Reactions with Clusters in Harmonic Oscillator Basis

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Reactions with Clusters in Harmonic Oscillator Basis

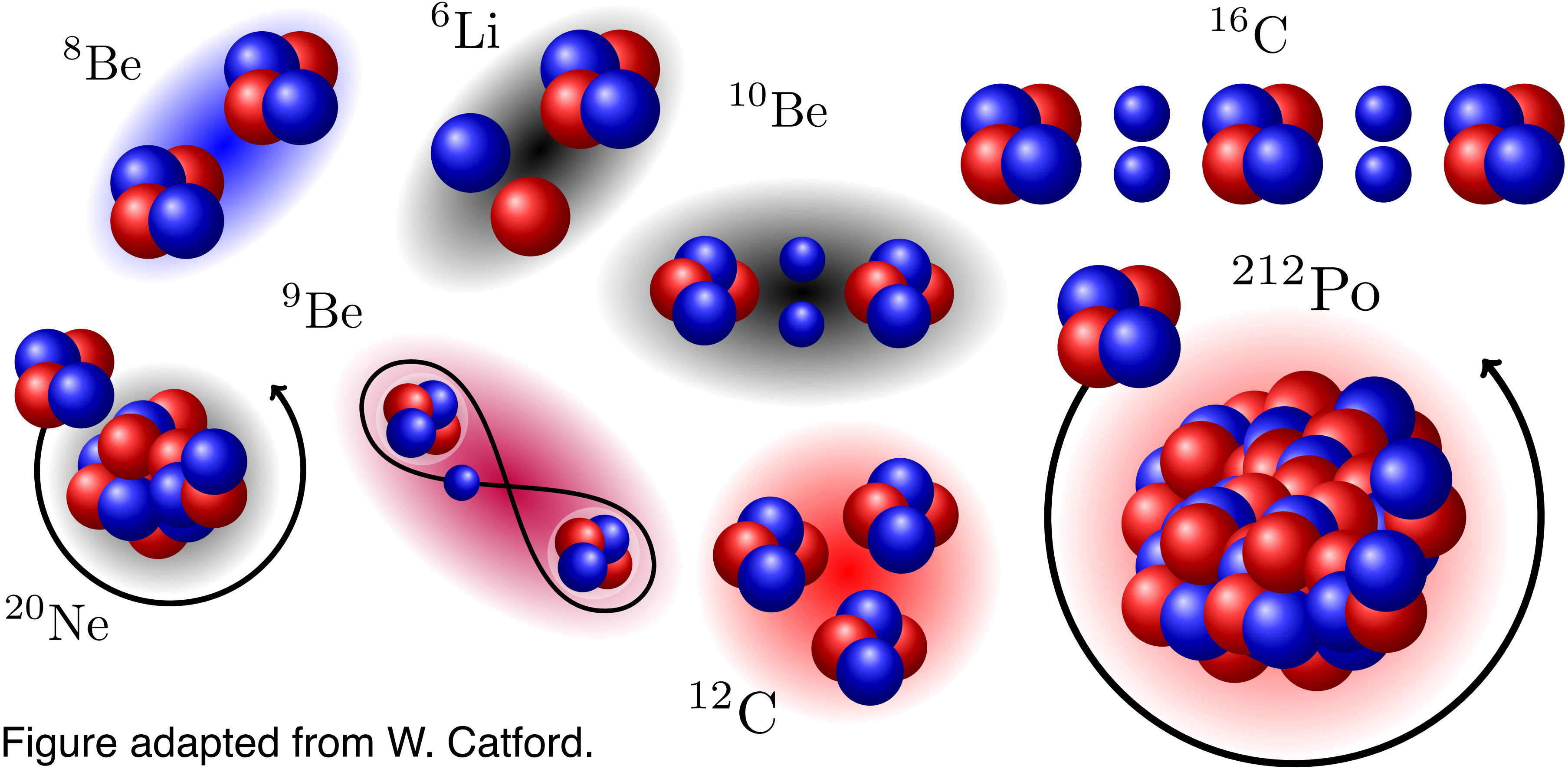

Figure adapted from W. Catford.

Goals:

- Starting from a bound state method (square integrable basis expansion), obtain scattering properties of the system.

- Generalize for scattering properties of many-body systems.

Outline:

- Introduction
- Scattering in Finite Bases
- Regularization
- Coulomb Scattering
- Simple example
- Channel Construction
- Many-body examples.

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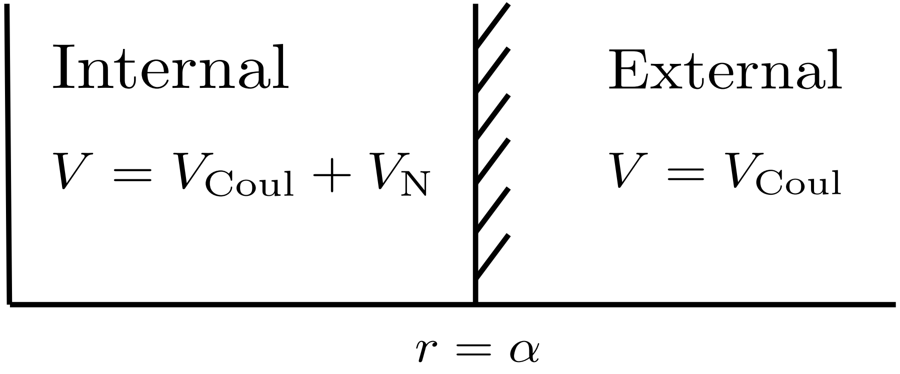


$$\left(\begin{array}{c|c} \mathcal{H}_{\mathcal{PP}} & \mathcal{H}^{(0)}_{\mathcal{PQ}} \\ \hline \mathcal{H}^{(0)}_{\mathcal{QP}} & \mathcal{H}^{(0)}_{\mathcal{QQ}} \end{array}\right)$$

$$N$$

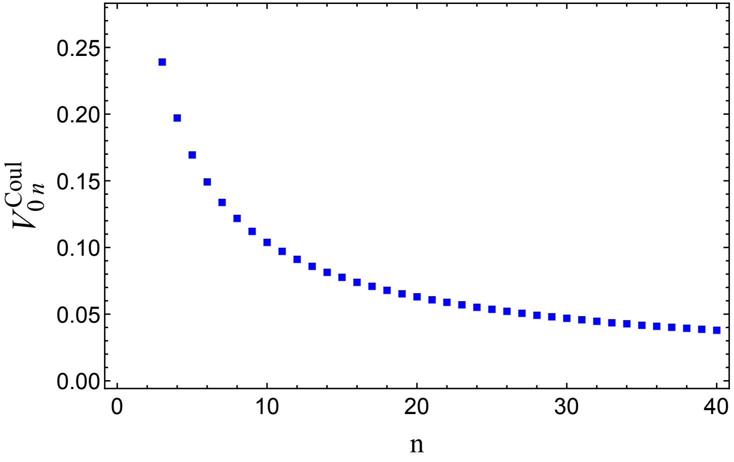
Internal P-space Hamiltonian contains interaction potential

External Q-space only has free components: $T + V_{\text{Coul}}$

Matching condition at some basis limit N. Potential matrix elements at limit ~ 0

$$\left(\begin{array}{c|c} \mathcal{H}_{\mathcal{PP}} & \mathcal{H}^{(0)}_{\mathcal{PQ}} \\ \hline \mathcal{H}^{(0)}_{\mathcal{QP}} & \mathcal{H}^{(0)}_{\mathcal{QQ}} \end{array}\right)$$

N



Implications

- Solving an approximate potential:

$$V = \sum_{nn'}^{N} |n\rangle V_{nn'} \langle n'|$$

- Coulomb matrix elements do not fall-off fast enough to ignore.
- Solution requires knowledge of expansion coefficients.

In order to match the internal part, we need to know what the free part looks like.

Regular Solution	Irregular Solution
$F_\ell(\eta, kr)$	$G_\ell(\eta, kr)$

Three-term recursion for neutral particle; infinite terms for charged.

$$\sum_{n'=0}^{\infty} (H^{(0)}_{nn'} - E\delta_{nn'}) F_{n'\ell}(\eta, k) = 0$$

For the regular solution, coefficients obtained through direct integration with basis function.

$$F_{n\ell}(\eta, k) = \int \phi^*_n(r) F_\ell(\eta, kr) dr$$

The irregular solution cannot be obtained as an expansion due to behavior near the origin.

$$G_\ell(\eta, kr) \sim r^{-\ell}$$

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At "infinity" (large n) the irregular expansion coefficients should obey the same recursion relations.
At the "origin" (n = 0) we add an inhomogeneity

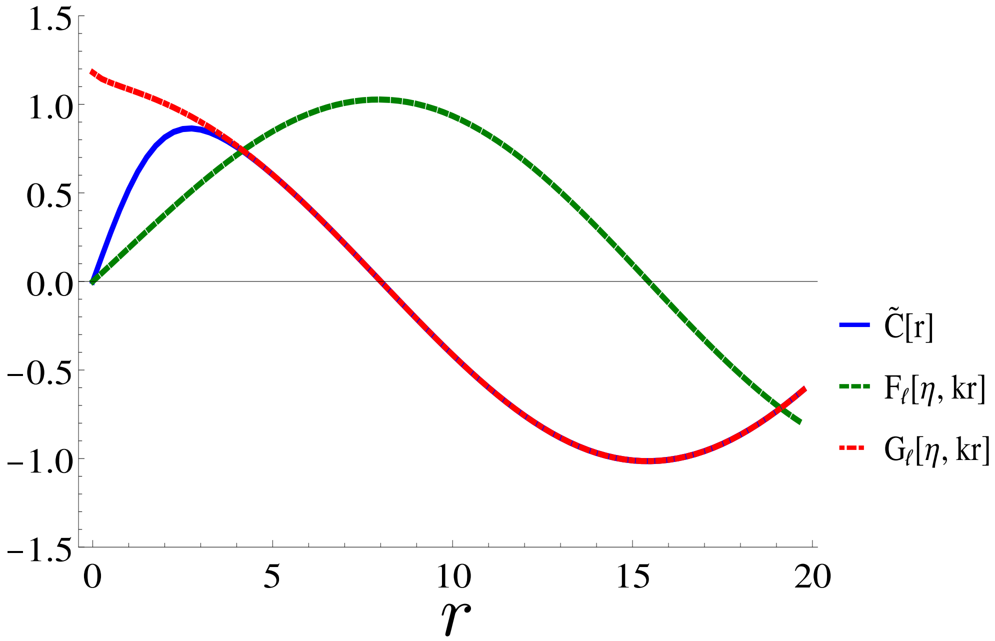
$$\sum_{n'=0}^{\infty}(H^{(0)}_{nn'} - E\delta_{nn'})G_{n'\ell}(\eta, k) = \beta\delta_{n0}$$

In r-space there is only one choice that preserves the form of the discrete equations

$$\left(H^{(0)} - E\right)\widetilde{C}_\ell(\eta, r) = \beta\phi_0(r)$$

Solve r-space problem via a Green's function

$$G(r, r') \sim F_\ell(\eta, kr_<)G_\ell(\eta, kr_>)$$



Good behavior at large distances, no divergence at small distances.

Strength of inhomogeneity fixed by requiring:

$$\widetilde{C}_\ell(\eta, r \to \infty) = G_\ell(\eta, kr)$$

$$\beta \sim 1/F_{0\ell}(\eta, k)$$

Coefficients can now be obtained by direct integration

$$G_{n\ell}(\eta, k) = \int \phi^*_{n\ell}(r)\widetilde{C}_\ell(\eta, r)dr$$

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The internal part is governed by the (matrix) equation:

$$\mathcal{H}_{\mathcal{P}\mathcal{P}'}\Psi_{\mathcal{P}'} + \mathcal{H}^{(0)}_{\mathcal{P}\mathcal{Q}}\Psi_{\mathcal{Q}} = E\Psi_{\mathcal{P}}$$

$$\left(\begin{array}{c|c} \mathcal{H}_{\mathcal{P}\mathcal{P}} & \mathcal{H}^{(0)}_{\mathcal{P}\mathcal{Q}} \\ \hline \mathcal{H}^{(0)}_{\mathcal{Q}\mathcal{P}} & \mathcal{H}^{(0)}_{\mathcal{Q}\mathcal{Q}} \end{array}\right)$$

$$N$$

For any P-space component we can use the resolvent

$$\mathcal{G}_{pp'} = \left[(E\mathrm{I} - H)^{-1}\right]_{pp'}$$

$$\Psi_p = \sum_{\substack{p'=0 \\ q\in\mathcal{Q}}}^{N} \mathcal{G}_{pp'} H^{(0)}_{p'q} \Psi_q$$

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Matching at the boundary N (summation implied)

$$\Psi_N = \mathcal{G}_{Np} H^{(0)}_{pq} \Psi_q$$

In the Q-space (outside) we have

$$\Psi_q = aF_{q\ell}(\eta, k) + bG_{q\ell}(\eta, k)$$

On the inside, we require that

$$\Psi_N = aF_{N\ell}(\eta, k) + bG_{N\ell}(\eta, k)$$

$$\tan\delta_\ell = \frac{b}{a} = -\frac{F_{N\ell} - \mathcal{G}_{Np} H^{(0)}_{pq} F_{q\ell}}{G_{N\ell} - \mathcal{G}_{Np} H^{(0)}_{pq} G_{q\ell}}$$

Special case: HORSE method

T_{NN+1}

$S_N(E)$ $\mathcal{G}_{NN}$ $S_{N+1}(E)$

$$\tan\delta_\ell = -\frac{F_{N\ell} - \mathcal{G}_{Np} H^{(0)}_{pq} F_{q\ell}}{G_{N\ell} - \mathcal{G}_{Np} H^{(0)}_{pq} G_{q\ell}}$$

$C_N(E)$ $\mathcal{G}_{NN}$ T_{NN+1} $C_{N+1}(E)$

Recover HORSE
exactly for neutral case.

But what about Coulomb?

Phase shifts for Coulomb problem require summation of F, G amplitudes over the infinite Q-space.

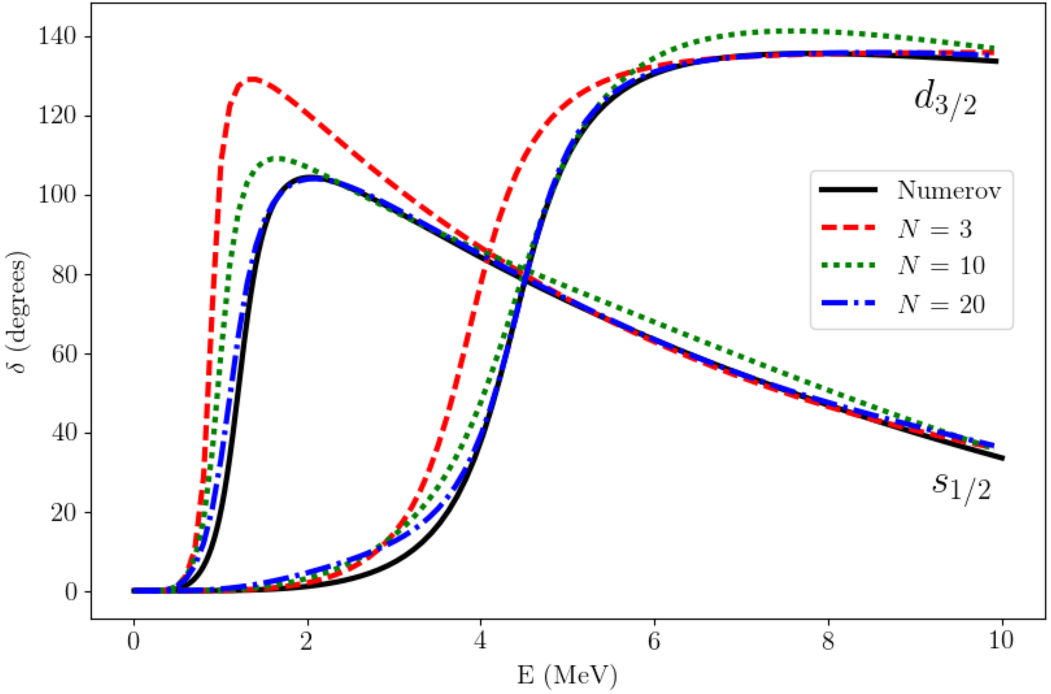
$$H^{(0)}_{pq} F_{q\ell} = \left(E\delta_{pp'} - H^{(0)}_{pp'}\right) F_{p'\ell}$$
$$H^{(0)}_{pq} G_{q\ell} = \left(E\delta_{pp'} - H^{(0)}_{pp'}\right) G_{p'\ell} + \beta\delta_{0p}$$

Summations over infinite Q-space can be converted to summations over finite P-space.

We are left with only P-space quantities that are known (semi-) analytically.

$$\tan\delta_\ell = -\frac{F_{N\ell} - \mathcal{G}_{Np}\left(EF_{p\ell} - H^{(0)}_{pp'}F_{p'\ell}\right)}{G_{N\ell} - \mathcal{G}_{Np}\left((E + \beta\delta_{0p})G_{p\ell} - H^{(0)}_{pp'}G_{p'\ell}\right)}$$

Does it work?



Woods-Saxon potential phase shifts converge with increasing size of basis.

Extrapolate resonance positions and widths from smaller calculations?

Can we modify matrix elements to accelerate convergence?

Note: We never specified a basis.

Why Harmonic Oscillator then?

Simple answer: Translational Invariance of Many-Body wave function.

Our goal is to describe scattering with clusters; we need to maintain translational invariance when constructing the relative motion channels.

Many-body channels are no longer orthogonal.

$$\mathcal{H}_{\mathcal{P}\mathcal{P}'}\Psi_{\mathcal{P}'} + \mathcal{H}^{(0)}_{\mathcal{P}\mathcal{Q}}\Psi_{\mathcal{Q}} = E\mathcal{N}_{\mathcal{P}\mathcal{P}'}\Psi_{\mathcal{P}'}$$

Norm Kernel imposes a second limit to the matching “radius”.

But first...

$$b_\mu^\dagger = \frac{1}{\sqrt{2m\omega\hbar}}(m\omega r_\mu - ip_\mu)$$

$$r_\mu = \sqrt{\frac{\hbar}{2m\omega}}(b_\mu^\dagger + b_\mu)$$

Many body case

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

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

Control single cluster
CM quantum numbers

ℓ, m with $\mathcal{B}_m^\dagger$

nodes with $\left[\mathcal{B}^\dagger \times \mathcal{B}^\dagger\right]_0^{(0)}$

$\mathcal{L}_m = \left[\mathcal{B}^\dagger \times \mathcal{B}\right]_m^{(1)}$

Recouple CM excited clusters
with Moshinsky Brackets

$$\psi_0(\mathbf{R})\mathcal{A}\psi_{n\ell\mu}(\rho)\Psi'_\alpha\Psi'_{\mathrm{D}} = \mathcal{A}\sum_{\substack{n_1 l_1\\ n_2 l_2}} \mathcal{M}^{n\ell 00;\ell}_{n_1 l_1 n_2 l_2}\left[\psi_{n_1 l_1}(\mathbf{R}_\alpha) \times \psi_{n_2 l_2}(\mathbf{R}_{\mathrm{D}})\right]^\ell_\mu \Psi'_\alpha\Psi'_{\mathrm{D}}$$

Many-body basis channels constructed with the boosting method are translationally invariant, fully antisymmetric and have definite HO relative motion.

Back to treating the Norm Kernel

$$\mathcal{H}_{\mathcal{P}\mathcal{P}'}\Psi_{\mathcal{P}'} + \mathcal{H}^{(0)}_{\mathcal{P}\mathcal{Q}}\Psi_{\mathcal{Q}} = E\mathcal{N}_{\mathcal{P}\mathcal{P}'}\Psi_{\mathcal{P}'}$$

The P-Space resolvent now becomes:

$$\mathcal{G}_{pp'} = \left[(E\mathcal{N} - H)^{-1}\right]_{pp'}$$

Need to be careful about summation only over Pauli allowed channels.

No change for asymptotic amplitudes F, G (only reduced mass).

Asymptotic matching:
Outside the matching "radius" assume Norm Kernel is Unit Matrix

$$\Psi_{\mathcal{Q}} = aF_{\mathcal{Q}} + bG_{\mathcal{Q}}$$

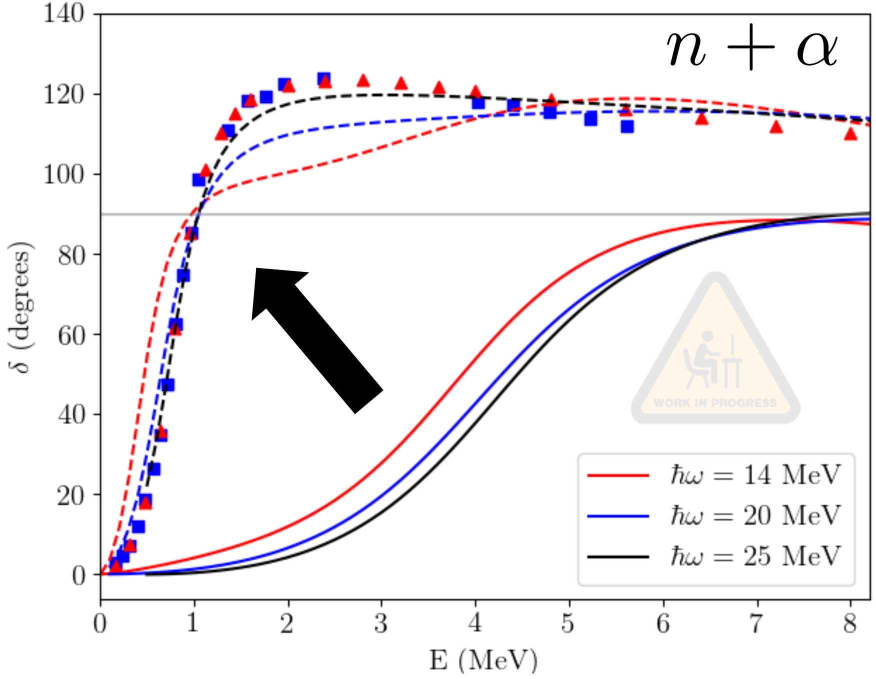
$$\mathcal{G}_{Np}H^{(0)}_{pq}F_q = \mathcal{G}_{Np}(EF_p - H^{(0)}_{pp'}F_{p'})$$

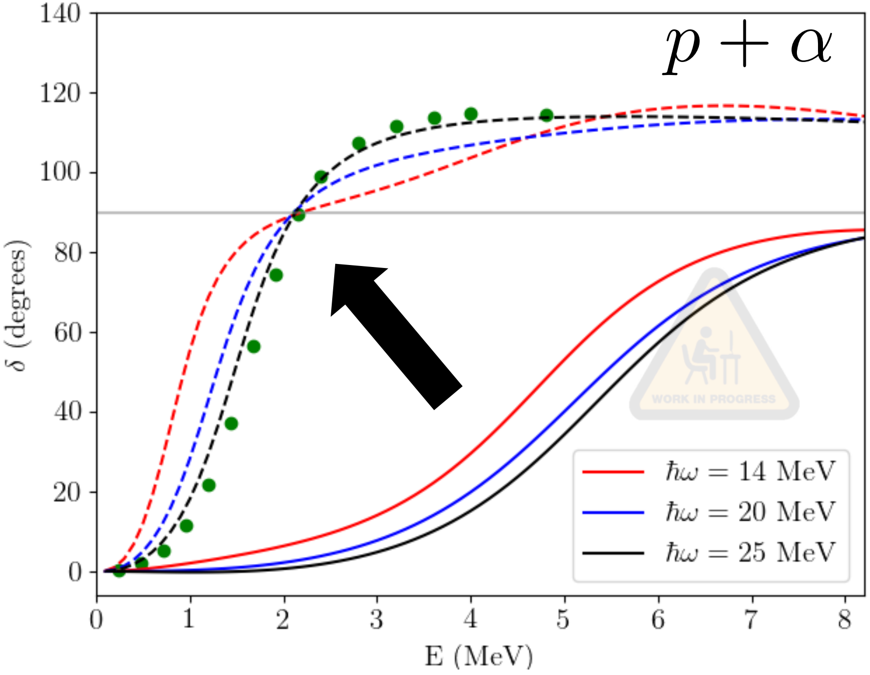
This P-Space summation has no forbidden channels

Internal part of matching

$$\Psi_N = \mathcal{N}^{-1/2}_{Np}\left(aF_p + bG_p\right)$$

Does it still work?

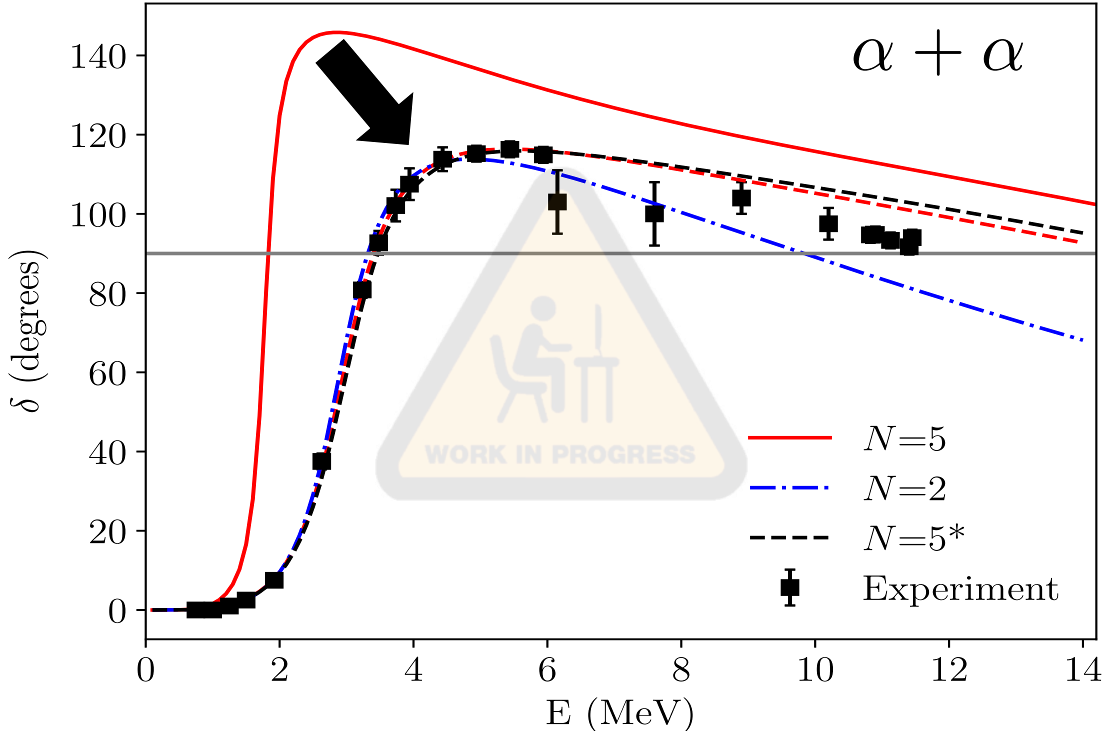




Experiment: Phys. Rev. 168, 1114 (1968)
Nucl. Phys. A287, 317 (1977)

Experiment: Nucl. Phys. A180, 225(1972)

What about heavier systems?



RGM Hamilton Kernel is heavily tri-diagonal

$$\begin{pmatrix} -31.8 & 21.9 & 0.15 & 0.50 & 0.03 \\ 21.9 & 6.12 & 38.0 & 0.40 & 0.77 \\ 0.15 & 38.0 & 41.0 & 53.6 & 0.67 \\ 0.50 & 0.40 & 53.6 & 73.4 & 68.5 \\ 0.03 & 0.77 & 0.67 & 68.5 & 104 \end{pmatrix}$$

Do the small off-tridiagonal matrix elements affect dynamics?

Experiment: Rev. Mod. Phys. 41, 247 (1969)

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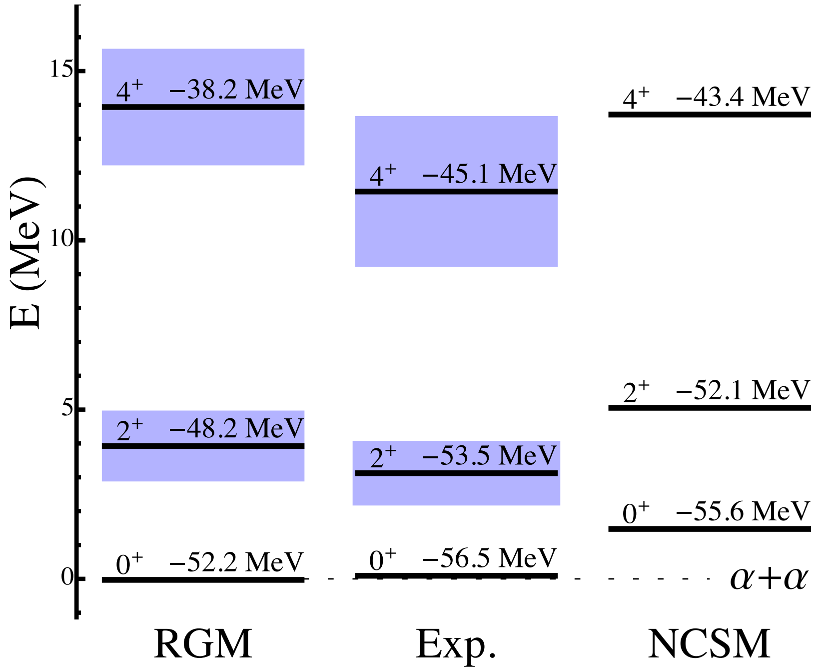
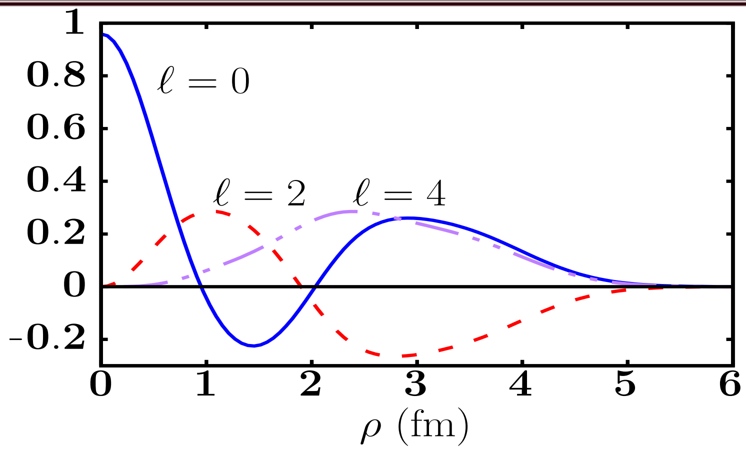
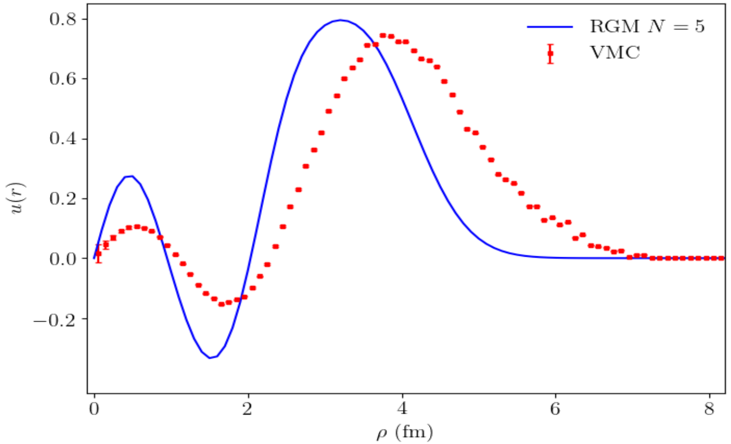
$$\Gamma = 2P_L(\rho_c)|g(\rho_c)|^2$$



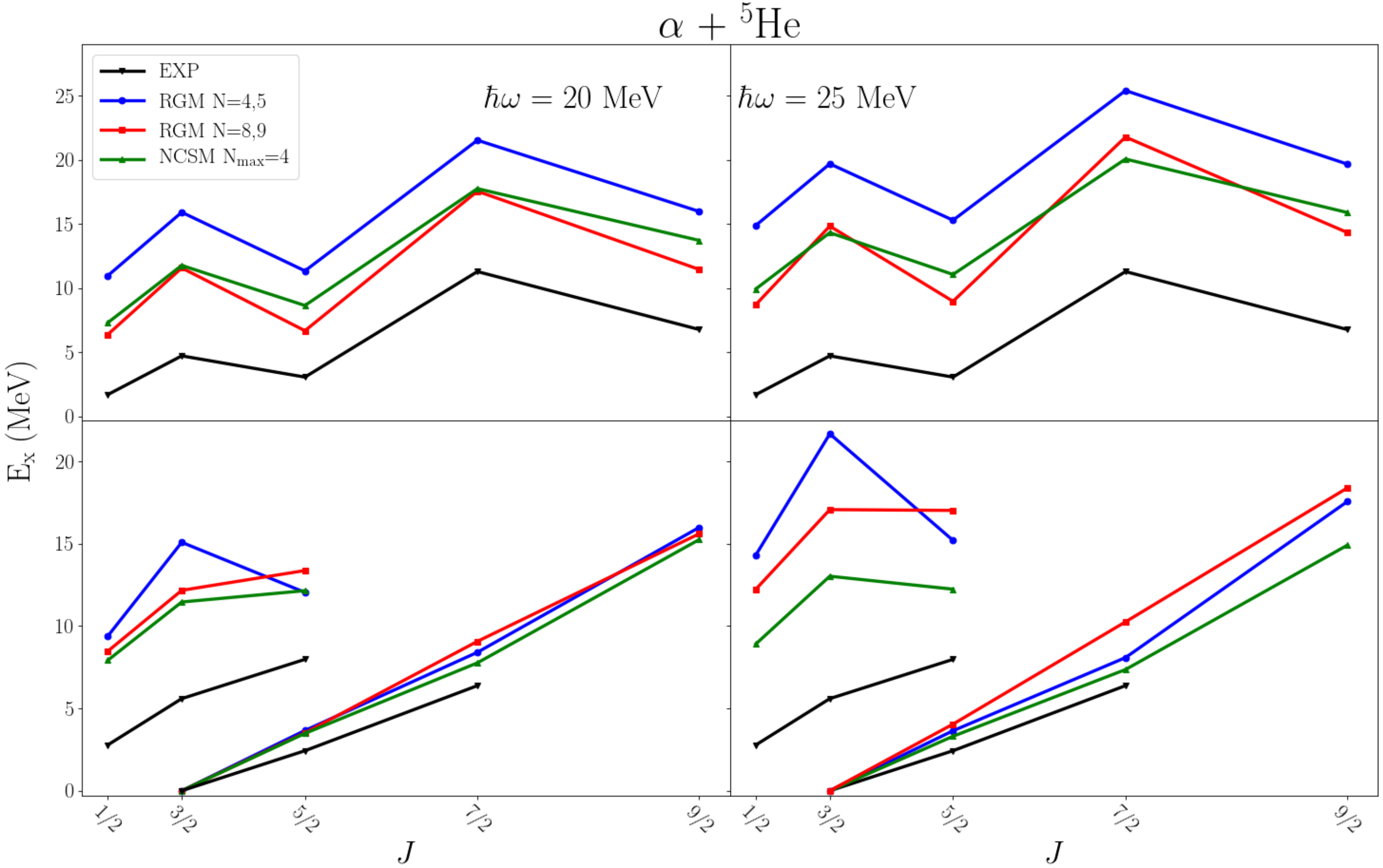




https://www.phy.anl.gov/theory/research/overlap_old/be8.aa

Reactions with Clusters in Harmonic Oscillator Basis

Need full three body extension for proper scattering study.



Summary:

- Successfully treated Coulomb part of the interaction in a square integrable basis expansion
- Using the boosting method, constructed many-body channels and evaluated phase shifts.

Outlook:

- Multi-channel S-matrix
- Ternary cluster systems

Coulomb wave functions:
Michel, CPC 176, 232 (2007)

Some References:

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Thanks to:
Theory: A. Volya, A. Shirokov, R. Wiringa
Interactions: J. Vary