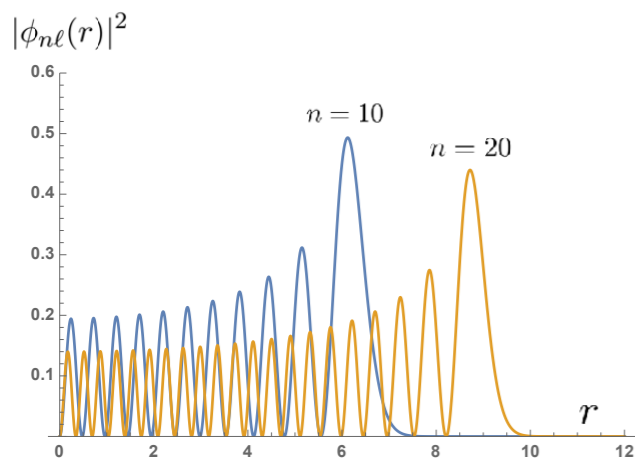


Resonating group method and reactions

$$\sum_n \mathcal{H}_{nn'}^{(\ell)} \chi_{n'} = E \sum_n \mathcal{N}_{nn'}^{(\ell)} \chi_{n'}$$

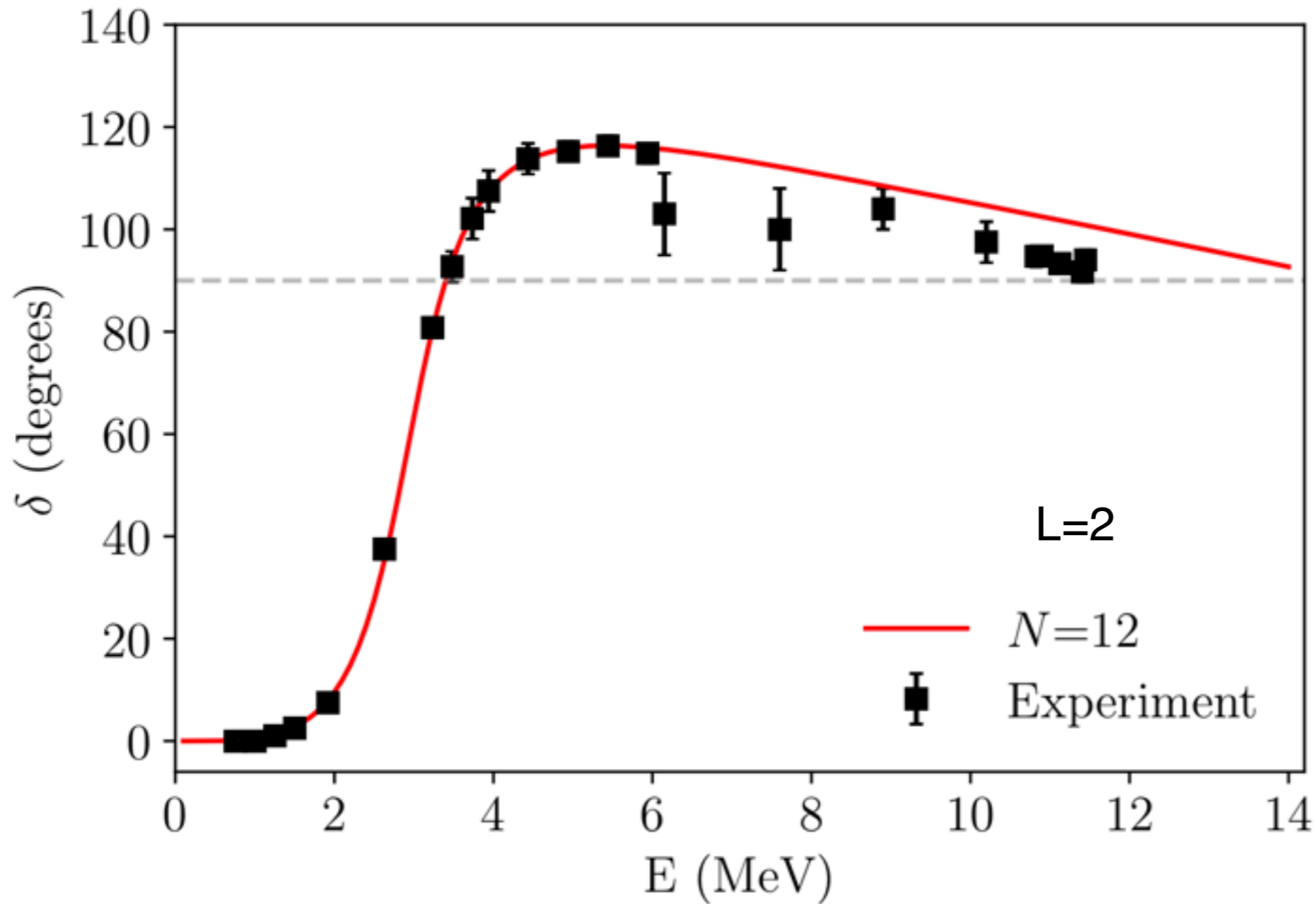
$$\begin{pmatrix} \mathcal{H}_{00} & \dots & \mathcal{H}_{0n} & 0 & 0 & 0 \\ \vdots & \ddots & \vdots & 0 & \vdots & \vdots \\ \mathcal{H}_{n0} & \dots & \mathcal{H}_{nn} & \mathcal{T}_{nn+1} & 0 & \vdots \\ 0 & 0 & \mathcal{T}_{n+1n} & \mathcal{T}_{n+1n+1} & \mathcal{T}_{n+1n+2} & 0 \\ 0 & \dots & 0 & \mathcal{T}_{n+2n+1} & \mathcal{T}_{n+2n+2} & \ddots \\ 0 & \dots & \dots & 0 & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \chi_0 \\ \vdots \\ \chi_n \\ x_{n+1} \\ x_{n+2} \\ \vdots \end{pmatrix} = E \begin{pmatrix} \mathcal{N}_{00} & \dots & \mathcal{N}_{0n} & 0 & 0 & 0 \\ \vdots & \ddots & \vdots & 0 & \vdots & \vdots \\ \mathcal{N}_{n0} & \dots & \mathcal{N}_{nn} & 0 & 0 & \vdots \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & \dots & 0 & 0 & 1 & 0 \\ 0 & \dots & \dots & 0 & 0 & \ddots \end{pmatrix} \begin{pmatrix} \chi_0 \\ \vdots \\ \chi_n \\ x_{n+1} \\ x_{n+2} \\ \vdots \end{pmatrix}$$

Asymptotic solution with phase shift



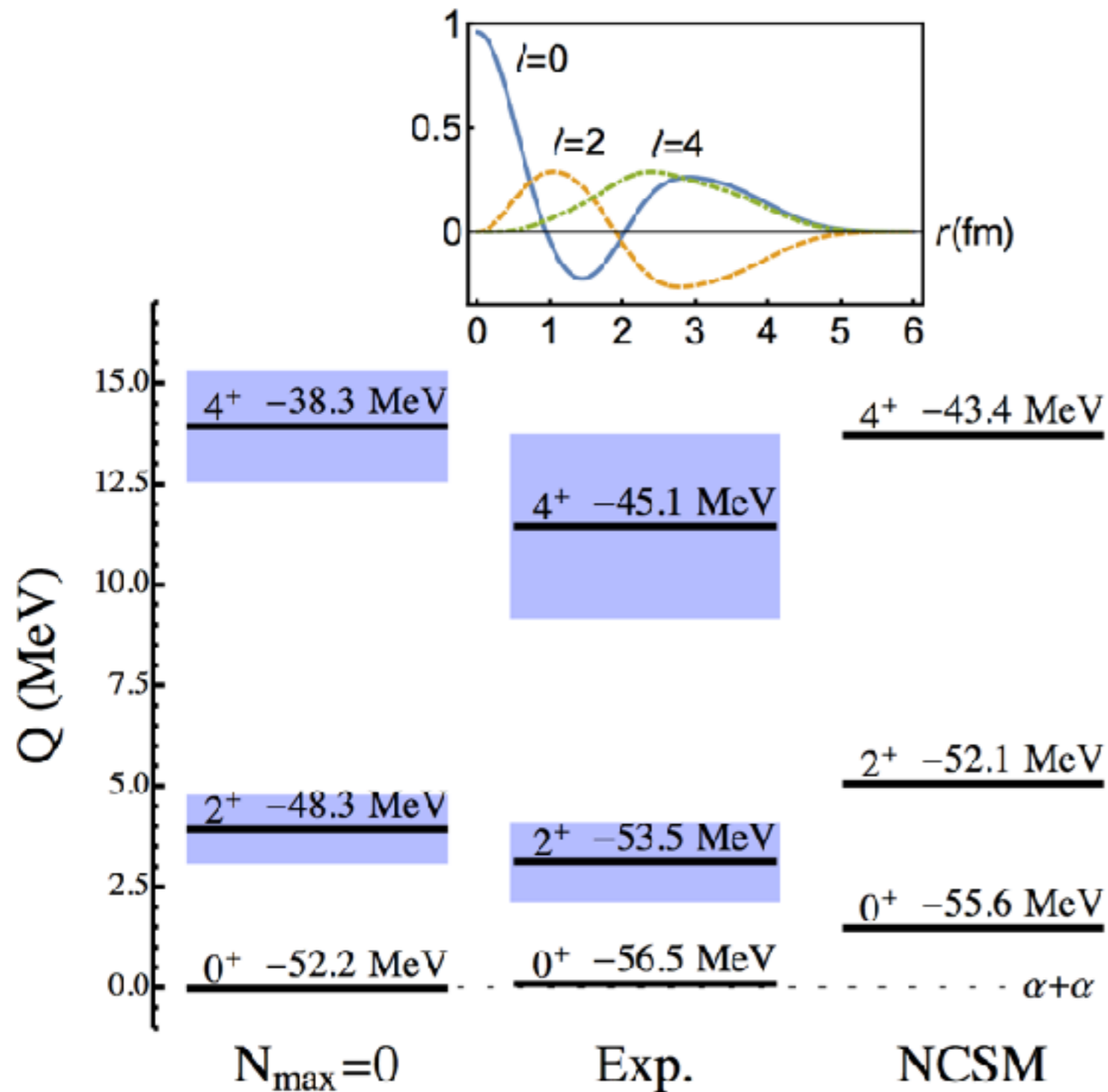
J-matrix (or HORSE) method: J. M. Bang, Annals of Physics **280**, 299 (2000)
 Experimental data: Phys. Rev. 168, 1114 (1968); Nucl. Phys. **A287**, 317 (1977)

alpha+alpha scattering phase shifts



Experimental data from S. A. Afzal, A. A. Z. Ahmad, and S. Ali, Rev. Mod. Phys. 41, 247 (1969).

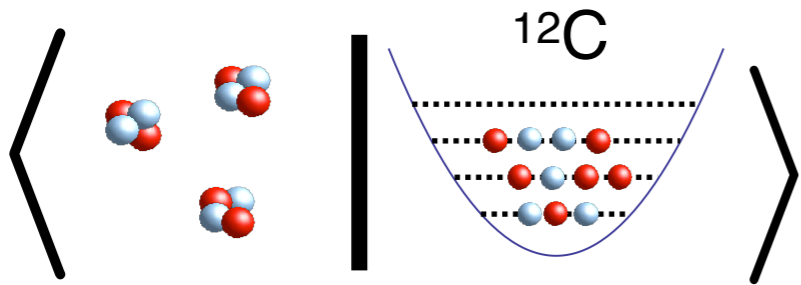
Resonating group method ${}^8\text{Be}$ results



		Theory	Exp.
$l=0$	ev	8.7	5.6
$l=2$	MeV	1.3	1.5
$l=4$	MeV	2.1	3.5

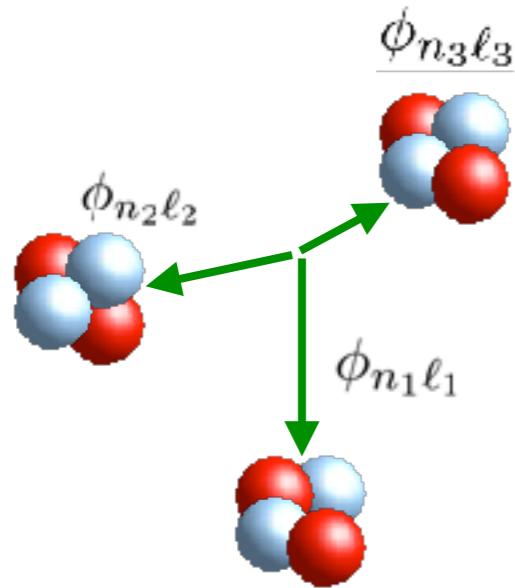
Spectroscopic amplitudes

parent	J^π	channel	$ \langle \Psi \mathcal{F}_e \rangle $
${}^8\text{Be}[4]$	0^+	$\alpha[0] + \alpha[0]$	0.905
${}^8\text{Be}[4]$	2^+	$\alpha[0] + \alpha[0]$	0.898
${}^8\text{Be}[4]$	4^+	$\alpha[0] + \alpha[0]$	0.874
${}^8\text{Be}[4]$	0^+	$\alpha[2] + \alpha[2]$	0.961
${}^8\text{Be}[4]$	2^+	$\alpha[2] + \alpha[2]$	0.957
${}^8\text{Be}[4]$	4^+	$\alpha[2] + \alpha[2]$	0.943
${}^{10}\text{Be}[4]$	0^+	${}^6\text{He}[0] + \alpha[0]$	0.844
${}^{10}\text{Be}[4]$	0^+	${}^6\text{He}[4] + \alpha[0]$	0.820
${}^{10}\text{Be}[4]$	2^+	${}^6\text{He}[0] + \alpha[0]$	0.834
${}^{10}\text{Be}[4]$	2^+	${}^6\text{He}[4] + \alpha[0]$	0.796
${}^{12}\text{C}[4]$	0_1^+	$\alpha[0] + \alpha[0] + \alpha[0]$	0.841
${}^{12}\text{C}[4]$	0_2^+	$\alpha[0] + \alpha[0] + \alpha[0]$	0.229

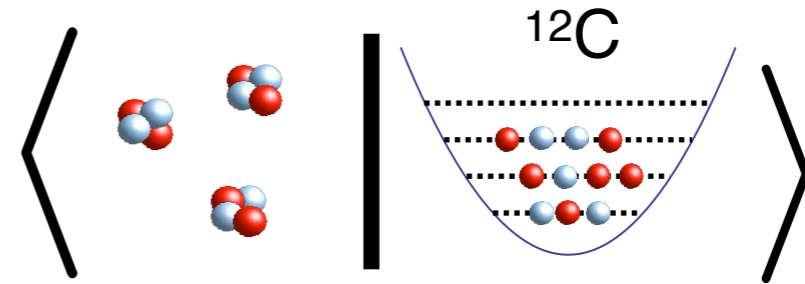


Spectroscopic amplitudes.

Ttriple-alpha RGM



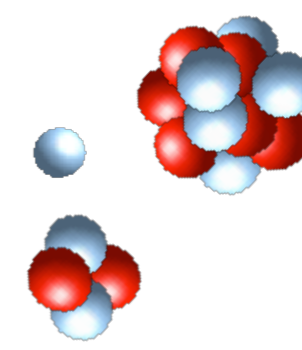
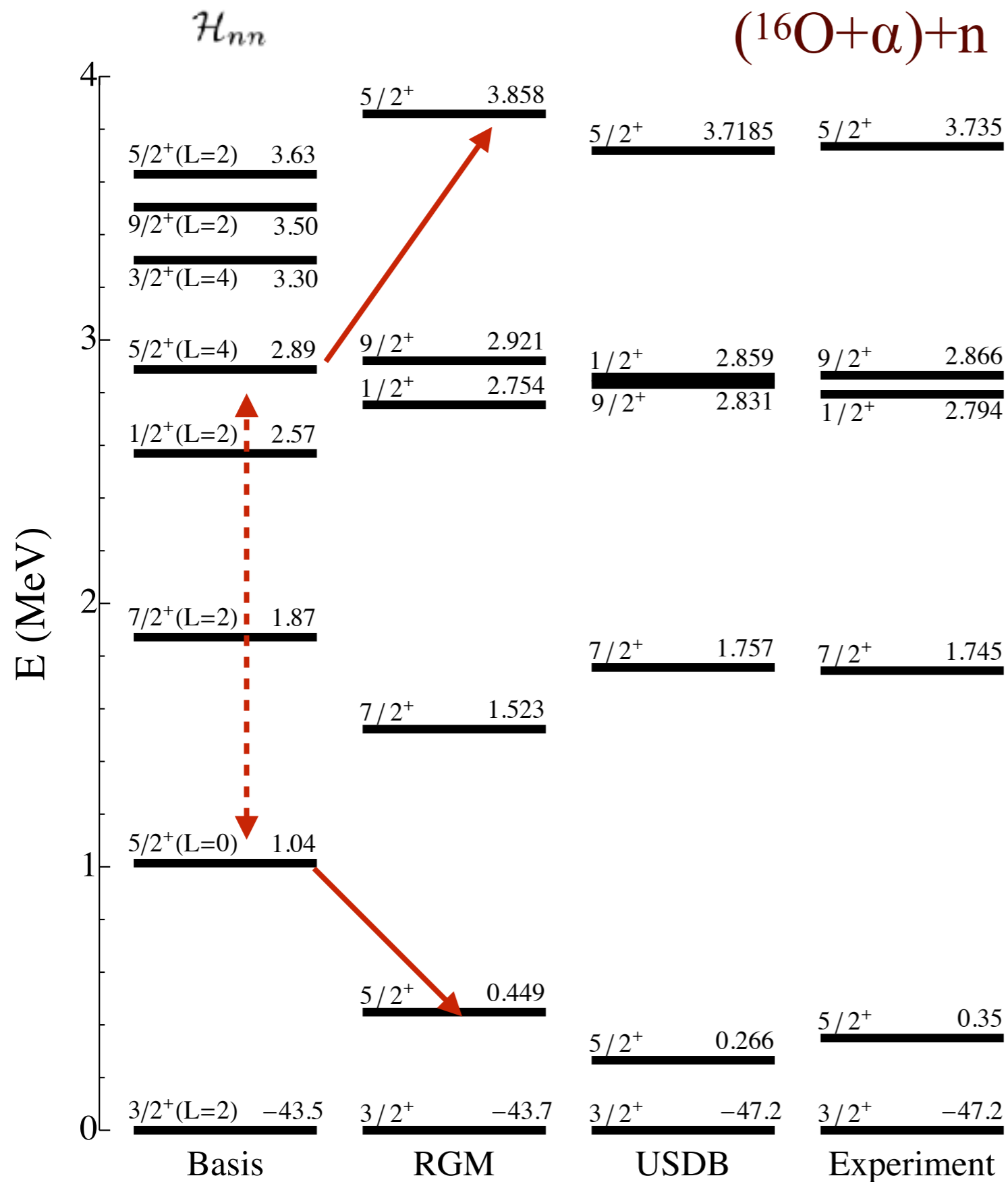
$N_{\max}(\text{rel})=12$



parent	channel	overlap
$^{12}\text{C}[4](0_1^+)$	$\alpha[0] + \alpha[0] + \alpha[0]$	0.841
$^{12}\text{C}[4](0_2^+)$	$\alpha[0] + \alpha[0] + \alpha[0]$	0.229

$$\left\langle \begin{array}{c} {}^8\text{Be} + \alpha \\ \alpha + \alpha + \alpha \end{array} \right\rangle^2 = 0.89$$

Molecular orbits ^{21}Ne



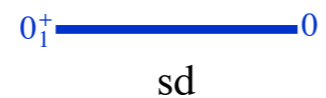
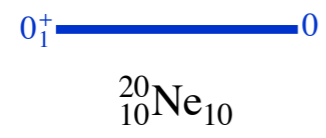
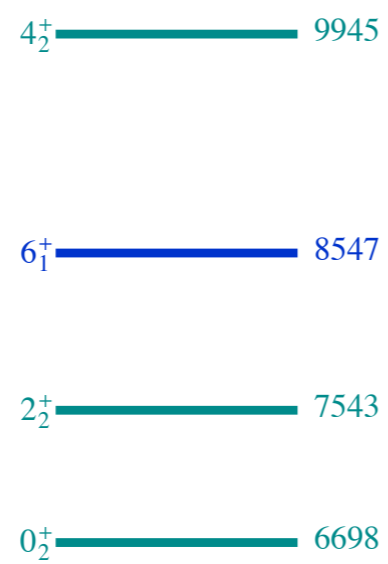
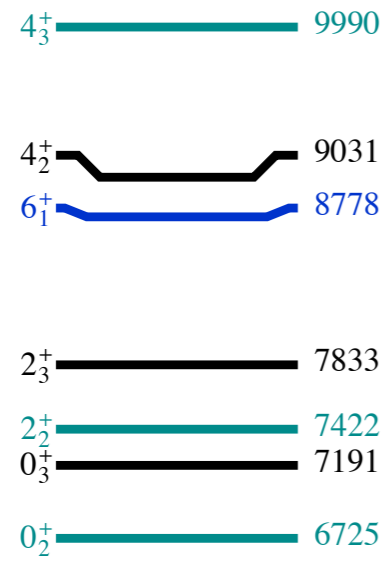
Weak-Coupling Behavior

J^π	$\mathcal{G}^{(new)}$			$\mathcal{G}^{(exp)}$		
	$\ell = 0$	$\ell = 2$	$\ell = 4$	$\ell = 0$	$\ell = 2$	$\ell = 4$
$3/2+$		1.0	0.18		1.0 ± 0.05	0.42 ± 0.04
$5/2+$	0.78	0.02	0.44	1.04 ± 0.41	...	0.32 ± 0.18
$7/2+$		0.9	0.14		0.91 ± 0.08	0.23 ± 0.04
$9/2+, 1/2+$		0.81	0.33		0.9 ± 0.05	0.29 ± 0.03

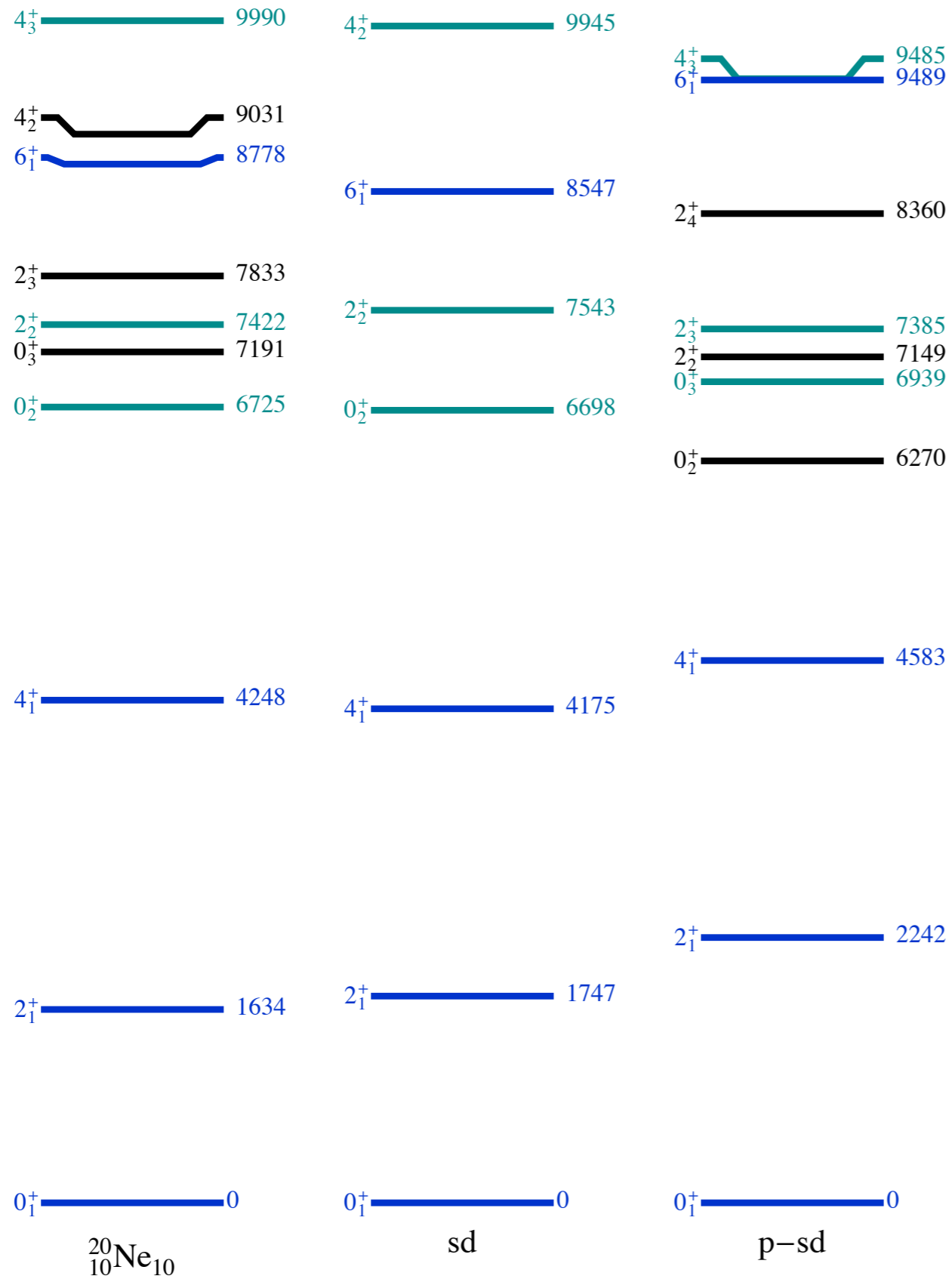
N. Anantaraman, J. P. Draayer, H. E. Gove, J. Toke, and H. T. Fortune. Alpha-particle stripping to ^{21}Ne . Phys.Rev. C18, 815 (1978); Phys.Lett. 74B, 199 (1978)

A. K. Nurmukhanbetova, V. Z. Goldberg, D. K. Nauruzbayev, M. S. Golovkov, A. Volya, Phys. Rev. C 100 (2019) 062802.

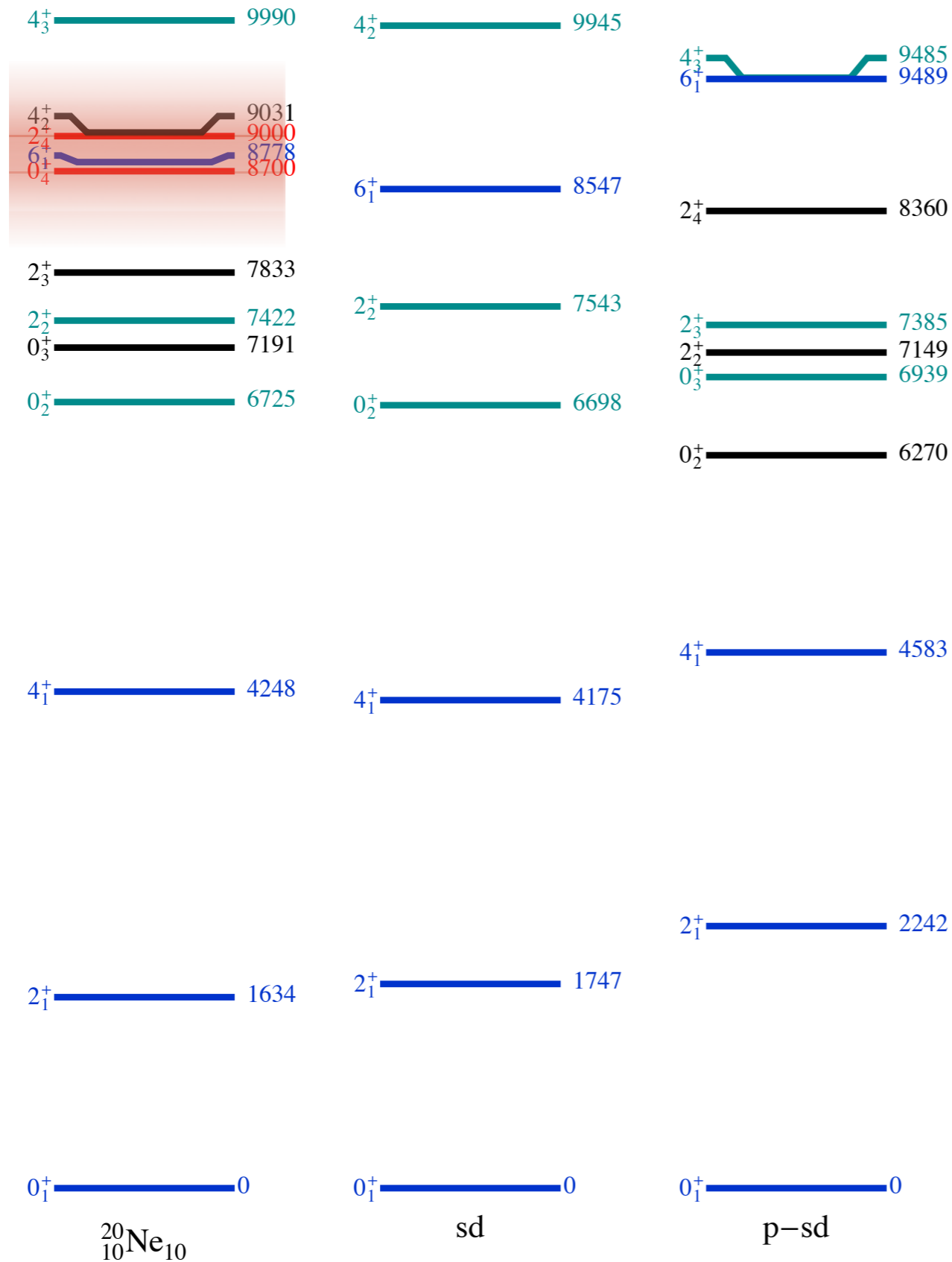
Clustering in ^{20}Ne



Clustering in ^{20}Ne

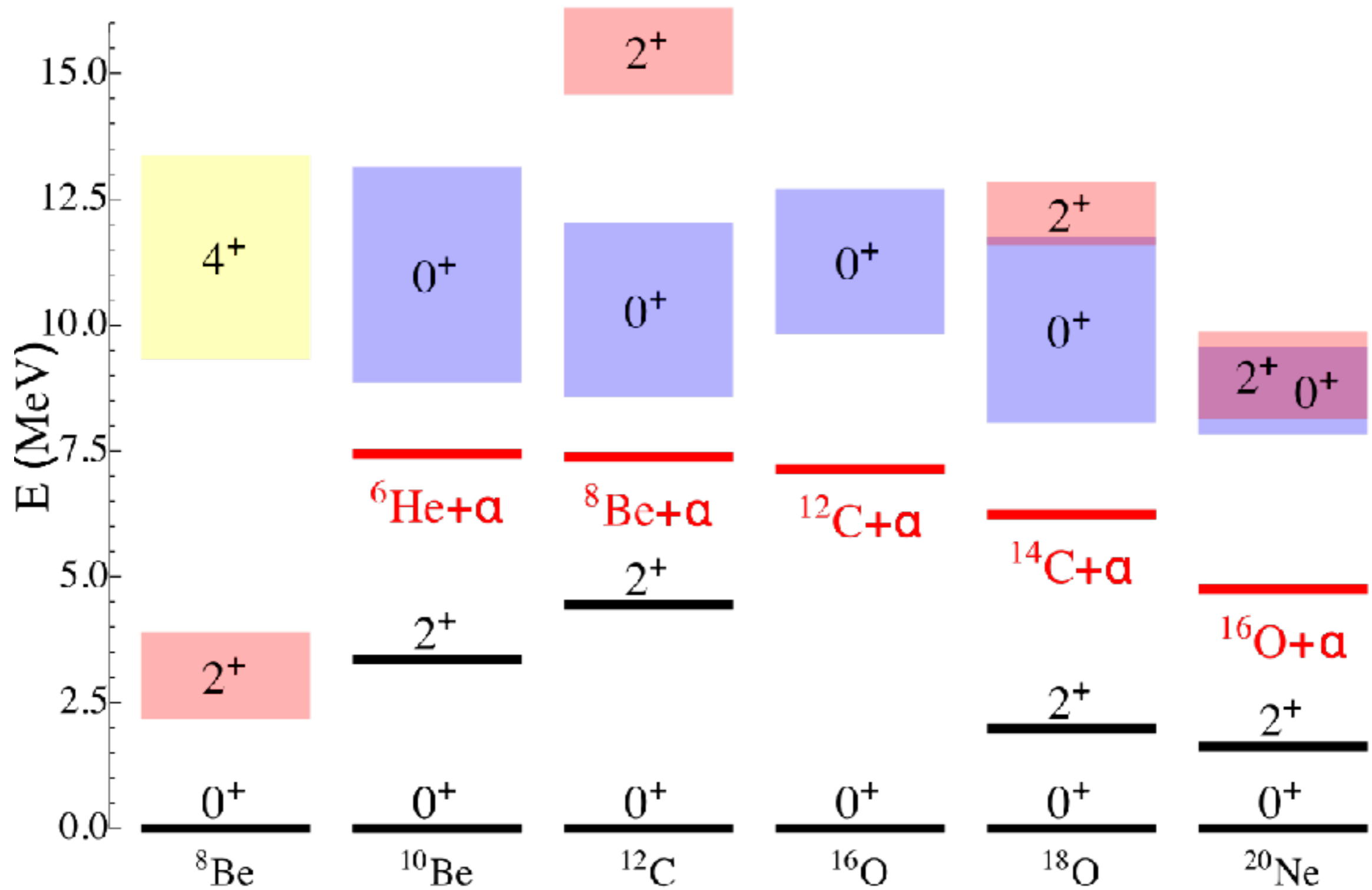


Clustering in ^{20}Ne

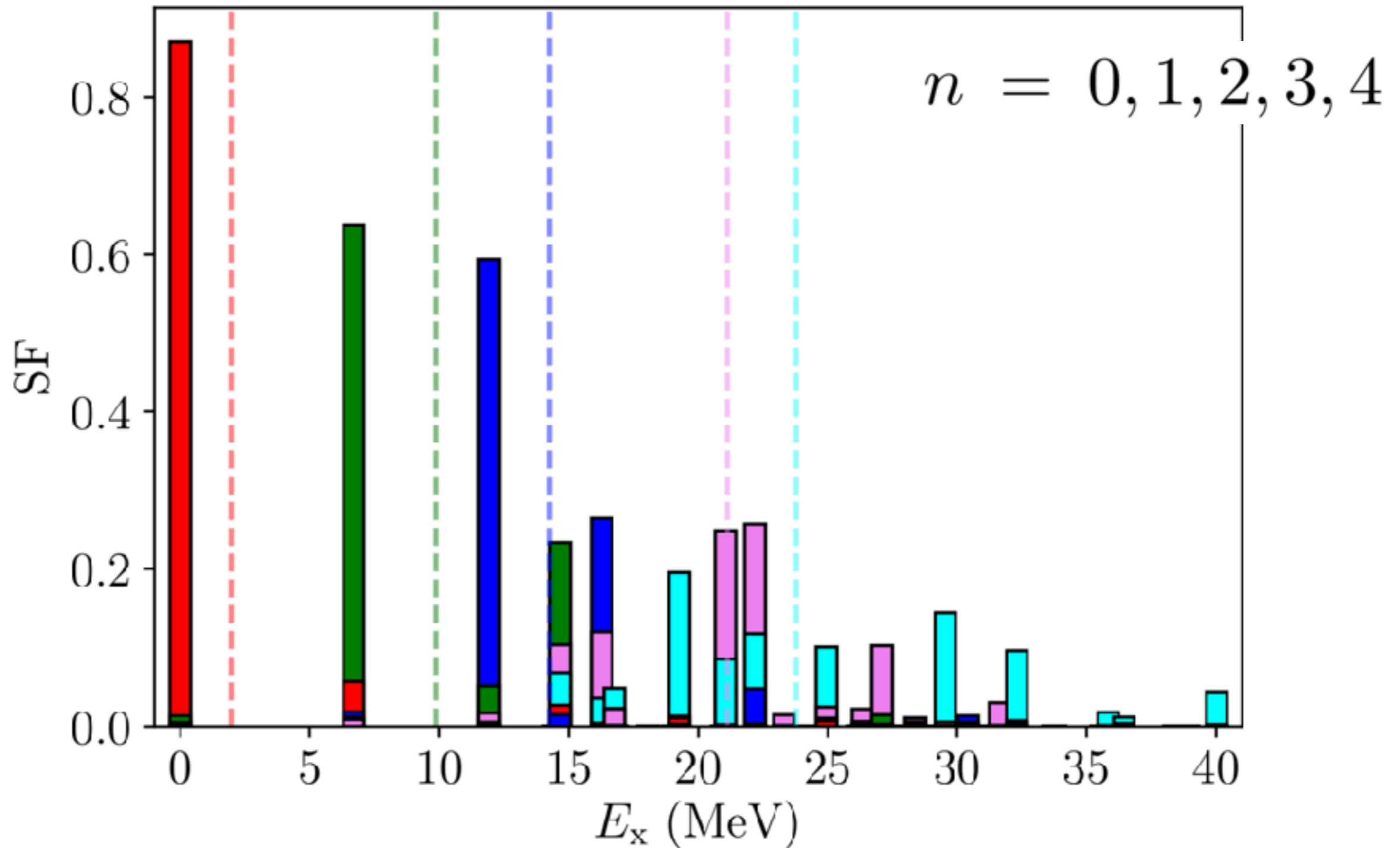


J	E MeV	Γ width	SF ex	SF th.
0+	0	0		0.73
2+	1.63	0		0.67
4+	4.25	0		0.62
0+	6.73	19	0.47	0.46
0+	7.19	3.4	0.02	0.10
2+	7.42	15	0.19	0.12
2+	7.83	2	0.01	0.09
0+	8.7	800	0.3	
6+	8.78	0.11	0.5	0.51
2+	9.00	800	0.86	

Clustering and continuum

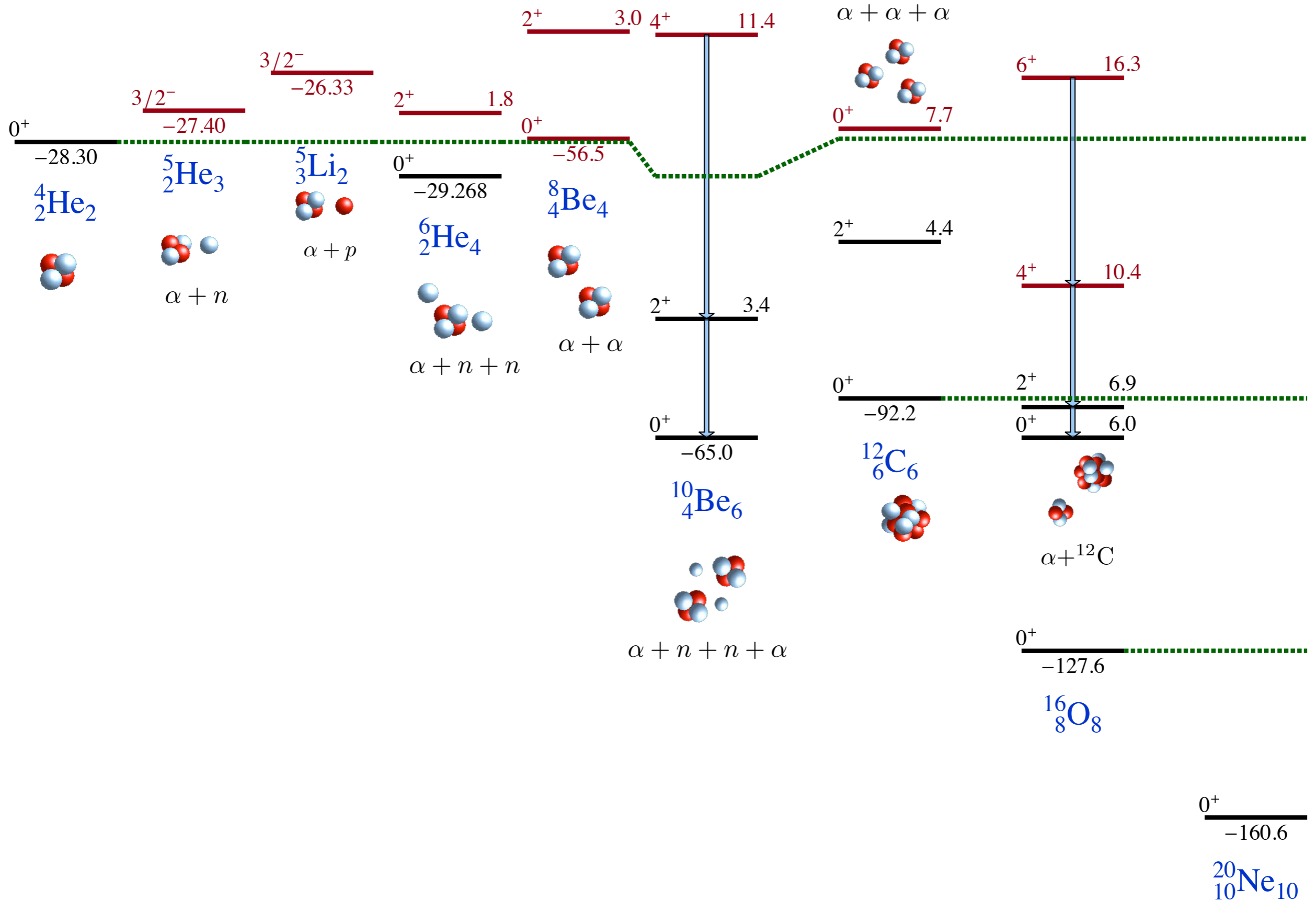


Searching for clustering strength

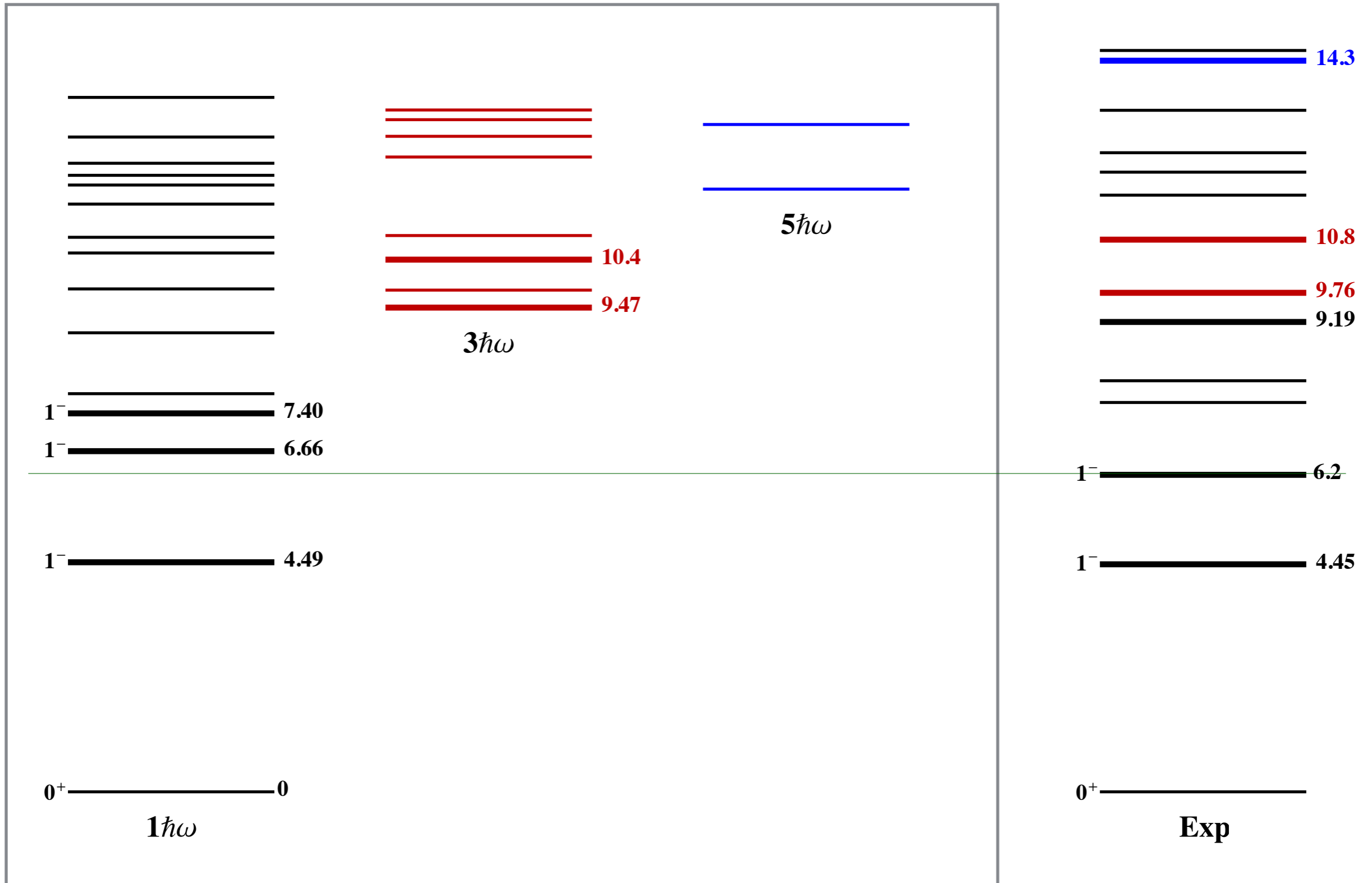


Distribution of dynamic spectroscopic factors for $^{20}\text{Ne} \rightarrow ^{16}\text{O}(\text{g.s.}) + \alpha$. The dashed lines correspond to the RGM energies for each decay channel.

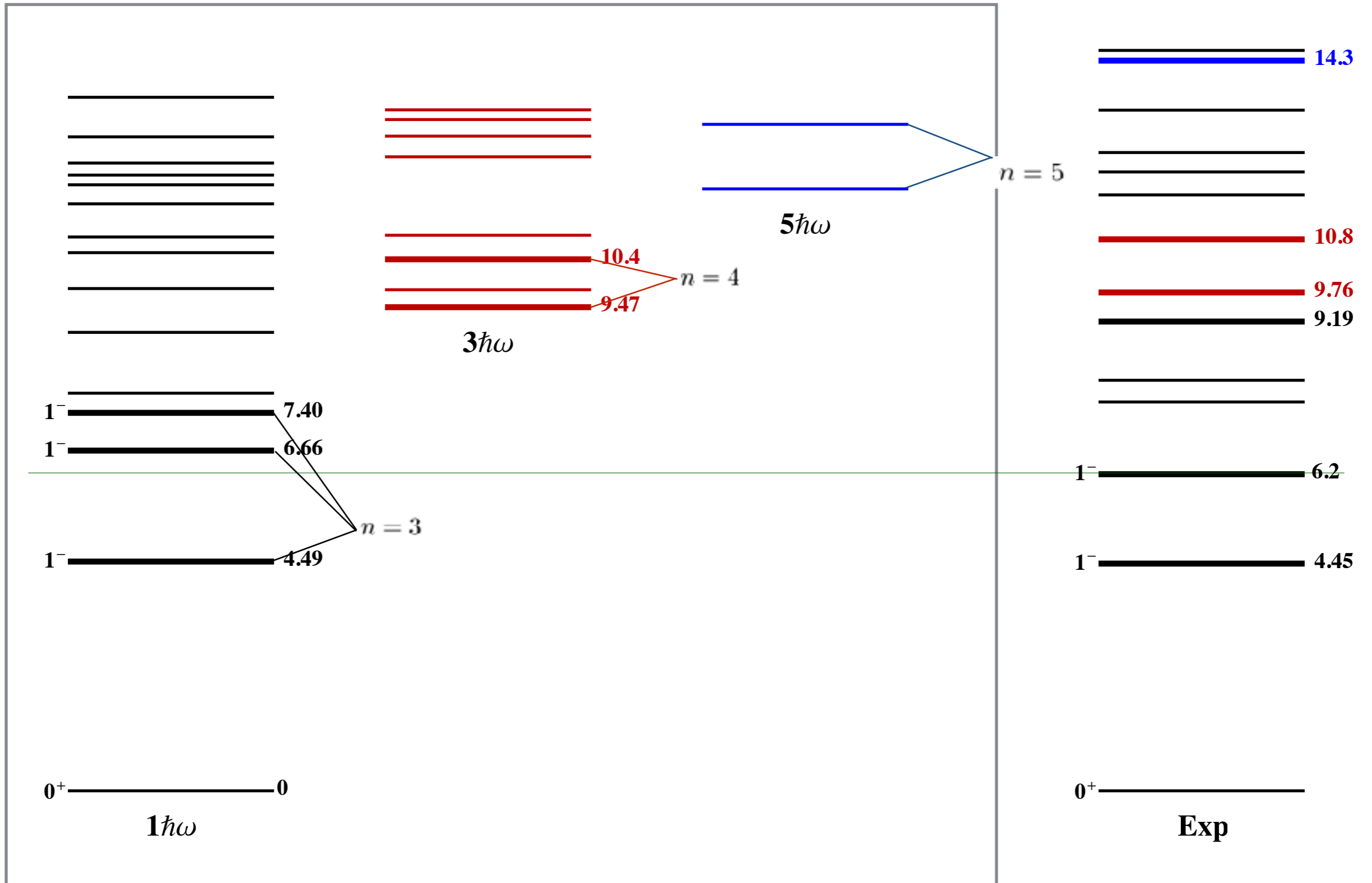
Clustering in light nuclei



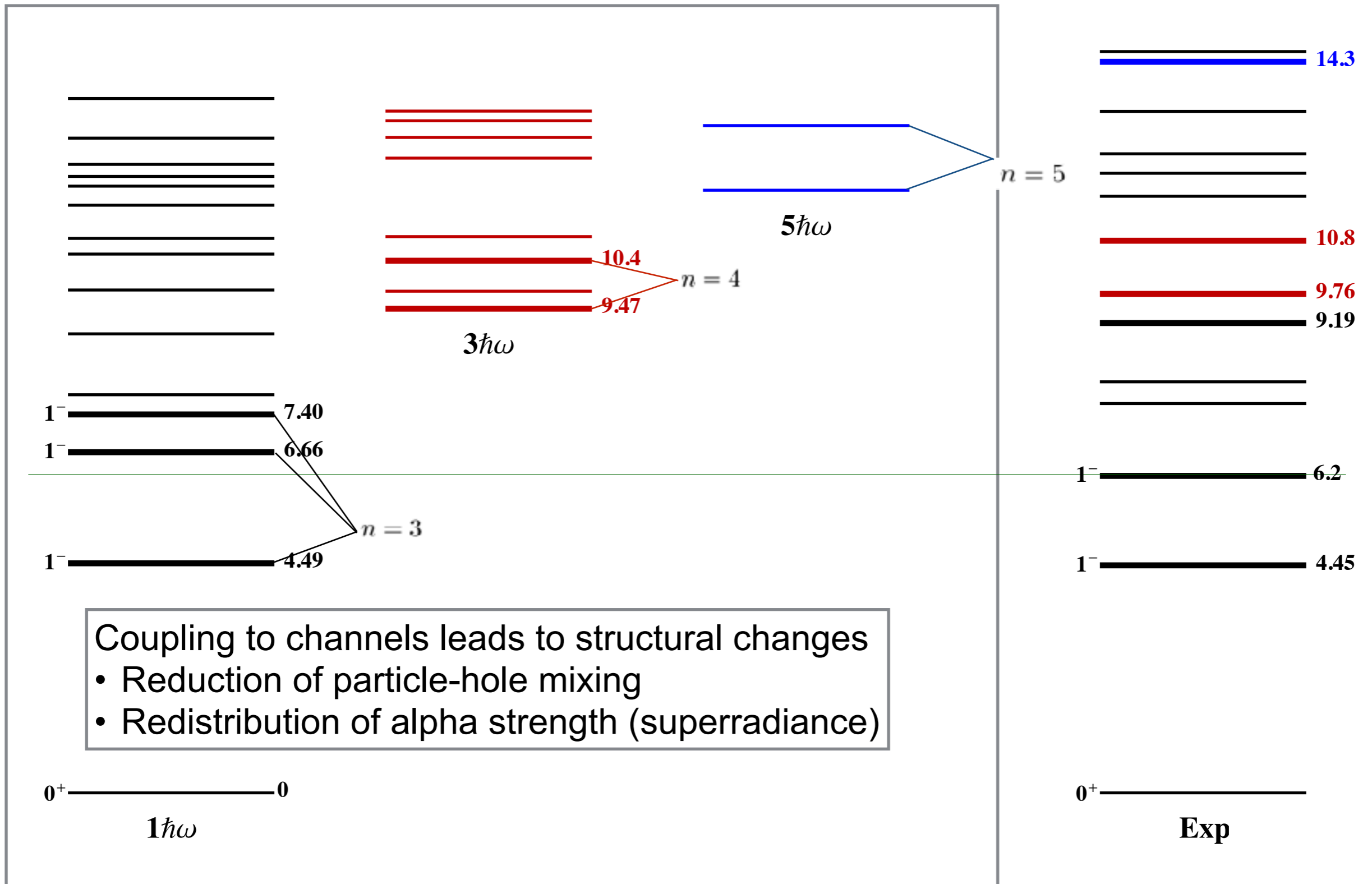
Channel coupling in ^{18}O $l=1$ channel



Channel coupling in ^{18}O $l=1$ channel



Channel coupling in ^{18}O $l=1$ channel



Thanks to all collaborators:

K Kravvaris and A. Volya, Phys. Rev. Lett, 119(6), 062501 (2017); Journal of Phys 863, 012016 (2017)

K. Kravvaris, A. Volya, Phys. Rev. C 100 (2019) 034321.

K Kravvaris Doctoral dissertation, Florida State University (2018)

A. Volya, et al. Phys. Rev. C 105 (2022) 014614.

V. Z. Goldberg, et al., Phys. Rev. C 105 (2022) 014615.

A. K. Nurmukhanbetova, et al, Phys. Rev. C 100 (2019) 062802.

D. K. Nauruzbayev, et al, Phys. Rev. C 96 (2017) 014322.

A. Volya and Y. M. Tchuvil'sky, Phys.Rev.C 91, 044319 (2015).

M. L. Avila, G. V. Rogachev, V. Z. Goldberg, E. D. Johnson, K. W. Kemper, Y. M. Tchuvil'sky, A. S. Volya, Phys. Rev. C 90 (2014) 024327.

A. M. Long, T. Adachi, M. Beard, G. P. A. Berg, Z. Buthelezi, J. Carter, M. Couder, R. J. Deboer, R. W. Fearick, S. V. Förtsch, J. Görres, J. P. Mira, S. H. T. Murray, R. Neveling, P. Papka, F. D. Smit, E. Sideras-Haddad, J. A. Swartz, R. Talwar, I. T. Usman, M. Wiescher, J. J. V. Zyl, A. Volya, Phys. Rev. C 95 (2017) 055803.

Resources: <https://www.volya.net/> (see research, clustering)

Funding: U.S. DOE contract DE-SC0009883.

