Microscopic description of nuclear reactions within Coupled Cluster and Gamow Shell Model theories

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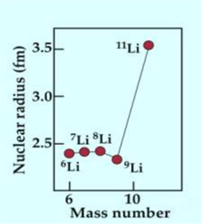
Scientific motivation

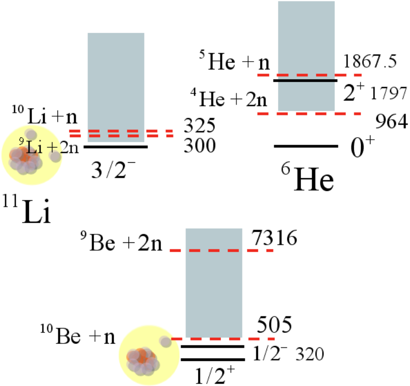
Experimental interest

Study of nuclei far from the valley of stability

SPIRAL-2 (GANIL), (EURISOL - Europe), FAIR (GSI), RIKEN (Japan), FRIB (USA)

Nuclei: halos (^{6}He, ^{8}B, ^{11}Be, ^{11}Li), resonant (^{7}He, ^{8}C, ^{9}Be)

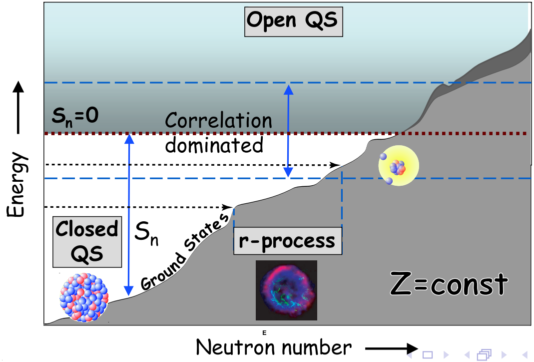




Open quantum systems

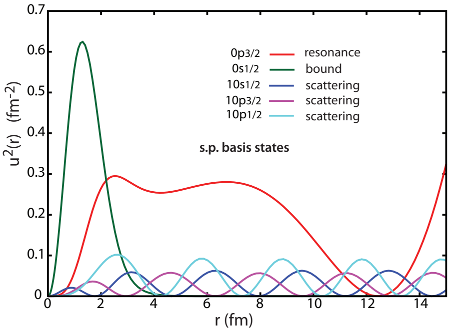
Open vs. closed systems

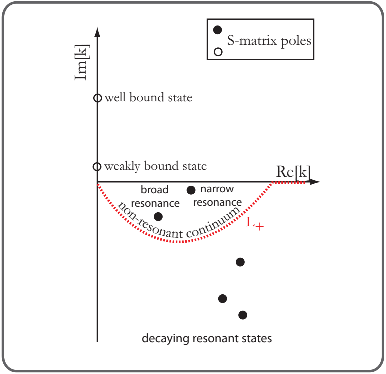
Open quantum system: interaction with an external environment
Distinguished part of a larger quantum system
Different physical properties from those of closed quantum systems:
small binding energy, halos, finite life-time
Molecules, quantum wires and dots, hadrons, microwave cavities



Outline

Berggren completeness relation



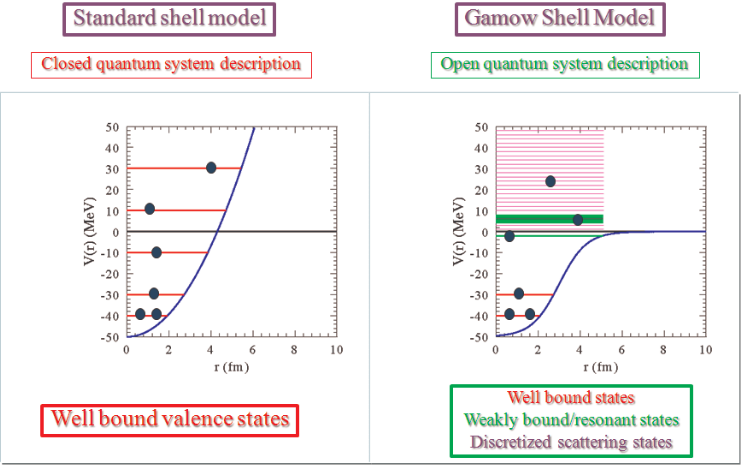


Asymptotic region

Pole states : $u(r) = u^+(r) = C^+ H^+_{\ell\eta}(kr)$

Scattering states: $u(r) = u^+(r) + u^-(r) = C^+ H^+_{\ell\eta}(kr) + C^- H^-_{\ell\eta}(kr)$

Gamow Shell Model (GSM)



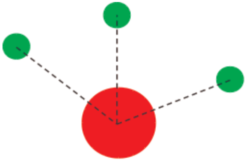
GSM within a core/valence particles picture

Cluster orbital shell model (COSM)

1. $3A$ particle $\neq 3(A-1)$ physical degrees of freedom $\Rightarrow$ spurious states
2. Lawson method: $H \to H + \lambda \left(\frac{P^2}{2M} + \frac{1}{2} M \omega^2 R^2 - \frac{3}{2} \hbar\omega \right)$

   Well-bound states only
3. COSM: use of relative core coordinates $\Rightarrow$ no center of mass excitation

   Appearance of a recoil term: $H \to H + \frac{1}{M_{core}} \sum_{i<j} \vec{p}_i \cdot \vec{p}_j$



$$\vec{r} = \vec{r}_{lab} - \vec{R}_{core}$$

Asymptotic normalization coefficient (ANC)

Overlap function

1. $I_{\ell j}(r) = \sum_{n \in (b,d)} \langle \Psi_A || a^\dagger_{n \ell j} || \Psi_{A-1} \rangle u_n(r) + \int_{L+} \langle \Psi_A || a^\dagger_{\ell j}(k) || \Psi_{A-1} \rangle u_k(r) dk$
2. $I_{\ell j}(r) \sim C_{\ell j} \frac{W_{-\eta, \ell+1/2}(2\kappa r)}{r}$ (bound), $C_{\ell j} \frac{H^{+}_{\ell,\eta}(kr)}{r}$ (resonant), $r \to +\infty$
3. $C_{\ell j}$: ANC

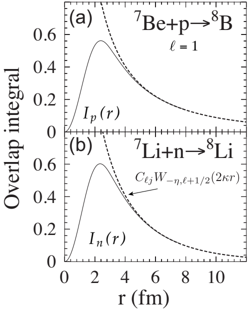
Reactions at low energy

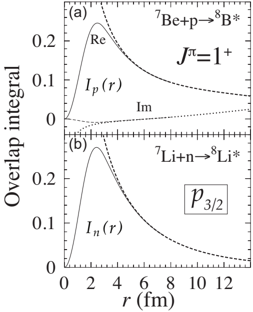
$\sigma \propto |C_{\ell j}|^2$: astrophysical reactions (radiative capture, transfer reactions, ...)

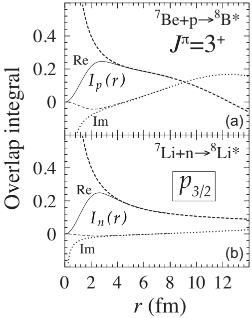
Theoretical description in different models

1. Standard models: Indirect determination of $C_{\ell j}$
   $|\Psi\rangle$: harmonic oscillator shell model, $a^\dagger|\Psi\rangle$: $u(r)$ from DWBA approximation
   (N.K. Timofeyuk, R.C. Johnson, A.M. Mukhamedzanov, Phys. Rev. Lett, **91** 232501 (2003))
2. GSM: Exact determination of ANCs
   (J. Okołowicz, N. Michel, W. Nazarewicz, M. Płoszajczak, Phys. Rev. C, **85** 064320 (2012))

ANCs in ^{7}Li and ^{8}B







1. Modified Surface Gaussian Interaction, ^{4}He core, COSM frame
2. Energies of ground and first excited states fitted to experimental data
3. Unbound states ANCs provide emission width: $\Gamma_{ANC} = (\hbar^2/\mu)\Re(k) \sum_{\ell j} |C_{\ell j}|^2$

   $\underline{^8\text{B } 1^+ \text{ state}}$: Γ_{GSM} = 24 keV, Γ_{ANC} = 23 keV, Γ_{exp} = 36 keV
   $\underline{^8\text{B } 3^+ \text{ state}}$: Γ_{GSM} = 275 keV, Γ_{ANC} = 258 keV, Γ_{exp} = 350 keV
   $\underline{^8\text{Li } 3^+ \text{ state}}$: Γ_{GSM} = 21 keV, Γ_{ANC} = 21 keV, Γ_{exp} = 32 keV

Comparisons of ANCs ratios for bound states

ANC ratio

1. $\mathcal{R} = |C_p/C_n|^2$ (N.K. Timofeyuk et al., Phys. Rev. Lett. **91**, 232501 (2003))
2. Interest: insensitive to model details, $\mathcal{R} \simeq \mathcal{R}_0 = \left| \frac{e^{i\sigma_\ell(-i\eta)} F_{\ell,-i\eta}(i\kappa_p R_f)}{\kappa_p R_f j_\ell(i\kappa_n R_f)} \right|^2$
3. Easier comparison with experimental data
4. Compared models: GSM and VMC (variational Monte Carlo)
   (K. Nollett and R. Wiringa, Phys. Rev. C **83** 041001 (2011))

Mirror pair	j^π	$\mathcal{R}_{\mathrm{GSM}}$	$\mathcal{R}_{\mathrm{VMC}}$	$\mathcal{R}_0$	$\mathcal{R}_{\mathrm{Exp.}}$
$({}^7\mathrm{Be}/{}^7\mathrm{Li})_{3/2^-}$	$1/2^-$	1.04	1.28	1.06	—
	$3/2^-$	1.06	1.29	1.06	—
	$1/2^- + 3/2^-$	1.06	1.29	1.06	—
$({}^8\mathrm{B}/{}^8\mathrm{Li})_{2^+}$	$1/2^-$	1.39	1.27	1.12	1.08 ± 0.18
	$3/2^-$	1.04	1.25	1.12	1.08 ± 0.15
	$1/2^- + 3/2^-$	1.04	1.25	1.12	1.08 ± 0.15
$({}^{17}\mathrm{F}/{}^{17}\mathrm{O})_{j^\pi}$	$5/2^+$	1.20	—	1.22	1.33 ± 0.20
	$1/2^+$	701	—	796	—

Comparisons of ANCs ratios with unbound states

Consideration of unbound proton state

1. $\mathcal{R}_\Gamma = (1/\hbar c)\ \Gamma_p/|C_n|^2 = |C_p/C_n|^2 \Re(\kappa_p)(\hbar c/\mu_p c^2)$

   (N.K. Timofeyuk et al., Phys. Rev. Lett. **91**, 232501 (2003))

2. Example: excited 1^+ state of ^{8}B and ^{8}Li in GSM.
   Good agreement with experimental data.

j^π	C_p	C_n	$\mathcal{R}_\Gamma$ (GSM)	$\mathcal{R}_\Gamma$ (Exp.)
$1/2^-$	$0.0322-i0.00138$	0.1379	0.0021	—
$3/2^-$	$0.0442-i0.00273$	0.2090	0.0018	—
$1/2^-+3/2^-$	0.0547	0.2504	0.0019	0.0022 ± 0.0002

Outline

Resonating Group Method with GSM (RGM-GSM): Theory

Generalities

1. Resonating Group Method:
   $\langle \Psi_{GSM;f} \otimes \Phi_{proj;f} | H | \Psi_{GSM;i} \otimes \Phi_{proj;i} \rangle$
   $\Rightarrow$ coupled-channel equations with coupling potentials

2. Fundamental equation for nucleon emission:
   $\langle \mathcal{A}\{ \langle \Psi_{T_f} |^{J_f} \langle r_f \; \ell_f \; j_f \; \tau_f | \}^J_M | H | \mathcal{A}\{ | \Psi_{T_i} \rangle^{J_i} | r_i \; \ell_i \; j_i \; \tau_i \rangle \}^J_M \rangle$

3. Fundamental equation for cluster emission:
   $\langle \mathcal{A}\{ \langle \Psi_{T_f} |^{J_f} \langle R^f_{CM} \; L^f_{CM} \; J^f_{int}; J^f_p | \}^J_M | H | \mathcal{A}\{ | \Psi_{T_i} \rangle |^{J_i} | R^i_{CM} \; L^i_{CM} \; J^i_{int}; J^i_p \rangle \}^J_M \rangle$

4. Advantages:
   No Jacobi coordinates (COSM),
   Antisymmetry exactly handled
   Fully microscopic
   Core arbitrary

One-body projectile treatment

1. Nucleon:
   Berggren basis expansion of one-body projectile
   $$|r\ell j\tau\rangle = \sum_n u_n(r)\ |u_n\ell j\tau\rangle$$

2. Composite:
   Linear combination of Slater determinants
   $$\{a^\dagger_{n\ell j\tau}|\Psi\rangle^{J_T}\}^J_M = \sum_i c_i|SD_i\rangle$$

3. Infinite range terms:
   Kinetic and Coulomb terms appear from $n \rightarrow +\infty$
   Analytical treatment of RGM matrix elements necessary
   Disappearance of antisymmetry at high $n \Rightarrow$ projectile and target factorize
   Kinetic and Coulomb terms handled with completeness of Berggren basis

Many-body projectile treatment (1/2)

1. Momentum space:
   Basis of momentum space cluster wave functions
   $$|\Psi_p\rangle = |R_{CM}, L_{CM}, J_{int}\rangle_{M_p}^{J_p} \rightarrow |K_{CM}, L_{CM}, J_{int}\rangle_{M_p}^{J_p}$$
2. Apparent solution:
   Direct Berggren basis expansion of projectile
   $$|K_{CM}, L_{CM}, J_{int}\rangle_{M_p}^{J_p} = \sum_i c_i |SD_i\rangle$$
3. Problem:
   Dirac delta normalization, center of mass/relative parts separation uncontrolled

Many-body projectile treatment (2/2)

1. Solution:
   finite-range of Hamiltonian ⇒ use of HO basis
   $$|K_{CM}, L_{CM}, J_{int}\rangle^{J_p}_{M_p} \rightarrow \sum_{N_{CM}} U^{HO}_{N_{CM},L_{CM}}(K_{CM}) |N_{CM}, L_{CM}, J_{int}\rangle^{J_p,M_p}_{HO}$$

2. HO many-body states generation:
   successive applications of $A^{\dagger}_{CM}$ on $|N_{CM} = 0, L_{CM} = 0\rangle |J_{int}, M_{int}\rangle$

3. CM scattering part:
   One-body problem ⇒ exact Dirac delta normalization
   $$U^{HO}_{N_{CM},L_{CM}}(K_{CM}) \text{ from } H_{CM} = \frac{{P_{CM}}^2}{2M_p} + U_{CM}(R_{CM})$$

4. Berggren basis expansion: $|K_{CM}, L_{CM}, J_{int}\rangle^{J_p,M_p}_{HO} = \sum_i c_i |SD_i\rangle$

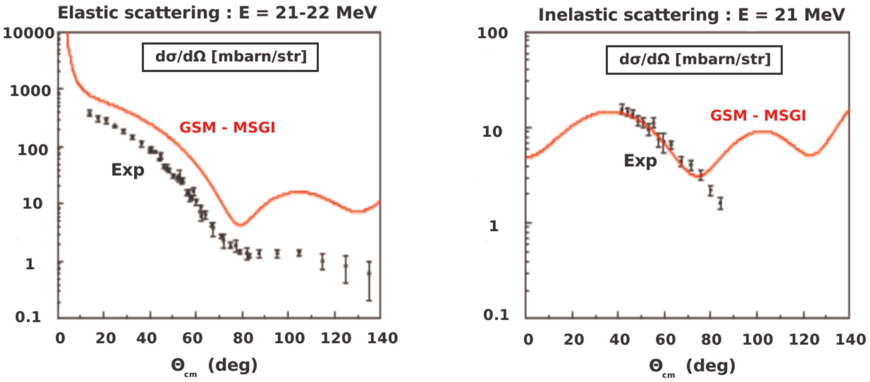
5. Coupled channel equations: similar to one-nucleon problem

Resonating Group Method with GSM (RGM-GSM): Applications

First applications of RGM-GSM

1. Nucleon scattering: $|\Phi_{proj}\rangle = |r \; \ell \; j\rangle$
2. Reactions of interest: ^{6}He(p,p')^{6}He and ^{18}Ne(p,p)^{18}Ne
3. Differential elastic and inelastic scattering cross sections calculated
4. Models
   Valence particles above ^{4}He/^{16}O core, p/sd valence space
   Modified Surface Gaussian interaction(MSGI): J, T-dependence

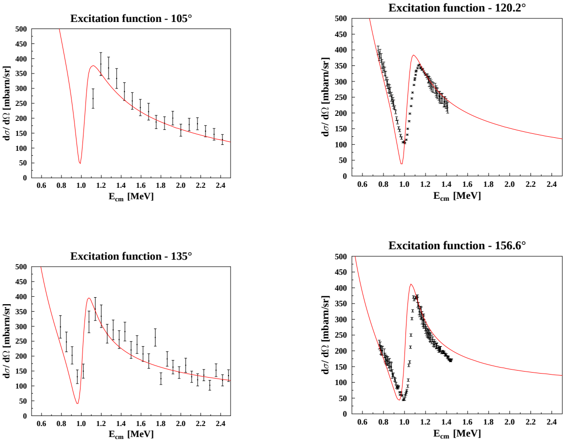
p+^{6}He at 21-22 MeV



1. Experimental elastic cross sections overall overestimation
2. Experimental inelastic cross sections well reproduced

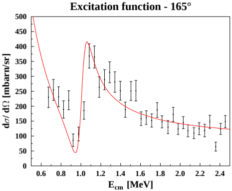
Y.Jaganathen, N.Michel, M.Płoszajczak, Proc. Int. Conf. "Horizons of Innovative Theories, Experiments and Supercomputing in Nuclear Physics" (2012)

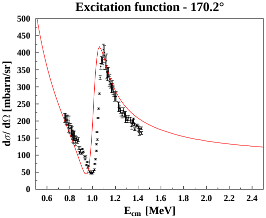
p+^{18}Ne (1/2)

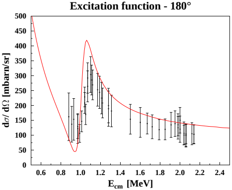


1. Experimental data very well reproduced
2. Continuum degrees of freedom less present in targets than in ^{6}He.

p+^{18}Ne (2/2)







Experimental data also reproduced at large angles

Y. Jaganathen, N. Michel, M. Płoszajczak, Phys. Rev. C **89**, 034624 (2014)

Radiative capture within GSM-RGM (1/2)

1. Radiative capture cross sections:
   $\sigma(E_{CM})$ function of electro-magnetic (EM) matrix elements

2. EM matrix elements for radiative capture in GSM-RGM:
   $\langle \mathcal{A}\{\langle\Psi_{T_f}|^{J_f}\langle u_f\ \ell_f\ j_f\ \tau_f|\}^{J'}||O^L||\mathcal{A}\{|\Psi_{T_i}\rangle^{J_i}|u_i\ \ell_i\ j_i\ \tau_i\rangle\}^J\rangle$

3. Problem:
   $\mathcal{A}\{|\Psi_{T_i}\rangle^{J_i}|u_i\ \ell_i\ j_i\ \tau_i\rangle\}^J_M$: many-body scattering state

   Slater determinant expansion with Berggren basis:
   only for bound and resonant states

   Antisymmetry apparently impossible to fulfill

Radiative capture within GSM-RGM (2/2)

1. Solution:
   Antisymmetry disappears at large r
   $O^L - O^L_{nas}$ localized $\Rightarrow$ HO expansion of $O^L - O^L_{nas}$
   $O^L \simeq O^L_{nas} + [O^L - O^L_{nas}]_{HO}$

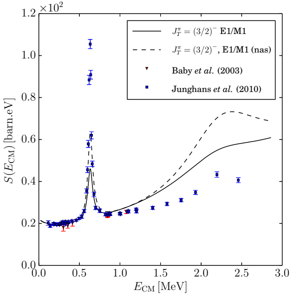
2. Treatment of $[O^L - O^L_{nas}]_{HO}$:
   Projection of $|u~\ell~j~\tau\rangle$ on HO basis $\Rightarrow \mathcal{A}\{|\Psi_T\rangle^J |u~\ell~j~\tau\rangle^{(HO)}\rangle\}^J_M$ localized
   $\Rightarrow$ Berggren basis expansion with Slater determinants possible
   $\Rightarrow$ Antisymmetry exactly fulfilled

3. Treatment of O^L_{nas}:
   $\langle[\langle\Psi_{T_f}|^{J_f}\langle u_f~\ell_f~j_f~\tau_f|]^{J'}||O^L_{nas}||[|\Psi_{T_i}\rangle^{J_i}|u_i~\ell_i~j_i~\tau_i\rangle]^J\rangle$
   $= A_T\langle\Psi^{J_f}_{T_f}||O^L||\Psi^{J_i}_{T_i}\rangle\langle u_f|u_i\rangle + A_p~\delta_{T_i T_f}~\langle u_f|O^L|u_i\rangle$

   Standard formulas involving GSM matrix elements and one-body radial integrals
   Tails of many-body wave functions exactly taken into account

4. Model
   Valence particles above ^{4}He core, p/sd valence space
   Effective interaction with central, spin-orbit and tensor parts

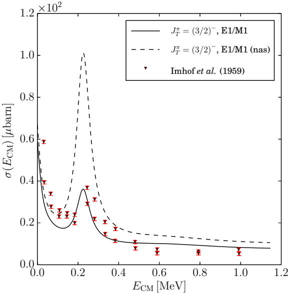
^{7}Be(p,γ)^{8}B reaction



1. Astrophysical factor $S(E_{CM}) = E_{CM}\ \sigma(E_{CM})\ \exp(2\pi\eta_{CM})$
2. Experimental data well reproduced at low energy, not at high energy
3. Effective charge for E1 almost equal to theoretical value
4. Asymptotical reaction at low energy: no antisymmetry

K. Fossez, N. Michel, Y. Jaganathen, M. Płoszajczak, in preparation

^{7}Li(n,γ)^{8}Li reaction



1. E1 and M1 transitions considered for cross section $\sigma(E_{CM})$
2. Experimental data well reproduced for all energies
3. Effective charge for E1: 15% larger than theoretical value
4. Antisymmetry greatly reduces cross section for all energies

K. Fossez, N. Michel, Y. Jaganathen, M. Płoszajczak, in preparation

Outline

1. Gamow Shell Model (GSM)
2. Nuclear reactions with GSM
3. Nuclear reactions with Coupled Clusters
4. Conclusion

Coupled-Cluster theory for closed-shell nuclei

Exponential ansatz for $|\Psi\rangle$

$|\Phi\rangle$: Hartree-Fock many-body state

$$|\Psi\rangle = e^{\hat{T}}|\Phi\rangle, \;\; \hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots + \hat{T}_A$$

$$\hat{T}_1 = \sum_{\substack{i<\epsilon_F \\ a>\epsilon_F}} t_i^a \hat{a}_a^\dagger \hat{a}_i, \hat{T}_2 = \frac{1}{2} \sum_{\substack{i<j<\epsilon_F \\ \epsilon_F<a<b}} t_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i.$$

Coupled-Cluster theory equations

$$\bar{H} = \exp(-T) \; H \; \exp(T)$$

$$\langle \Phi_p | \bar{H} | \Phi \rangle = 0$$

$$\bar{H}|\Phi\rangle = E|\Phi\rangle$$

1. Coupled-Cluster theory is fully microscopic and size extensive
2. Low computational cost (CCSD scales as $n_o^2 n_u^4$)
3. Use of realistic Hamiltonians:
   N^3LO two-body force, three-body force averaged in nuclear matter
4. Nuclei in the vicinity of closed-shell systems only

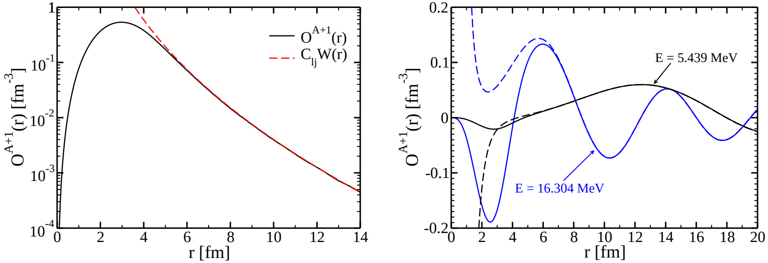
(G. Hagen, N. Michel, Phys. Rev. C **86**, 021602(R) (2012))

Reactions with Coupled-Cluster theory

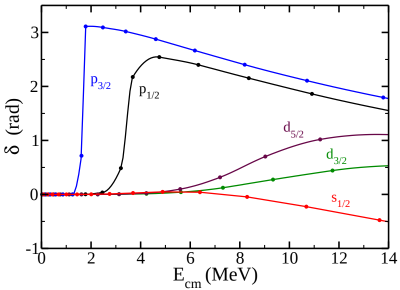
Overlap functions and continuum coupling

$$O_A^{A+1}(\ell j;r) = \sum_n \langle \Phi_A || L^{A+1} \bar{a}^{\dagger}_{n\ell j} || \Phi_A \rangle u_{n\ell j}(r)$$

1. ℓj: Berggren basis $\Rightarrow$ continuum coupling included in ^{41}Sc
2. Nuclear correlations (ab-initio calculation), proper asymptotic for $O_A^{A+1}(\ell j;r)$
3. Example: $f_{7/2}$ bound and scattering proton overlap functions

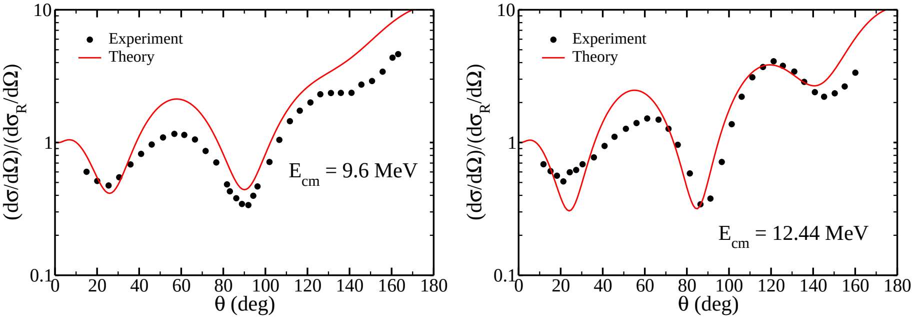


^{40}Ca(p,p)^{40}Ca elastic scattering phase shifts



1. Phase shifts extracted from overlap functions
2. $p_{3/2}, p_{1/2}$ resonances at 1.6 MeV and 3.4 MeV $\Leftrightarrow$ calculated resonant states
3. $\underline{p_{3/2}}$: narrow resonant state at $E = 1.61$ MeV, $\Gamma = 2$ keV
4. $\underline{p_{1/2}}$: broad resonant state at $E = 3.42$ MeV, $\Gamma = 400$ keV
5. $\underline{\ell \geq 3}$: spurious resonant states appear $\Rightarrow$ suppressed

^{40}Ca(p,p)^{40}Ca elastic scattering cross sections



Ratio of proton and Rutherford differential cross sections

1. Good overall agreement with experimental data
2. Minima and maxima of cross sections reproduced
3. No fitting procedure: Hamiltonian interaction is the only input
4. Overestimation at large angles: no high $\ell's$, deuteron, ..., channels

Outline

Conclusion

GSM for reaction calculations

1. GSM: Shell model with Berggren basis continuum included at basis level
2. Application to ANCs: ^{7}Be, ^{7}Li, ^{8}B, ^{8}Li studied in GSM
3. Reactions within GSM: Structure fully included in reaction theory with RGM
   ^{6}He(p,p')^{6}He, ^{18}Ne(p,p)^{18}Ne, ^{7}Be(p,γ)^{8}B, ^{7}Li(n,γ)^{8}Li considered
4. Elastic and inelastic scattering within CC: ^{40}Ca(p,p)^{40}Ca
5. Good overall reproduction of experimental data

Perspectives

1. Ab-initio GSM/CC:
   Consideration of a larger set of nuclei
2. Reactions within GSM and CC:
   Inclusion of scattering channels and many-body clusters
3. Reactions within GSM:
   COSM formalism $\Rightarrow$ GSM close to closed-shell nuclei