Microscopic R-Matrix approaches

FRIB-Theory Alliance workshop: From bound states to the continuum

Connecting bound state calculations with scattering and reaction theory

Sofia Quaglioni

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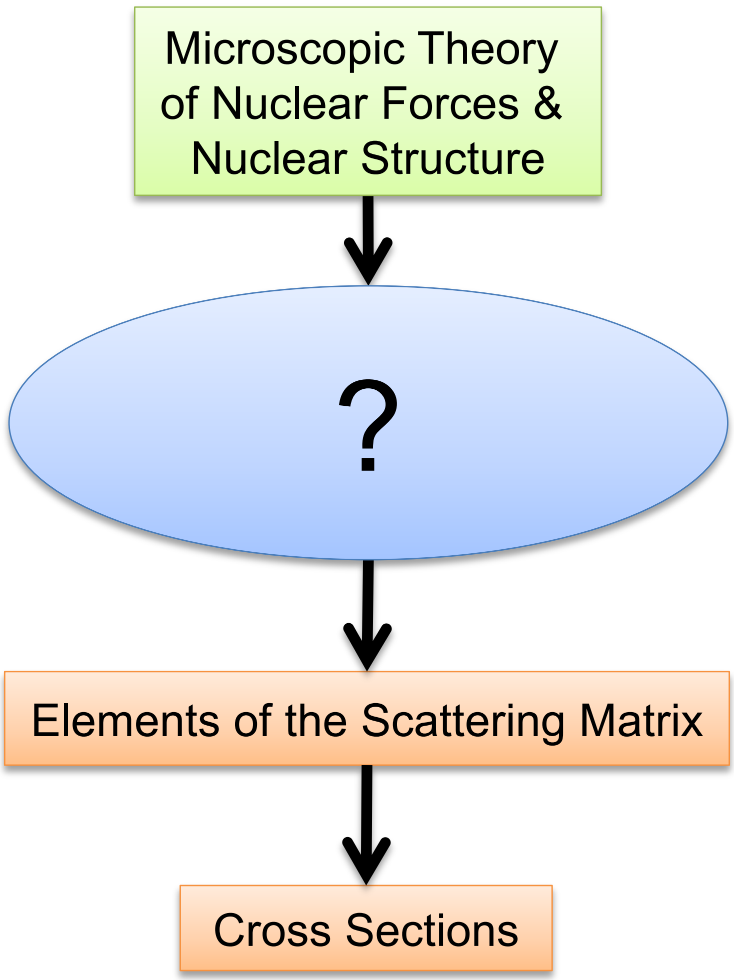
Content



- R-Matrix theory
- Resonating Group Method
  - Implemented within the no-core shell model
  - No-core shell model with continuum
- Generator Coordinate Method
- Microscopic R-Matrix combined with Density Functional Theory

R-Matrix theory provides a rigorous framework for bridging *ab initio* many-body and collision theory

Known interactions in external region (Coulomb functions)

Projectile-Target interactions in the internal Region

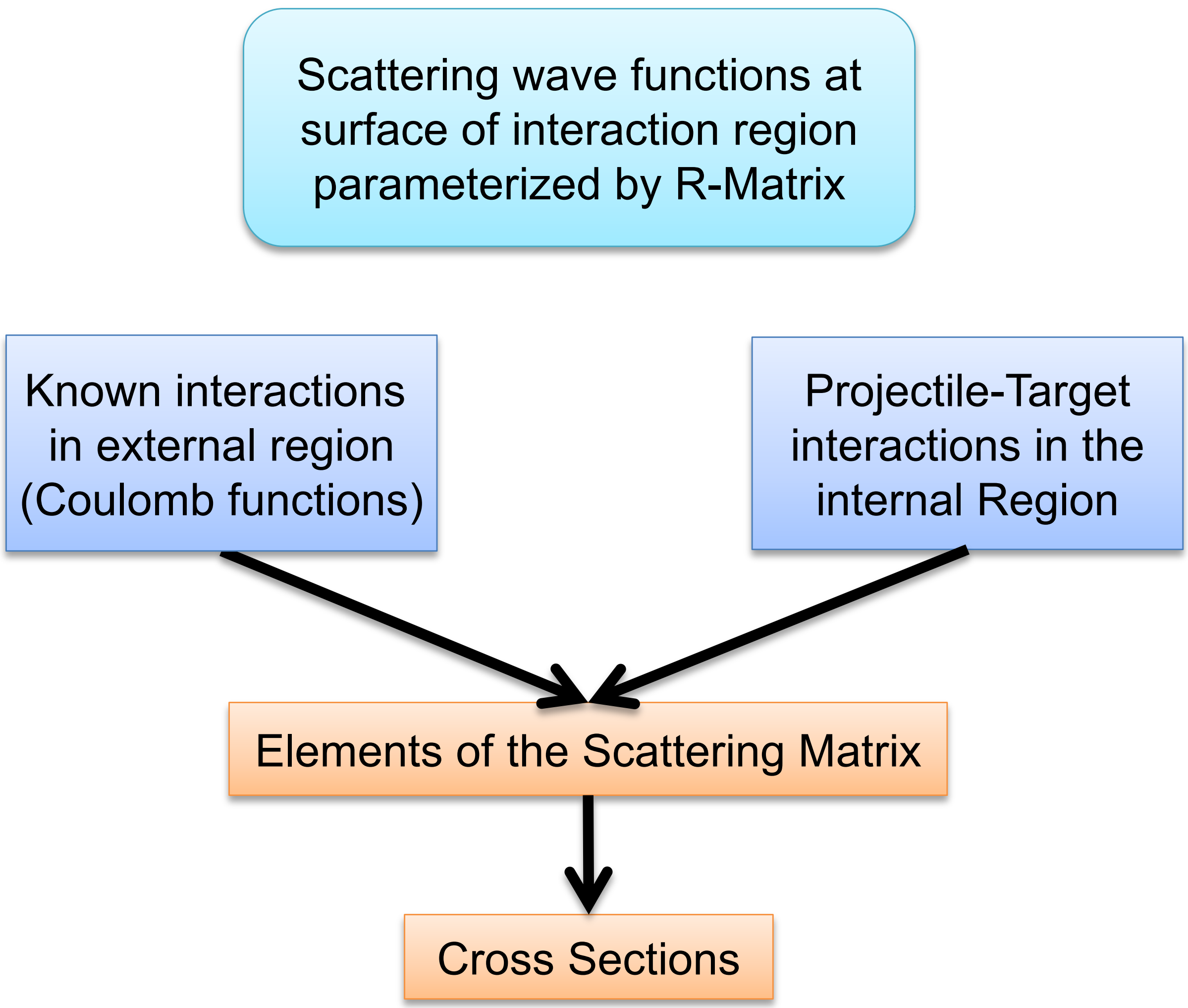
↓

Elements of the Scattering Matrix

↓

Cross Sections

R-Matrix theory provides a rigorous framework for bridging *ab initio* many-body and collision theory



In its phenomenological incarnation experimental cross sections are fitted in terms of the R-matrix parameters

<u>Phenomenological R-Matrix:</u>

Set of parameters completely defining the R-matrix

Known interactions in external region (Coulomb functions)

Projectile-Target interactions in the internal Region

Elements of the Scattering Matrix

Cross Sections

Vary parameters until best fit of experimental cross sections

The values and properties of the R-matrix parameters can be predicted on the basis of a microscopic theory

<u>Microscopic R-Matrix:</u>

Microscopic Theory of Nuclear Forces & Nuclear Structure

↓

Known interactions in external region (Coulomb functions)

Projectile-Target interactions in the internal Region

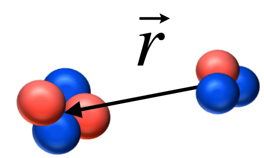
↓

Elements of the Scattering Matrix

↓

Cross Sections

Need an approach to describe dynamics between clusters of nucleons



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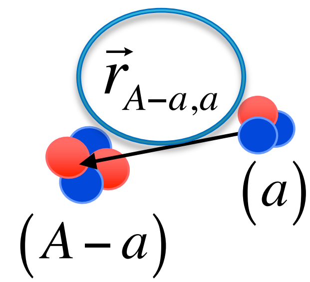
e.g.: Resonating Group Method

Binary Cluster Resonating Group Method

- Trial wave function ($\nu \equiv \left\{A-a\ \alpha_1 I_1^{\pi_1} T_1; a\ \alpha_2 I_2^{\pi_2} T_2; s\ell\right\}$):

$$|\Psi^{J^\pi T}\rangle = \sum_\nu \int dr\, r^2 \frac{\gamma_\nu^{J^\pi T}(r)}{r} \hat{\mathcal{A}}_\nu \, |\Phi_{\nu r}^{J^\pi T}\rangle$$



Relative vector

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

Binary Cluster Resonating Group Method

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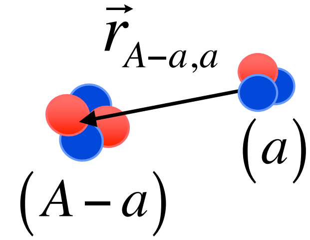

Translational invariant channel basis

$$|\Phi_{\nu r}^{J^\pi T}\rangle = \boxed{\left[\left(\left| A-a\ \alpha_1 I_1^{\pi_1} T_1 \right\rangle \left| a\ \alpha_2 I_2^{\pi_2} T_2 \right\rangle \right)^{(sT)} Y_\ell(\hat{r}_{A-a,a}) \right]^{(J^\pi T)} \frac{\delta(r - r_{A-a,a})}{r r_{A-a,a}}}$$

- Target and projectile wave functions are **both translational invariant**

Binary Cluster Resonating Group Method

- Trial wave function ($\nu \equiv \left\{A-a\ \alpha_1 I_1^{\pi_1} T_1; a\ \alpha_2 I_2^{\pi_2} T_2; s\ell\right\}$):

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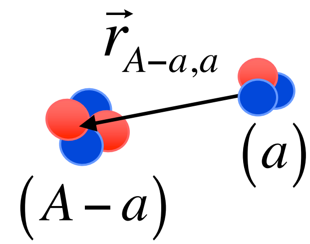


Inter-cluster antisymmetrizer

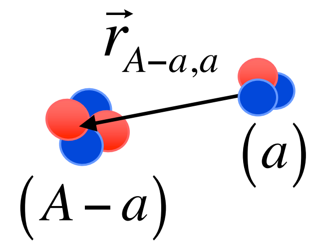
$$\hat{\mathcal{A}}_\nu = \sqrt{\frac{(A-a)!a!}{A!}} \left(1 + \sum_{P \neq id} (-)^p P\right)$$

- Antisymmetrizes wave function for exchanges of nucleons across clusters
- Note that $\vec{r}_{A-a,a}$ changes under the action of the antisymmetrizer

Binary Cluster Resonating Group Method

- Trial wave function ($\nu \equiv \left\{A-a\ \alpha_1 I_1^{\pi_1} T_1; a\ \alpha_2 I_2^{\pi_2} T_2; s\ell\right\}$):

$$|\Psi^{J^\pi T}\rangle = \sum_\nu \int dr\, r^2 \frac{\gamma_\nu^{J^\pi T}(r)}{r} \hat{\mathcal{A}}_\nu \, |\Phi_{\nu r}^{J^\pi T}\rangle$$



Unknown amplitudes

RGM equations

$$\sum_\nu \int dr\, r^2 \left[\mathcal{H}_{\nu'\nu}^{J^\pi T}(r',r) - E\, \mathcal{N}_{\nu'\nu}^{J^\pi T}(r',r)\right] \frac{\gamma_\nu^{J^\pi T}(r)}{r} = 0$$

$$\left\langle \Phi_{\nu' r'}^{J^\pi T} \right| \hat{\mathcal{A}}_{\nu'} H \hat{\mathcal{A}}_\nu \left| \Phi_{\nu r}^{J^\pi T} \right\rangle \qquad \left\langle \Phi_{\nu' r'}^{J^\pi T} \right| \hat{\mathcal{A}}_{\nu'} \hat{\mathcal{A}}_\nu \left| \Phi_{\nu r}^{J^\pi T} \right\rangle$$

Hamiltonian kernel **Overlap (or norm) kernel**

Solving the RGM equations …

- The RGM equations can be orthogonalized (see PRC 79, 044606)

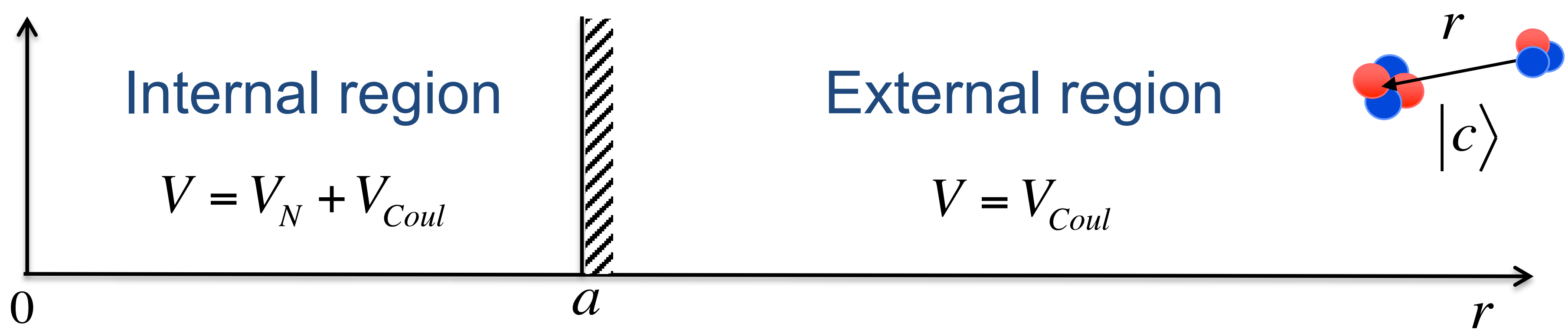
$$\sum_{\nu'} \int dr' r'^2 \left[N^{-\frac{1}{2}} H N^{-\frac{1}{2}} \right]_{\nu\nu'} (r,r') \frac{u_{\nu'}(r')}{r'} = E \frac{u_\nu(r)}{r}$$

  - This removes the energy dependence from the 'effective' projectile-target potential (see below)

- In the end, one is left with a set of integral-differential coupled channel equations with a non-local potential of the type:

$$\left[T_{rel}(r) + \bar{V}_{Coul}(r) - \underbrace{(E - \varepsilon_{\alpha_1} - \varepsilon_{\alpha_2})}_{E_\nu} \right] u_\nu(r) + \sum_{\nu'} \int dr' r' \; W_{\nu\nu'}(r,r') \; u_{\nu'}(r') = 0$$

… with the R-Matrix method



Expansion on a basis (square-integrable)

$$u_c(r) = \sum_n A_{cn} f_n(r)$$

Bound state asymptotic behavior

$$u_c(r) = C_c W(k_c r)$$

Scattering state asymptotic behavior

$$u_c(r) = \frac{i}{2} v_c^{-\frac{1}{2}} \left[\delta_{ci} I_c(k_c r) - S_{ci} O_c(k_c r)\right]$$

… with the R-Matrix method

- R-matrix formalism conveniently expressed with the help of the Bloch surface operator

$$L_c = \frac{\hbar^2}{2\mu_c}\delta(r-a)\left(\frac{d}{dr} - \frac{B_c}{r}\right)$$

Boundary parameters

- System of Bloch-Schrödinger equations:

$$\left[\hat{T}_{rel}(r) + L_c + \overline{V}_{Coul}(r) - (E - E_c)\right] u_c(r) + \sum_{c'} \int dr'\, r' W_{cc'}(r,r')\, u_{c'}(r') = L_c u_c(r)$$

$$u_c(r) = \sum_n A_{cn} f_n(r)$$

asymptotic form for large r

… with the R-Matrix method

- We can choose:

$$B_c = k_c a \frac{W'(k_c a)}{W(k_c a)} \Rightarrow L_c u_c^{ext}(r) = 0$$

- After projection (from the left) on the basis $f_n(r)$:

$$\sum_{c'n'} \left[C_{cn,c'n'} - E\, \delta_{cn,c'n'} \right] A_{c'n'} = 0$$

$$\boxed{\left\langle f_n \middle| \hat{T}_{rel}(r) + L_c + \bar{V}_{Coul}(r) \middle| f_{n'} \right\rangle \delta_{cc'} + \left\langle f_n \middle| W_{cc'}(r,r') \middle| f_{n'} \right\rangle}$$

Bound states

- We can choose:

$$B_c = k_c a \frac{W'(k_c a)}{W(k_c a)} \Rightarrow L_c u_c^{ext}(r) = 0$$

- After projection (from the left) on the basis $f_n(r)$:

$$\sum_{c'n'} \left[C_{cn,c'n'} - E\,\delta_{cn,c'n'} \right] A_{c'n'} = 0$$

Eigenvalue problem

- Start with $E = 0$ and solve iteratively (k_c depends on the energy!)

- Convergence in few iterations

Scattering states

- We can choose: $B_c = 0$

- After projection (from the left) on the basis $f_n(r)$:

$$\sum_{c'n'} \left[C_{cn,c'n'} - (E - E_c)\delta_{cn,c'n'} \right] A_{c'n'} = \frac{\hbar^2 k_c}{2\mu_c v_c^{1/2}} \left\langle f_n \middle| L_c \middle| I_c \delta_{ci} - S_{ci} O_c \right\rangle$$

1) Solve for A_{cn}

2) Match internal and external solutions at channel radius, *a*

$$\sum_{c'} R_{cc'} \frac{k_{c'} a}{\sqrt{\mu_{c'} v_{c'}}} \left[I'_{c'}(k_{c'}a)\delta_{ci} - S_{c'i} O'_{c'}(k_{c'}a) \right] = \frac{1}{\sqrt{\mu_c v_c}} \left[I_c(k_c a)\delta_{ci} - S_{ci} O_c(k_c a) \right]$$

Scattering states

- In the process introduce R-matrix, projection of the Green's function operator on the channel-surface functions

$$R_{cc'} = \sum_{nn'} \frac{\hbar}{\sqrt{2\mu_c a}} f_n(a) \left[C - EI\right]^{-1}_{cn,c'n'} \frac{\hbar}{\sqrt{2\mu_{c'} a}} f_{n'}(a)$$

3) Solve for the scattering matrix: $S = Z^{-1} Z^{*}$

with: $Z_{cc'} = \left(k_{c'} a\right)^{-1} \left[O_c(k_c a)\delta_{cc'} - k_{c'} a \, R_{cc'} \; O'_{c'}(k_{c'} a)\right]$

- Phase shifts, cross sections are computed from the scattering matrix

Scattering states

- The R-matrix takes a simple pole-expansion form, in terms of energy levels E_λ and (energy independent) partial widths $\gamma_{\lambda c}$

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E} \quad \text{with} \quad \gamma_{\lambda c} = \sum_{nn'} \frac{\hbar}{\sqrt{2\mu_c a}} f_n(a) B_{cn,\lambda}$$

Change from f_n basis to eigenvectors of matrix C

3) Solve for the scattering matrix: $S = Z^{-1}Z^*$

with: $Z_{cc'} = \left(k_{c'}a\right)^{-1}\left[O_c(k_c a)\delta_{cc'} - k_{c'}a\, R_{cc'}\; O'_{c'}(k_{c'}a)\right]$

- Phase shifts, cross sections are computed from the scattering matrix

Scattering states

- The R-matrix takes a simple pole-expansion form, in terms of energy levels E_λ and (energy independent) partial widths $\gamma_{\lambda c}$

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E}$$

In phenomenological theory:
E_λ and $\gamma_{\lambda c}$ used as fitting parameters
(typically use a few channels)

3) Solve for the scattering matrix: $S = Z^{-1} Z^*$

with: $Z_{cc'} = \left(k_{c'}a\right)^{-1}\left[O_c(k_c a)\delta_{cc'} - k_{c'}a\, R_{cc'}\ O'_{c'}(k_{c'}a)\right]$

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Scattering states

- The R-matrix takes a simple pole-expansion form, in terms of energy levels E_λ and (energy independent) partial widths $\gamma_{\lambda c}$

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E}$$

In *ab initio* theory:
E_λ and $\gamma_{\lambda c}$ computed from first principles
(typically large number of channels)

3) Solve for the scattering matrix: $S = Z^{-1} Z^*$

with: $Z_{cc'} = \left(k_{c'}a\right)^{-1}\left[O_c(k_c a)\delta_{cc'} - k_{c'}a\, R_{cc'}\ O'_{c'}(k_{c'}a)\right]$

- Phase shifts, cross sections are computed from the scattering matrix

If target and projectile are obtained within the *ab initio* NCSM, one arrives at the *ab initio* NCSM/RGM approach

- Jacobi channel states in the harmonic oscillator (HO) space:

$$\left|\Phi^{J^\pi T}_{\nu n}\right\rangle = \left[\left(\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle \left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle\right)^{(sT)} Y_\ell(\hat{r}_{A-a,a})\right]^{(J^\pi T)} R_{n\ell}(r_{A-a,a})$$

- Notes:
  - Formally, the coordinate space channel sates given by:

$$\left|\Phi^{J^\pi T}_{\nu r}\right\rangle = \sum_n R_{n\ell}(r) \left|\Phi^{J^\pi T}_{\nu n}\right\rangle$$

    – I used the closure properties of HO radial wave functions

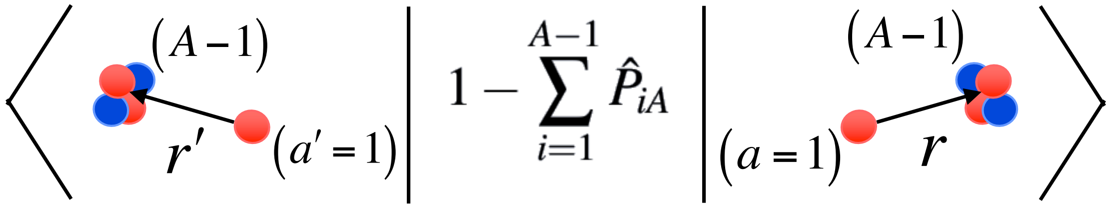
$$\delta(r - r_{A-a,a}) = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

  - Again: target and projectile are both translational invariant eigenstates
    – Works for the projectiles up to ^{4}He
    – Not practical if we want to describe reactions with p-shell targets!

In practice, expansion is truncated and is only used for short-range components of NCSM/RGM kernels

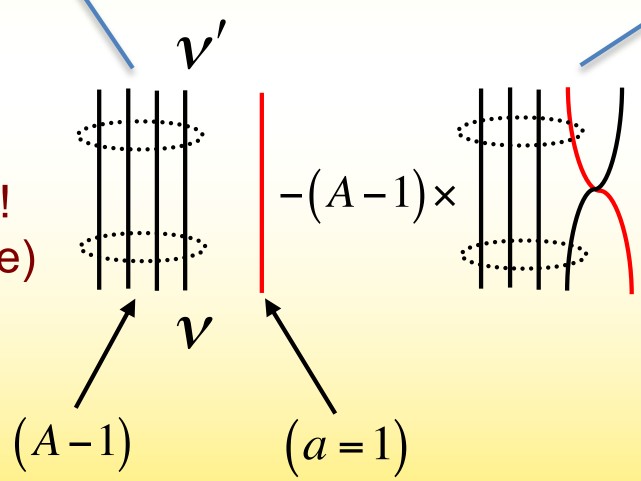
An example: the RGM norm kernel for nucleon-nucleus channel states

$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} \hat{A}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle =$$



$$N^{\text{RGM}}_{\nu'\nu}(r',r) = \delta_{\nu'\nu}\frac{\delta(r'-r)}{r'r} - (A-1)\sum_{n'n} R_{n'\ell'}(r')R_{n\ell}(r)\left\langle \Phi^{J^\pi T}_{\nu' n'} \middle| \hat{P}_{A-1,A} \middle| \Phi^{J^\pi T}_{\nu n} \right\rangle$$

Direct term:
Treated exactly!
(in the full space)



Exchange term:
Obtained in the model space!
(**Short-range** many-body correction due to the exchange of particles)

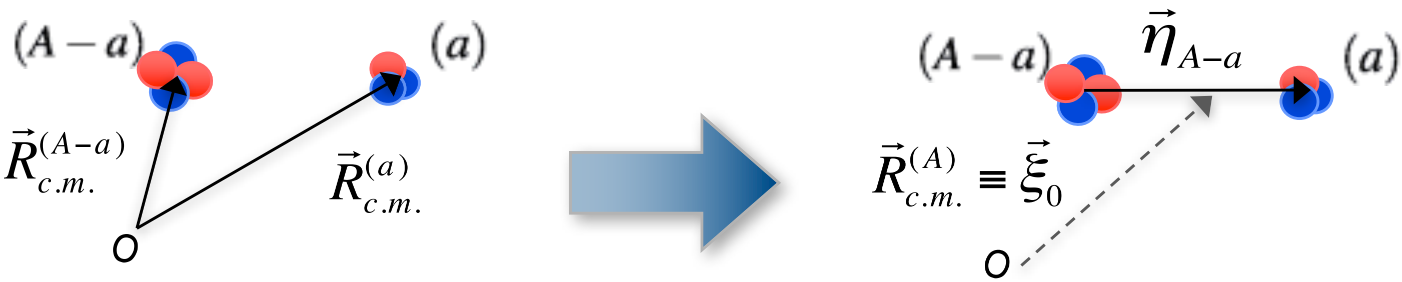
$$\delta(r-r_{A-a,a}) = \sum_n R_{n\ell}(r)R_{n\ell}(r_{A-a,a})$$

Define Slater-Determinant (SD) channel states in which the target is described by a SD eigenstates

$$\left|\Phi^{J^\pi T}_{\nu n}\right\rangle_{SD} = \Bigg[\Big(\underbrace{\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle_{SD}}_{\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle \varphi_{00}\left(\vec{R}^{(A-a)}_{c.m.}\right)} \left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle\Big)^{(sT)} Y_\ell\left(\hat{R}^{(a)}_{c.m.}\right)\Bigg]^{(J^\pi T)} R_{n\ell}\left(R^{(a)}_{c.m.}\right)$$

Vector proportional to the c.m. coordinate of the A-a nucleons

Vector proportional to the c.m. coordinate of the a nucleons



$$\left(\varphi_{00}\left(\vec{R}^{(A-a)}_{c.m.}\right)\varphi_{n\ell}\left(\vec{R}^{(a)}_{c.m.}\right)\right)^{\ell} = \sum_{n_r \ell_r, NL} \left\langle 00, n\ell, \ell \middle| n_r \ell_r, NL, \ell\right\rangle_{d=\frac{a}{A-a}} \left(\varphi_{n_r \ell_r}\left(\vec{\eta}_{A-a}\right)\varphi_{NL}\left(\vec{\xi}_0\right)\right)^{\ell}$$

c.m. motion

In this ‘SD’ channel basis, translation-invariant matrix elements are mixed with c.m. motion …

- More in detail:

c.m. motion

$$\left|\Phi^{J^\pi T}_{\nu n}\right\rangle_{SD} = \sum_{n_r \ell_r, NL, J_r} \hat{\ell}\hat{J}_r (-1)^{s+\ell_r+L+J} \begin{Bmatrix} s & \ell_r & J_r \\ L & J & \ell \end{Bmatrix} \langle 00, n\ell, \ell | n_r \ell_r, NL, \ell \rangle_{d=\frac{a}{A-a}} \left[\left|\Phi^{J_r^\pi T}_{\nu_r n_r}\right\rangle \varphi_{NL}(\vec{\xi}_0) \right]^{(J^\pi T)}$$

- The spurious motion of the c.m. is mixed with the intrinsic motion

$$\boxed{{}_{SD}\left\langle \Phi^{J^\pi T}_{\nu' n'} \left| \hat{O}_{t.i.} \right| \Phi^{J^\pi T}_{\nu n} \right\rangle_{SD}} = \sum_{n_r' \ell_r', n_r \ell_r, J_r} \left\langle \Phi^{J_r^\pi T}_{\nu_r' n_r'} \left| \hat{O}_{t.i.} \right| \Phi^{J_r^\pi T}_{\nu_r n_r} \right\rangle$$

Interested in this

$$\boxed{\begin{aligned} &\times \sum_{NL} \hat{\ell}\hat{\ell}'\hat{J}_r^2 (-1)^{s+\ell-s'-\ell'} \begin{Bmatrix} s & \ell_r & J_r \\ L & J & \ell \end{Bmatrix} \begin{Bmatrix} s' & \ell_r' & J_r \\ L & J & \ell' \end{Bmatrix} \\ &\times \langle 00, n\ell, \ell | n_r \ell_r, NL, \ell \rangle_{d=\frac{a}{A-a}} \langle 00, n'\ell', \ell' | n_r' \ell_r', NL, \ell' \rangle_{d'=\frac{a'}{A-a'}} \end{aligned}}$$

Compute these

… but they can be extracted exactly from the 'SD' matrix elements by applying the inverse of the mixing matrix

- More in detail:

c.m. motion

$$\left|\Phi^{J^\pi T}_{\nu n}\right\rangle_{SD} = \sum_{n_r \ell_r, NL, J_r} \hat{\ell}\hat{J}_r (-1)^{s+\ell_r+L+J} \begin{Bmatrix} s & \ell_r & J_r \\ L & J & \ell \end{Bmatrix} \langle 00, n\ell, \ell | n_r \ell_r, NL, \ell \rangle_{d=\frac{a}{A-a}} \left[\left|\Phi^{J_r^{\pi_r} T}_{\nu_r n_r}\right\rangle \varphi_{NL}(\vec{\xi}_0) \right]^{(J^\pi T)}$$

- The spurious motion of the c.m. is mixed with the intrinsic motion

Matrix inversion

$${}_{SD}\left\langle \Phi^{J^\pi T}_{f_{SD}} \middle| \hat{O}_{t.i.} \middle| \Phi^{J^\pi T}_{i_{SD}} \right\rangle_{SD} = \sum_{i_R f_R} M^{J^\pi T}_{i_{SD} f_{SD}, i_R f_R} \left\langle \Phi^{J^\pi T}_{f_R} \middle| \hat{O}_{t.i.} \middle| \Phi^{J^\pi T}_{i_R} \right\rangle$$

Calculate these

Interested in these

Working within the 'SD' channel basis we can access reactions involving p-shell targets

- Can use second quantization representation
  - Matrix elements of translational operators can be expressed in terms matrix elements of density operators on the target eigenstates
  - E.g., the matrix elements appearing in the RGM norm kernel for nucleon-nucleus channel states:

$$
{}_{SD}\left\langle \Phi^{J^\pi T}_{\nu' n'} \middle| P_{A-1,A} \middle| \Phi^{J^\pi T}_{\nu n} \right\rangle_{SD} = \frac{1}{A-1} \sum_{jj'K\tau} \hat{s}\hat{s}'\hat{j}\hat{j}'\hat{K}\hat{\tau} (-1)^{I_1'+j'+J} (-1)^{T_1+\frac{1}{2}+T}
$$

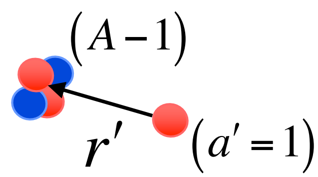
$$
\times \begin{Bmatrix} I_1 & \frac{1}{2} & s \\ \ell & J & j \end{Bmatrix} \begin{Bmatrix} I_1' & \frac{1}{2} & s' \\ \ell' & J & j' \end{Bmatrix} \begin{Bmatrix} I_1 & K & I_1' \\ j' & J & j \end{Bmatrix} \begin{Bmatrix} T_1 & \tau & T_1' \\ \frac{1}{2} & T & \frac{1}{2} \end{Bmatrix}
$$

One-body density matrix elements

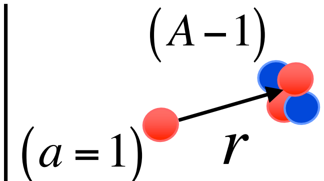
$$
\times \boxed{ {}_{SD}\left\langle A-1\ \alpha_1' I_1'^{\pi_1'} T_1' \middle\| \left(a^{+}_{n\ell j \frac{1}{2}} \tilde{a}_{n'\ell' j' \frac{1}{2}} \right)^{(K\tau)} \middle\| A-1\ \alpha_1 I_1^{\pi_1} T_1 \right\rangle_{SD} }
$$

The RGM (2-body) Hamiltonian kernel for nucleon-nucleus channel states

$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \left| \hat{A}_{\nu'} H \hat{A}_{\nu} \right| \Phi^{J^\pi T}_{\nu r} \right\rangle = \Bigg\langle$$



$$\left| H \left(1 - \sum_{i=1}^{A-1} \hat{P}_{iA} \right) \right|$$

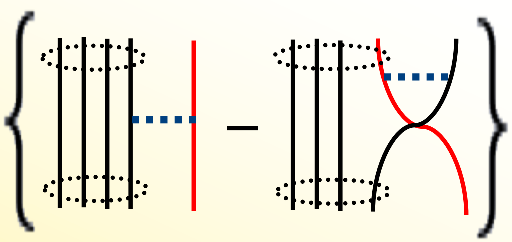
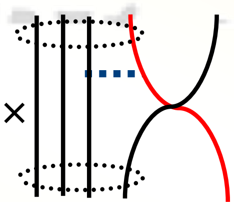


$$\Bigg\rangle$$

$$H^{J^\pi T}_{\nu'\nu}(r',r) = \left[T_{rel}(r) + \bar{V}_{Coul}(r) + \varepsilon^{I_1'^{\pi_1'} T_1'}_{\alpha_1'} \right] N^{J^\pi T}_{\nu'\nu}(r',r)$$

$$+ (A-1) \sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \left| V_{A-1,A} \left(1 - \hat{P}_{A-1,A} \right) \right| \Phi^{J^\pi T}_{\nu n} \right\rangle$$

$$- (A-1)(A-2) \sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \left| \hat{P}_{A-1,A} V_{A-2,A-1} \right| \Phi^{J^\pi T}_{\nu n} \right\rangle$$

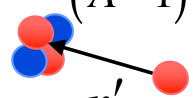
$+(A-1)\times$  $-(A-1)(A-2)\times$ 

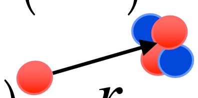
Direct potential: in the model space (interaction is locaized!)

Exchange potential: in the model space

The RGM (2-body) Hamiltonian kernel for nucleon-nucleus channel states

$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} H \hat{A}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left\langle (A-1) \;\; r' \;\; (a'=1) \middle| H\left(1-\sum_{i=1}^{A-1}\hat{P}_{iA}\right) \middle| (a=1) \;\; r \;\; (A-1) \right\rangle$$





$$H^{J^\pi T}_{\nu'\nu}(r',r) = \left[T_{rel}(r) + \bar{V}_{Coul}(r) + \varepsilon^{I_1'^{\pi_1'} T_1'}_{\alpha_1'}\right] N^{J^\pi T}_{\nu'\nu}(r',r)$$

$$+(A-1)\sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \middle| V_{A-1,A}\left(1-\hat{P}_{A-1,A}\right) \middle| \Phi^{J^\pi T}_{\nu n} \right\rangle$$

$$-(A-1)(A-2)\sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \middle| \hat{P}_{A-1,A} V_{A-2,A-1} \middle| \Phi^{J^\pi T}_{\nu n} \right\rangle$$

$$\propto \; {}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \middle| a^+ a \middle| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD} \qquad \propto \; {}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \middle| a^+ a^+ a a \middle| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

Direct potential: in the model space (interaction is localized!)

Exchange potential: in the model space

The RGM three-nucleon force kernel for nucleon-nucleus channel states

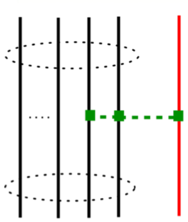
$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \right| \hat{A}_{\nu'} V^{NNN} \hat{A}_{\nu} \left| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left\langle \begin{matrix}(A-1)\\ r' \quad (a'=1)\end{matrix} \right| V^{NNN} \left(1 - \sum_{i=1}^{A-1} \hat{P}_{iA}\right) \left| \begin{matrix}(A-1)\\ (a=1) \quad r\end{matrix} \right\rangle$$

$$\mathcal{V}^{NNN}_{\nu'\nu}(r,r') = \sum R_{n'l'}(r') R_{nl}(r) \left[\frac{(A-1)(A-2)}{2} \langle \Phi^{J^\pi T}_{\nu' n'} | V_{A-2A-1A}(1 - 2P_{A-1A}) | \Phi^{J^\pi T}_{\nu n} \rangle \right.$$

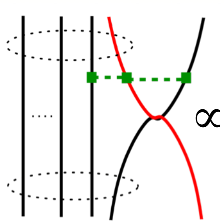
$$\left. -- \frac{(A-1)(A-2)(A-3)}{2} \langle \Phi^{J^\pi T}_{\nu' n'} | P_{A-1A} V_{A-3A-2A-1} | \Phi^{J^\pi T}_{\nu n} \rangle \right] .$$

Direct potential: in the model space (interaction is localized!)

Exchange potential: in the model space (interaction is localized!)

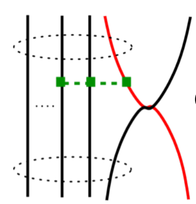


(a)



(b)

$$\propto {}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \right| a_i^+ a_j^+ a_l a_k \left| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

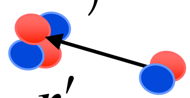


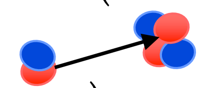
(c)

$$\propto {}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \right| a_h^+ a_i^+ a_j^+ a_m a_l a_k \left| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

The RGM norm kernel for deuteron-nucleus channel states

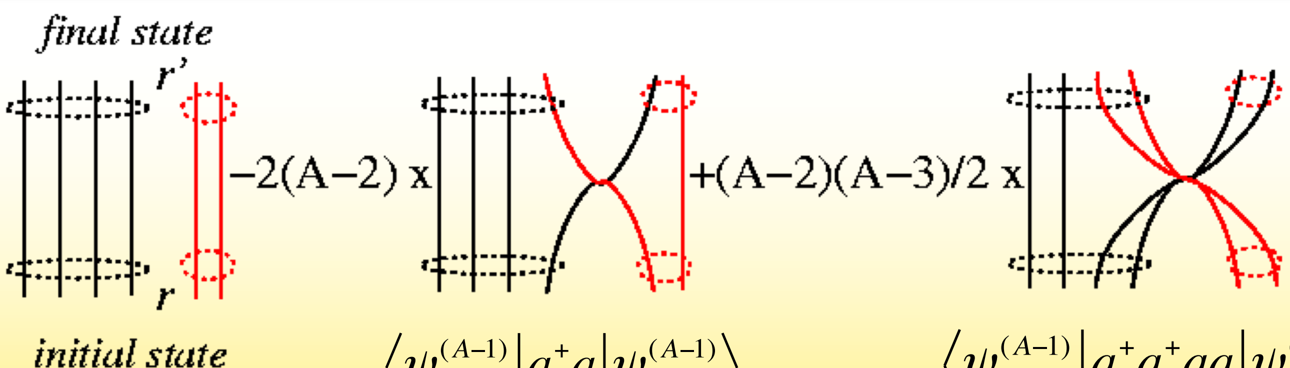
$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \right| \hat{A}_{\nu'} \hat{A}_{\nu} \left| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left\langle (A-2)\; r' \; (a'=2) \right| 1 - \sum_{i=1}^{A-2} \sum_{k=A-1}^{A} \hat{P}_{ij} + \sum_{i<j=1}^{A-2} \hat{P}_{i,A} \hat{P}_{j,A-1} \left| (a=2)\; r \; (A-2) \right\rangle$$





$$N^{J^\pi T}_{\nu'\nu}(r',r) = \delta_{\nu'\nu} \frac{\delta(r'-r)}{r'r} - 2(A-2) \sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \right| \hat{P}_{A-2,A} \left| \Phi^{J^\pi T}_{\nu n} \right\rangle$$

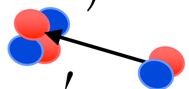
$$+ \frac{(A-2)(A-3)}{2} \sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \right| \hat{P}_{A-2,A} \hat{P}_{A-3,A-1} \left| \Phi^{J^\pi T}_{\nu n} \right\rangle$$



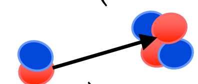
$${}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \right| a^+ a \left| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD} \qquad {}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \right| a^+ a^+ a a \left| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

The RGM (2-body) Hamiltonian kernel for deuteron-nucleus channel states

$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} H \hat{A}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left\langle (A-2) \right.$$

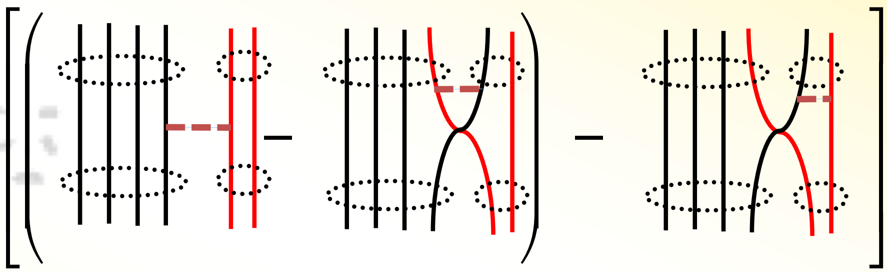


$$r' \quad (a'=2) \left| H \left(1 - \sum_{i=1}^{A-2} \sum_{k=A-1}^{A} \hat{P}_{ij} + \sum_{i<j=1}^{A-2} \hat{P}_{i,A} \hat{P}_{j,A-1} \right) \right| (A-2)$$



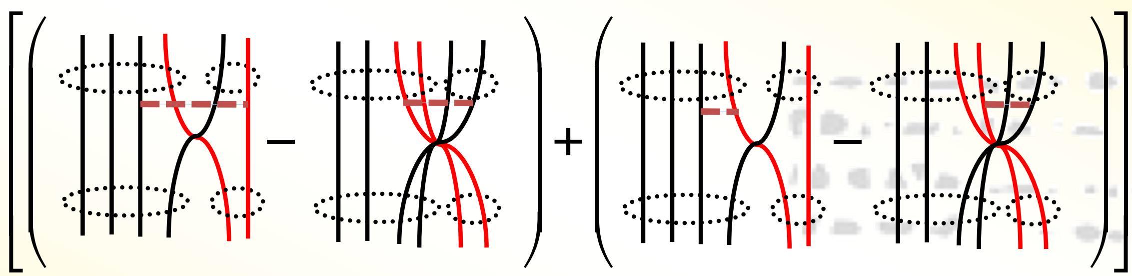
$$(a=2) \quad r \left. \right\rangle$$

$= 2(A-2)$



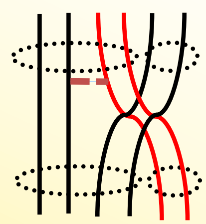
$${}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \middle| a^+ a \middle| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

$-2(A-2)(A-3)$



$${}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \middle| a^+ a^+ a a \middle| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

$+2(A-2)(A-3)(A-4)$



$${}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \middle| a^+ a^+ a^+ a a a \middle| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

Some considerations on the NCSM/RGM

1) Enables exact removal of spurious motion of the center of mass

2) Successfully applied to nucleon-nucleus, deuterium-nucleus, ^{3}H/^{3}He-nucleus collisions, (*d*,*N*) transfer reactions, radiative capture reactions

3) Has been extended to the description of three-cluster dynamics

4) Projectile wave function always in Jacobi coordinates: the formalism depends on the number of nucleons in the projectile

5) Requires the calculation of one-body, two-body, three-body and even higher-body densities of the target depending on Hamiltonian (2-body versus 3-body), number of nucleons in the projectile

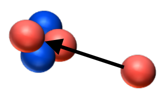
6) For p-shell targets three- and higher-body densities cannot be precomputed and stored, have to be computed on the fly

7) Limitation: tends to underestimate short-range many-body correlations

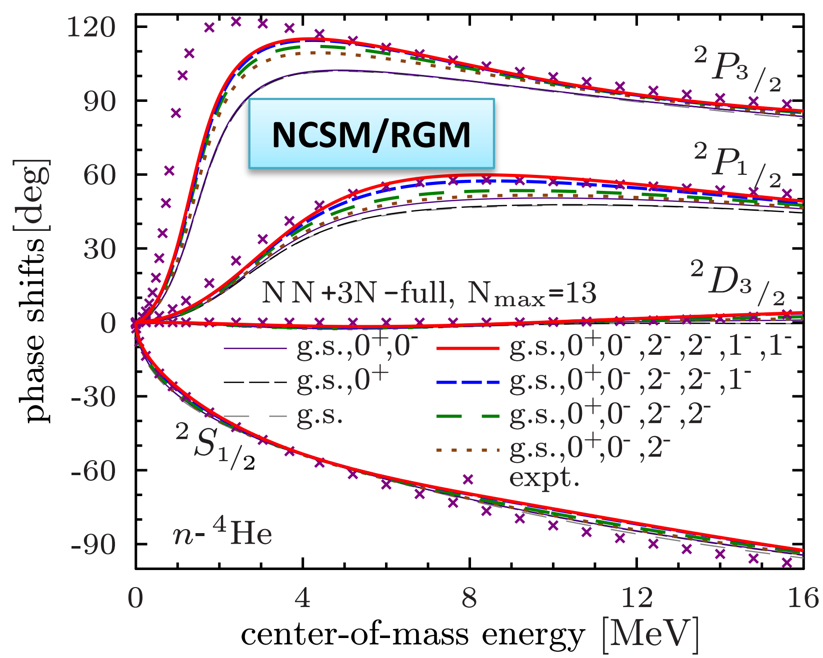
Short-range many-body correlations are recovered through cluster excitations

- Are the ^{4}He excited states really needed to accurately describe the n+^{4}He continuum?

- Yes … the ^{4}He core polarization is non negligible.
  - SRG-evolved chiral NN+3N with λ = 2.0 fm^{-1}
  - Very large (N_{max} = 13) model space
  - Up to first 7 states of ^{4}He
  - Not sufficient!



n+^{4}He Scattering Phase Shifts



Convergence with number of ^{4}He eigenstates

G. Hupin, J. Langhammer, P. Navratil, S. Quaglioni, A. Calci, And R. Roth, Phys. Rev. C **88**, 054622 (2013)

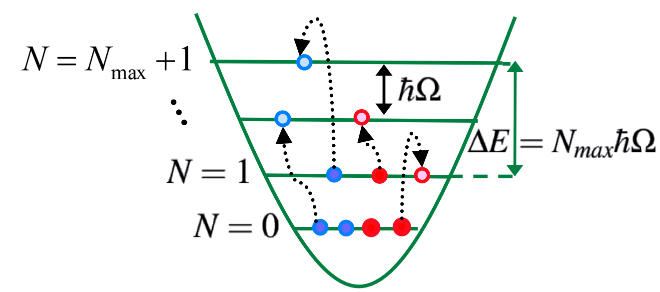
Ab initio no-core shell model with continuum (NCSMC)

- Seeks many-body solutions in the form of a generalized cluster expansion

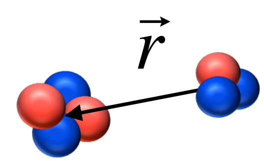
$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \overbrace{\left|^{(A)} \, , \lambda \right\rangle}^{\text{NCSM eigenstates}} + \sum_{\nu} \int d\vec{r}\, u_{\nu}(\vec{r})\, \hat{A}_{\nu} \overbrace{\left|_{(A-a)} \ \vec{r} \ \ _{(a)} \, , \nu \right\rangle}^{\text{NCSM/RGM continuous states}}$$

Unknowns

- *Ab initio* no-core shell model (NCSM):
  - Clusters' structure, short range

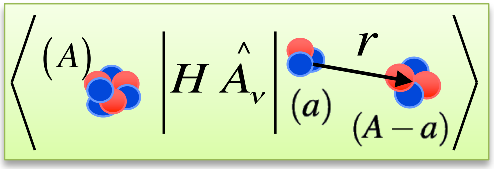


- Resonating-group method (RGM):
  - Dynamics between clusters, long range

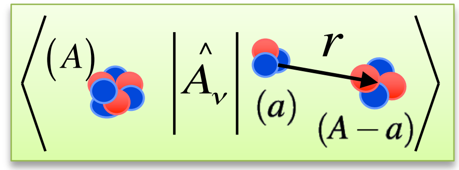


Discrete and continuous variational amplitudes are determined by solving the coupled NCSMC equations

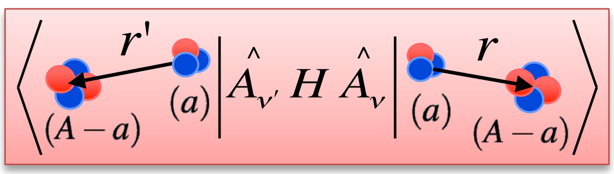
$E_\lambda^{NCSM} \, \delta_{\lambda\lambda'}$

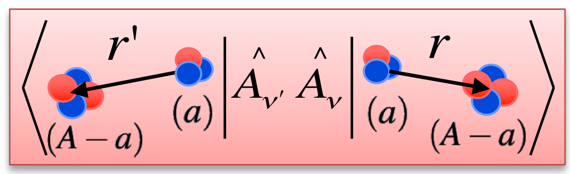


$\delta_{\lambda\lambda'}$



$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix} \begin{pmatrix} c \\ u \end{pmatrix} = E \begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix} \begin{pmatrix} c \\ u \end{pmatrix}$$

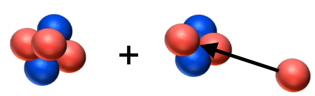




- Scattering matrix (and observables) from matching solutions to known asymptotic with microscopic *R*-matrix on Lagrange mesh

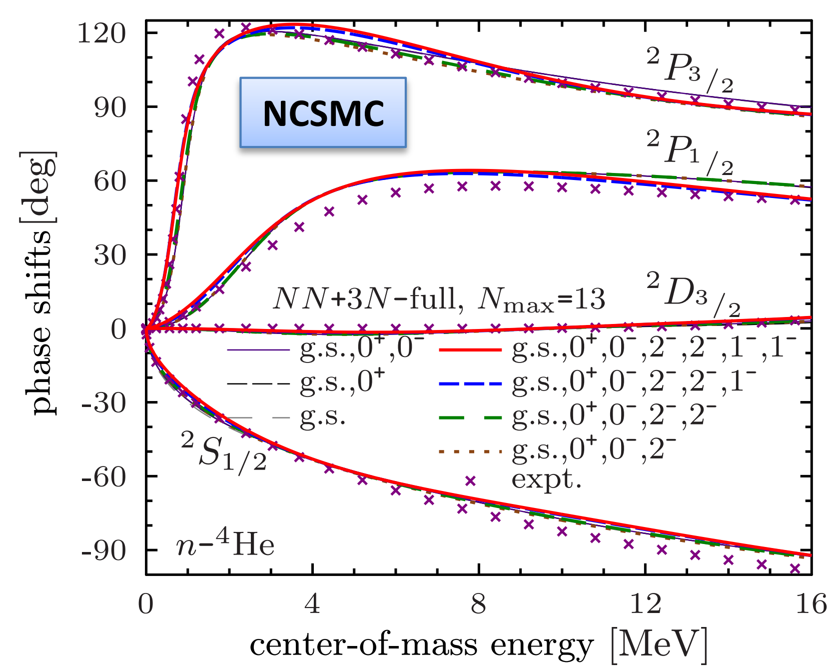
NCSM states account for short-range many-body correlations (cluster excitations)

- Are the ^{4}He excited states really needed to accurately describe the n+^{4}He continuum?
- … No. Eigenstates of the ^{5}He compound nucleus can compensate for missing ^{4}He excitations
  - Same as before + up to first 14 ^{5}He states
  - Excellent convergence!



^{4}He core polarization is non negligible. ^{5}He states essential to describe resonances

n+^{4}He Scattering Phase Shifts



Convergence with number of ^{4}He eigenstates

G. Hupin, S. Quaglioni, and P. Navratil, JPC Conf. Proc. in print, (2015)

Some considerations on the NCSMC

1) Efficient simultaneous description of short-range many-body and long-range cluster correlations

2) Successfully applied to nucleon-nucleus, deuterium-nucleus, ^{3}H/^{3}He-nucleus collisions, (*d*,*N*) transfer reactions, radiative capture reactions

3) Has been extended to the description of three-cluster dynamics

4) Formalism requirements are similar to NCSM/RGM

5) Exploring normal-ordering approximation of 3N force

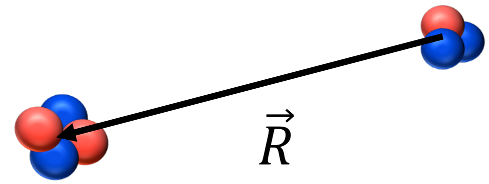
6) Exploring more efficient on the fly calculation of density matrix elements

7) Another possibility: Controlled approximation of densities?

Microscopic R-Matrix theory in a Generator Coordinate basis

- Two-center HO shell model

$$\Psi_{\nu K_1 K_2}(\vec{R}) = \sum_j c^j_{\nu K_1 K_2} \Phi^{(SD)j}_{\nu K_1 K_2}(\vec{R})$$

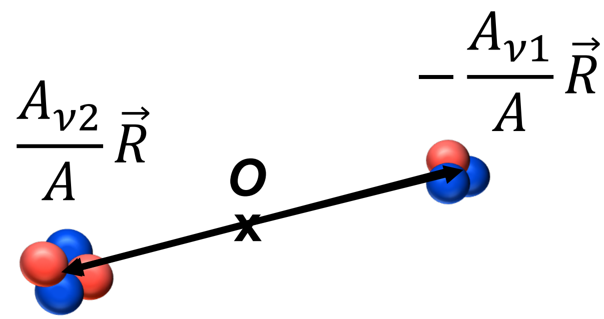


- Antisymmetrization is trivial
- However, single-particle basis states no longer orthogonal
  - $A_{\nu 1}$ centered at $\frac{A_{\nu 2}}{A}\ \vec{R}$
  - $A_{\nu 2}$ centered at $-\frac{A_{\nu 1}}{A}\ \vec{R}$
- Needs angular momentum and parity projection

$$\Psi^{J\pi}_{\nu K_1 K_2}(\vec{R}) = \hat{P}^J_{MK}\, \frac{1}{2}\left(1 + \pi \hat{P}\right)\, \Psi_{\nu K_1 K_2}(\vec{R})$$

Microscopic R-Matrix theory in a Generator Coordinate basis

- Two-center HO shell model



$$\Psi_{\nu K_1 K_2}(\vec{R}) = \sum_j c^j_{\nu K_1 K_2} \Phi^{(SD)j}_{\nu K_1 K_2}(\vec{R})$$

- Antisymmetrization is trivial

- However, single-particle basis states no longer orthogonal
  - $A_{\nu 1}$ centered at $\frac{A_{\nu 2}}{A}\ \vec{R}$
  - $A_{\nu 2}$ centered at $-\frac{A_{\nu 1}}{A}\ \vec{R}$

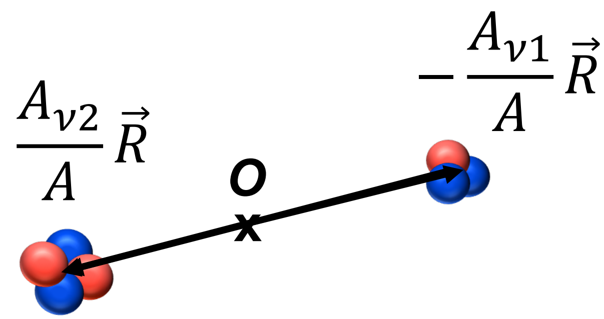
- Needs angular momentum and parity projection

$$\Psi^{J\pi}_{\nu K_1 K_2}(\vec{R}) = \hat{P}^J_{MK}\,\frac{1}{2}\left(1 + \pi\hat{P}\right)\,\Psi_{\nu K_1 K_2}(\vec{R})$$

Microscopic R-Matrix theory in a Generator Coordinate basis

- It can be demonstrated that

$$\left|\Psi^{J\pi}_{\nu K_1 K_2}(R)\right\rangle \propto \sum_{s\ell} \hat{A}_\nu u^{J\pi}_{\nu s\ell K_1 K_2}(r_\nu, R)\left|\Phi^{J\pi}_{\nu s\ell}\right\rangle$$



- Generator Coordinate Method (GCM) ansatz for the wave function in the internal region:

$$\left|\Psi^{J\pi}\right\rangle = \sum_{\nu K_1 K_2} \int \left|\Psi^{J\pi}_{\nu K_1 K_2}(R)\right\rangle f^{J\pi}_{\nu K_1 K_2}(R) R^2 dR \approx \sum_{\nu K_1 K_2 n} \left|\Psi^{J\pi}_{\nu K_1 K_2}(R_n)\right\rangle f^{J\pi}_{\nu K_1 K_2}(R_n)$$

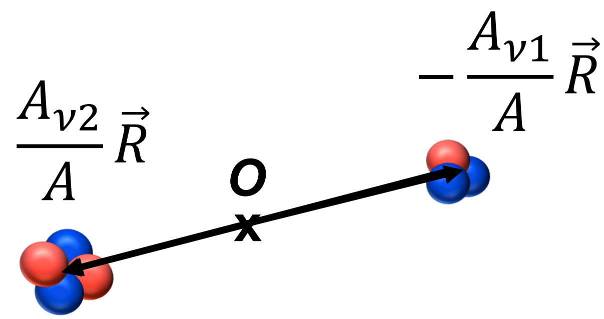
- Equivalent to RGM:

$$\gamma^{J\pi}_{\nu s\ell}(r_\nu) = \sum_{K_1 K_2} f^{J\pi}_{\nu K_1 K_2}(R) u^{J\pi}_{\nu s\ell K_1 K_2}(r_\nu, R)\, R^2 dR$$

Microscopic R-Matrix theory in a Generator Coordinate basis

- It can be demonstrated that

$$\left|\Psi^{J\pi}_{\nu K_1 K_2}(R)\right\rangle \propto \sum_{s\ell} \hat{A}_\nu u^{J\pi}_{\nu s\ell K_1 K_2}(r_\nu, R)\left|\Phi^{J\pi}_{\nu s\ell}\right\rangle$$



- Generator Coordinate Method (GCM) ansatz for the wave function in the internal region:

$$\left|\Psi^{J\pi}\right\rangle = \sum_{\nu K_1 K_2} \int \left|\Psi^{J\pi}_{\nu K_1 K_2}(R)\right\rangle f^{J\pi}_{\nu K_1 K_2}(R) R^2 dR \approx \sum_{\nu K_1 K_2 n} \left|\Psi^{J\pi}_{\nu K_1 K_2}(R_n)\right\rangle f^{J\pi}_{\nu K_1 K_2}(R_n)$$

- GCM equations:

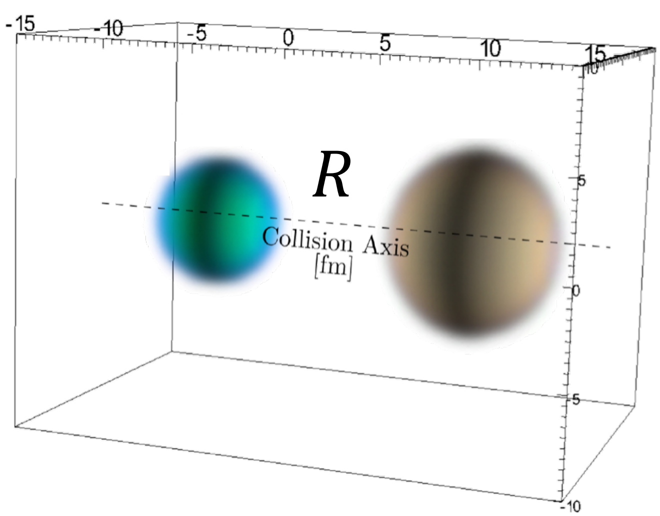
$$\sum_{\alpha}\left[H_{\alpha'\alpha}(R_{n'}, R_n) - E\, N_{\alpha'\alpha}(R_{n'}, R_n)\right] f^{J\pi}_{\alpha}(R_n) = 0$$

Ab initio reaction theory for medium-mass nuclei?

- NCSMC within symmetry adapted basis?
- NCSMC-inspired formalism?
  - Use target densities computed within coupled-cluster or IM-SRG
  - Approximate removal of center of mass motion
- GCM-inspired formalism?
  - Valence-space IM-SRG or similar ‘ab initio shell model’ wave functions
- ...

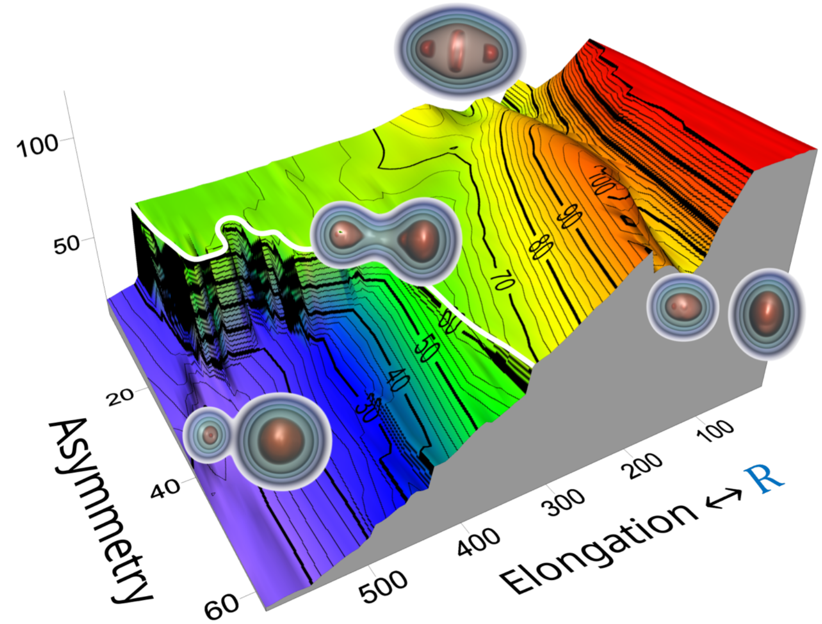
Microscopic R-Matrix with Density Functional Theory

1) **Static projectile-target solutions:** Density Functional Theory (DFT) accounts for Pauli principle, microscopic nuclear interactions



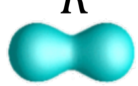
Builds on methods for fission theory

(in collaboration with N. Schunck)

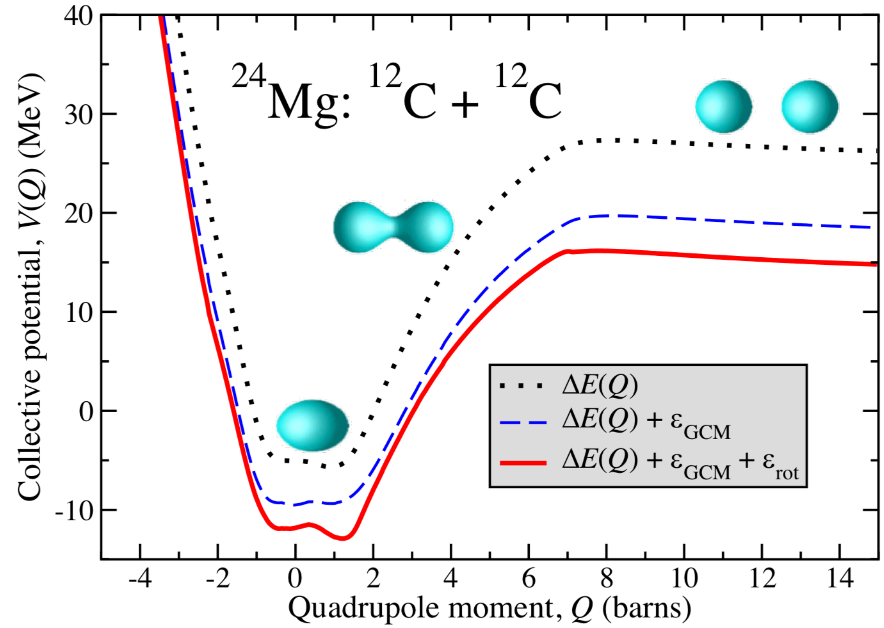


Microscopic R-Matrix with Density Functional Theory

2) **Projectile-target dynamics:** Generator coordinate method (GCM) with Gaussian overlap approximation maps the many-body problem into a collective Schrödinger-like equation for the relative motion

$|\Psi\rangle = \int \Big|$ R  $\Big\rangle\, \chi(R)\, dR$

$$\left(-\frac{1}{2}\frac{d}{dR}\frac{\hbar^2}{\boldsymbol{M}(\boldsymbol{R})}\frac{d}{dR} + \boldsymbol{V}(\boldsymbol{R}) - E\right)\chi(R) = 0$$



(Q is a proxy for R)

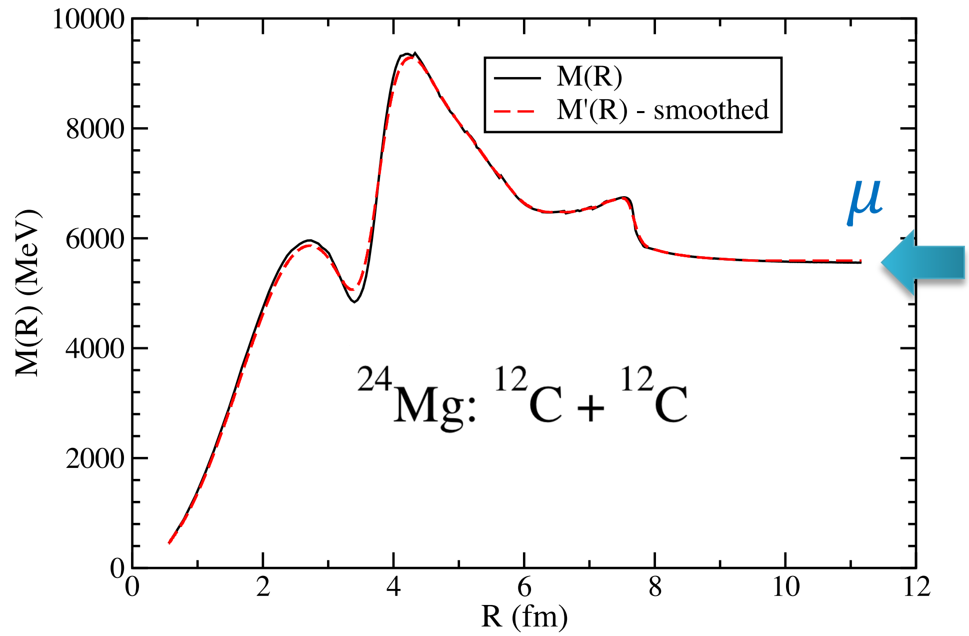
Similar to: Berger & Gogny, NPA**333**, 302

Microscopic R-Matrix with Density Functional Theory

2) **Projectile-target dynamics:**
Generator coordinate method (GCM) with Gaussian overlap approximation maps the many-body problem into a collective equation for the relative-motion amplitudes

$$|\Psi\rangle = \int \left| \, R \, \right\rangle \chi(R)\, dR$$

$$\left(-\frac{1}{2}\frac{d}{dR}\frac{\hbar^2}{\boldsymbol{M(R)}}\frac{d}{dR} + \boldsymbol{V(R)} - E\right)\chi(R) = 0$$



Similar to: Berger & Gogny, NPA**333**, 302

Microscopic R-Matrix with Density Functional Theory

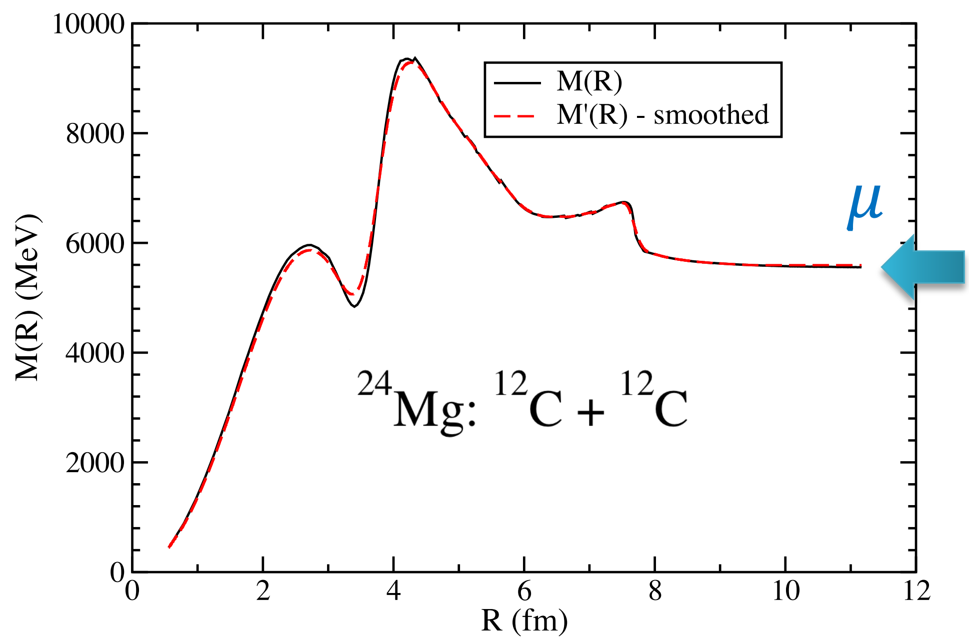
3) **Point canonical transformation:** Maps the GCM+GOA equation into a Schrödinger-like equation for a relative motion wave function:

$$\left(-\frac{1}{2}\frac{d}{dR}\frac{\hbar^2}{\boldsymbol{M(R)}}\frac{d}{dR}+\boldsymbol{V(R)}-E\right)\chi(R)=0$$

– Change of variables:

$$r=\mu^{-\frac{1}{2}}\int_0^R\sqrt{M(x)}dx$$

$$\chi(R)=[M(R)/\mu]^{\frac{1}{4}}\psi(r)$$

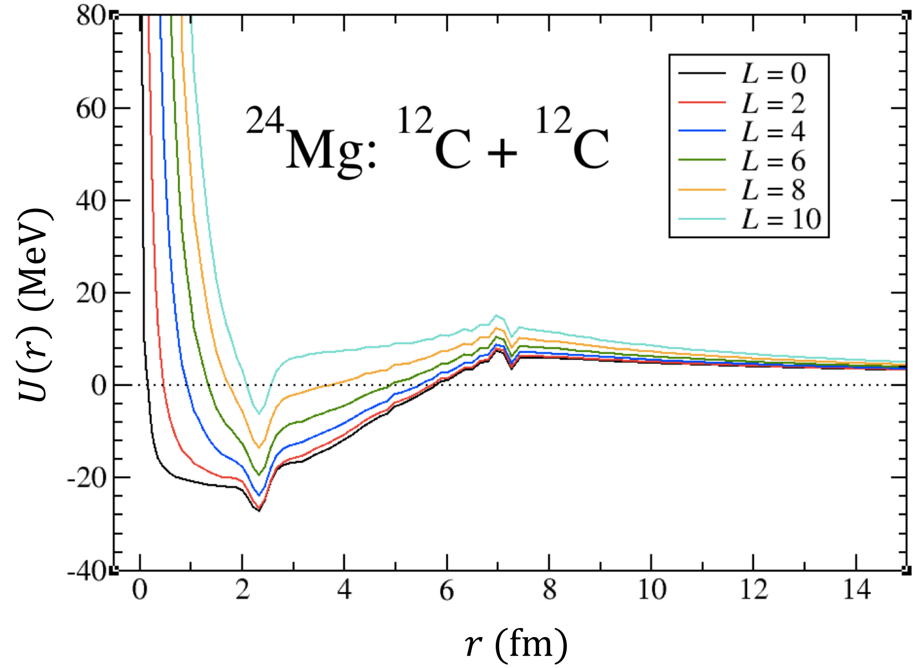


Microscopic R-Matrix with Density Functional Theory

3) **Point canonical transformation:** Maps the GCM+GOA equation into a Schrödinger-like equation for a relative motion wave function

$$\left(-\frac{1}{2}\frac{d}{dR}\frac{\hbar^2}{\boldsymbol{M(R)}}\frac{d}{dR}+\boldsymbol{V(R)}-E\right)\chi(R)=0$$

$$\left\{\frac{d^2}{dr}-\frac{2\mu}{\hbar^2}[U(r)-E]\right\}\psi(r)=0$$



$$U(r)=V(R)+\frac{L(L+1)\hbar^2}{2I(R)}$$

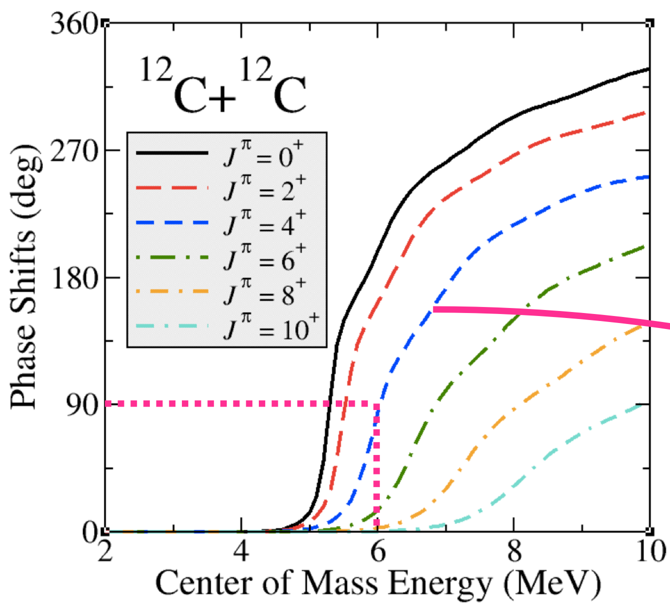
$$+\frac{\hbar^2}{8M(R)}\left[\frac{7}{4}\left(\frac{M'(R)}{M(R)}\right)^2-\frac{M''(R)}{M(R)}\right]$$

- New potential depends on the derivative of the collective mass

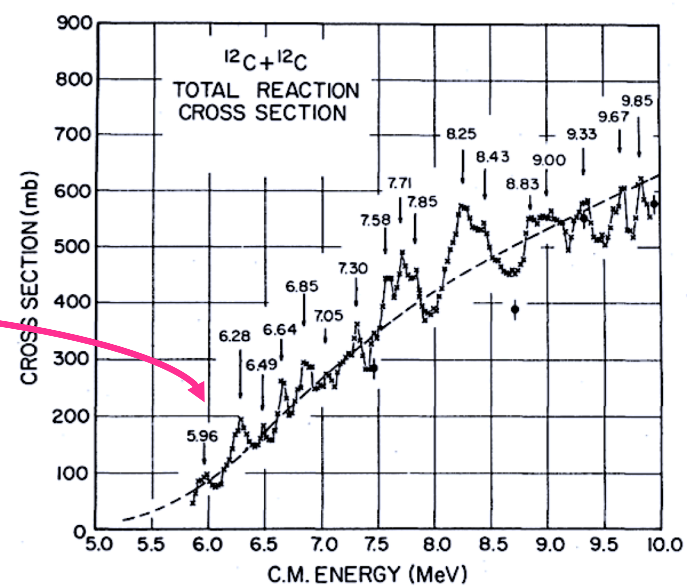
Microscopic R-Matrix with Density Functional Theory

- Present results obtained by including only 0^+ ground-state DFT solutions for $^{24}Mg(^{12}C+^{12}C)$
- Preliminary results for the low-energy resonances are encouraging

Phase shifts



Total cross section



A more quantitative description requires the inclusion of excitations of the $^{24}Mg(^{12}C+^{12}C)$

Conclusions

- R-Matrix theory provides a rigorous framework for bridging many-body bound-state calculations and collision theory
- Today there are several implementations of it, I only mentioned a few
- The RGM or equivalently the GCM provide a convenient explicit treatment of clustering, facilitate matching with asymptotic solutions
  - Present different challenges
- It should be possible to combine R-Matrix theory with ab initio methods for medium-mass nuclei
- Attempt to combine R-Matrix theory with Density Functional Theory