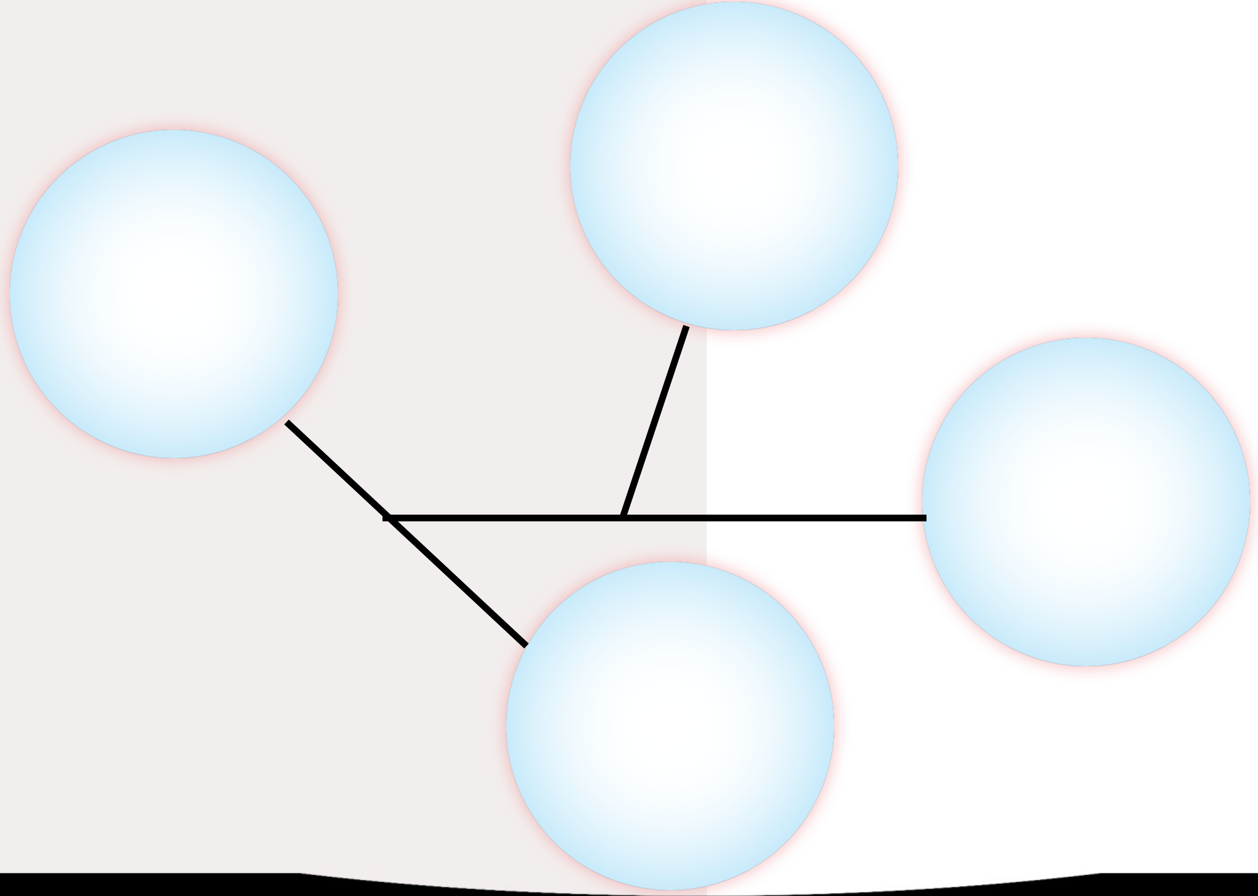
Complex scaling method for multiple particle collisions



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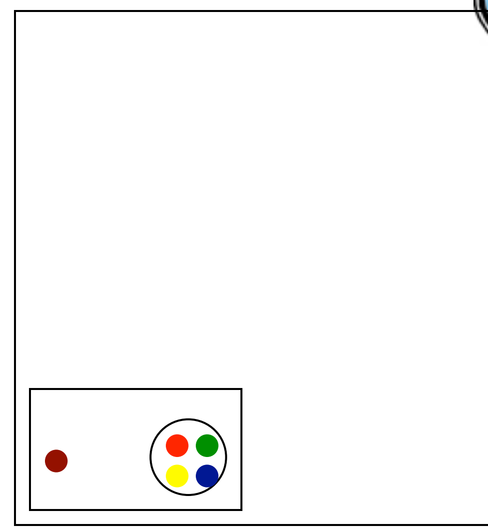
Bound states

- Wave function of finite size (bound to the box)

Variational method, multiple ways to discretize wave function and solve the Schrödinger eq.

Scattering

- Configuration space wave functions extend to infinity.

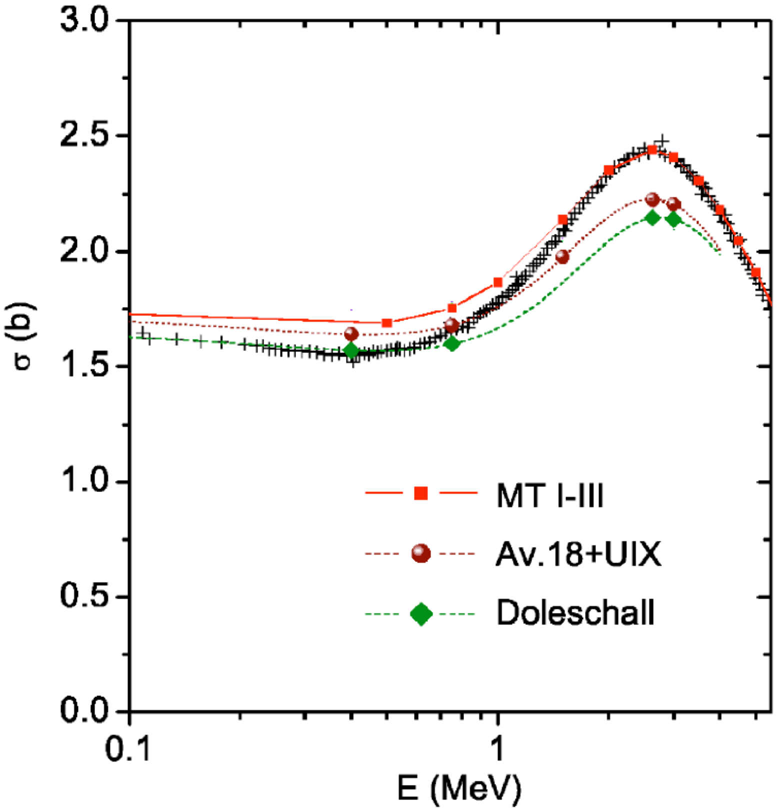


Singularities in momentum space…

Scattering requires a much more « fine tuning » of the interactions

When all bound states are OK, $V_{NN}+V_{NNN}$ can still fail there !!!

e.g. n + ^{3}H



PHYSICAL REVIEW C **70**, 044002 (2004)

A dream: to solve scattering problem with a similar ease as bound state one (avoiding complex singularities or boundary conditions)

- Lorentz integral transform *(inclusive process)*

  *N. Barnea, V. D. Efros, W. Leidemann, and G. Orlandini, Phys. Rev. C **63**, 057002 (2001)*

- Complex energy method in momentum space

  *E. Uzu, H. Kamada, and Y. Koike, Phys. Rev. C **68**, 061001 (2003)*
  *A. Deltuva and A. C. Fonseca, Phys. Rev. C **86**, 011001(2012)*

- Momentum lattice technique

  *O. A. Rubtsova, V. N. Pomerantsev, and V. I. Kukulin, Phys. Rev. C **79**, 064602 (2009)*

- Continuum discretization *(above break-up threshold?)*

  *A. Kievsky, M. Viviani, and L. E. Marcucci, Phys. Rev. C **85**, 014001 (2012).*

- Complex scaling method

  B.Giraud, K.Kato and A. Ohnishi, J. of Phys. A37 (2004),11575 (passing via spectral function)

  Y.Suzuki, W.Horiuchi, D.Baye, PTP,123 (2010) (passing via spectral function)

Complex scaling method (2b scattering)

J. Nuttal and H. L. Cohen, Phys. Rev. ***188*** *(1969) 1542*

Driven radial Schrödinger equation:

$$\Psi_l(r) = \Psi_l^{in}(r) + \Psi_l^{sc}(r)$$

$$\frac{\hbar^2}{2\mu}\left(-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + V_l(r) - k^2\right)\Psi_l^{sc}(r) = -V_l^s(r)\Psi_l^{in}(r)$$

$$\Psi_l(r\to\infty) = \hat{j}_l(kr) + A_l(k)\exp(ikr - l\frac{\pi}{2})$$

$$\Psi_l(r\to\infty) = F_l(kr) + A_l(k)\exp(ikr - l\frac{\pi}{2} - \eta\ln(2kr))$$

$$\Psi_l^{in}(r) \qquad \Psi_l^{sc}(r\to\infty)$$

Complex scaling: $r \longrightarrow re^{i\theta}$

$$\frac{\hbar^2}{2\mu}\left(-\frac{d^2}{e^{2i\theta}dr^2} + \frac{l(l+1)}{e^{2i\theta}r^2} + V_l(re^{i\theta}) - k^2\right)\widetilde{\Psi}_l^{sc}(r) = -V_l^s(re^{i\theta})\Psi_l^{in}(re^{i\theta})$$

Exp. bound by the short range pot. term V^s

$$\widetilde{\Psi}_l^{sc}(r\to\infty) \sim \exp(ikr) \sim \exp(-kr\sin\theta)$$

Exp. bound if $\theta<\pi/2$

$$\widetilde{H}x = b$$

Extraction of amplitudes:

- From the asymptote of the solution

$$A_l(k) = \widetilde{\Psi}_l^{sc}(r\to\infty)/\exp(ikre^{i\theta} + \ldots)$$

- Using Green's theorem

$$A_l(k) \sim \int \Psi_l^{in}(re^{i\theta})V_l^s(re^{i\theta})(\widetilde{\Psi}_l^{sc}(r) + \Psi_l^{in}(re^{i\theta}))e^{i\theta}dr$$

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Complex scaling method (Resonances)

Analiticity of the potential, limitation of the scaling angle:

$$V(r) \sim \exp(-\mu r^n) \longrightarrow \exp(-\mu r^n e^{in\theta})$$

Starts to diverge for $\theta > \pi/(2n)$

M. Rittby, N. Elander and E. Brandas, Phys. Rev. A 24 (1981) 1636

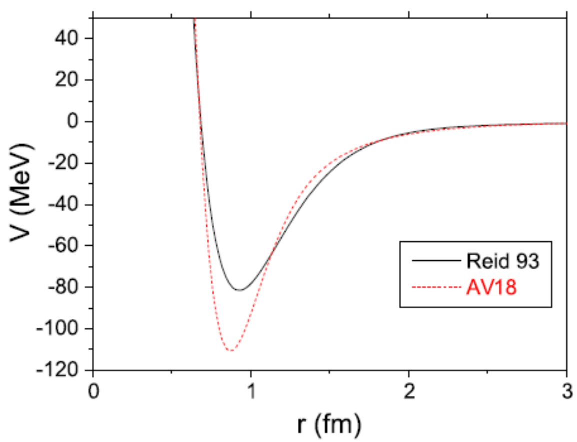
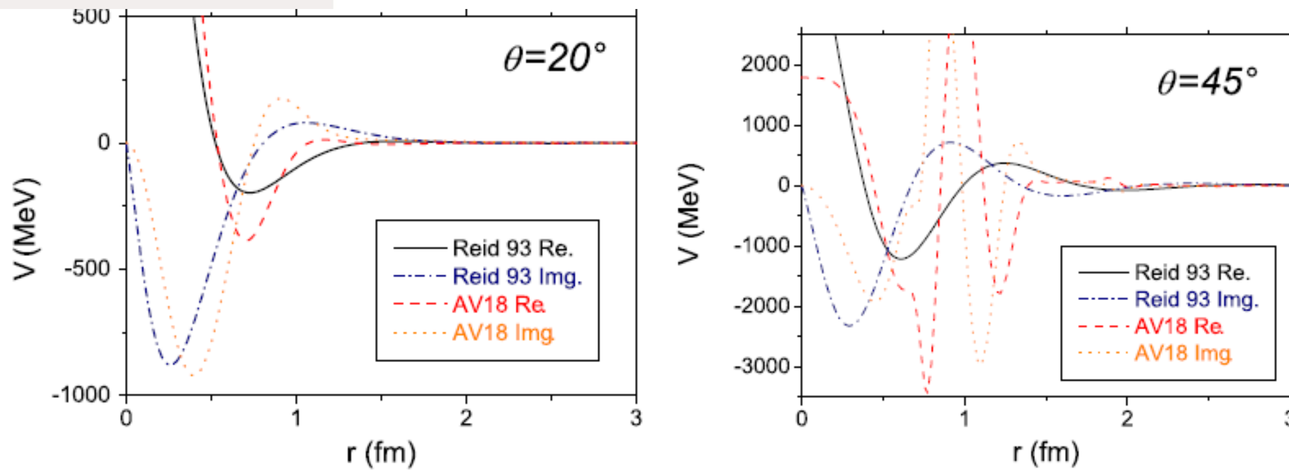


FIG. 1. (Color online) Reid 93 and AV18 $^1S_0$ *nn* potentials.



Hardcore propagates! Sets upper limit on angle θ.

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Complex scaling method (2b scattering)

Solution obtained by imposing $\varphi(r_{max})=0$ condition at the border r_{max} of the finite grid. Using spline discretization technique.

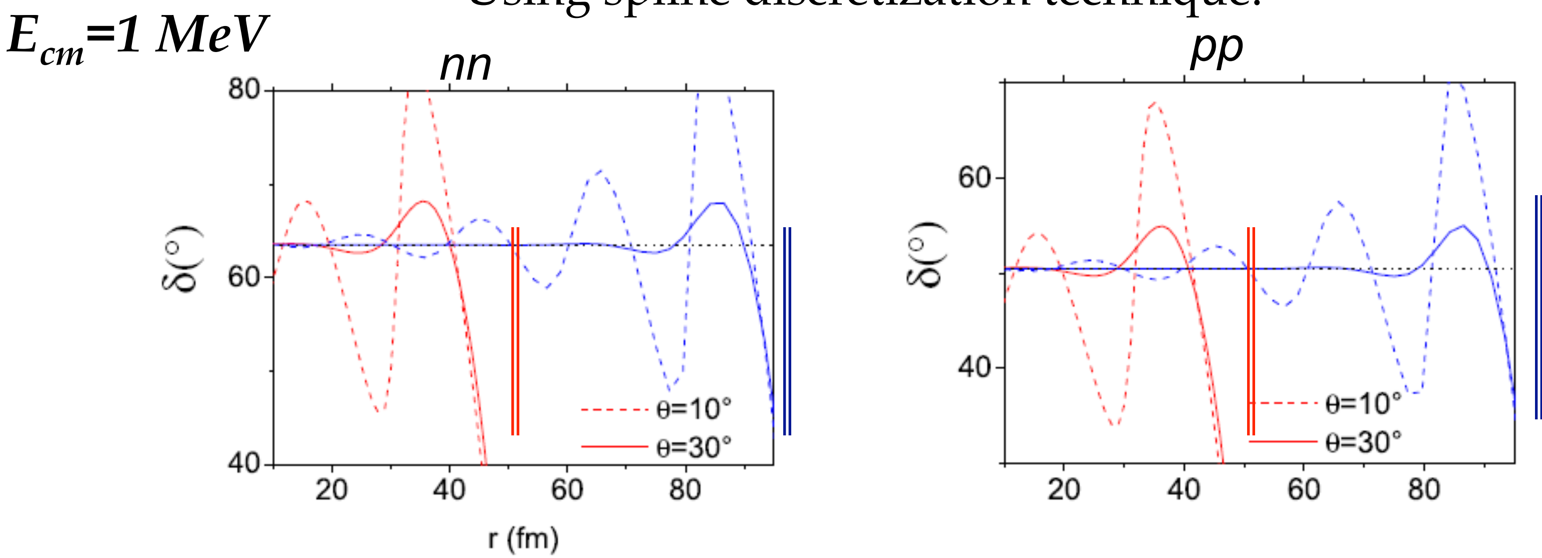
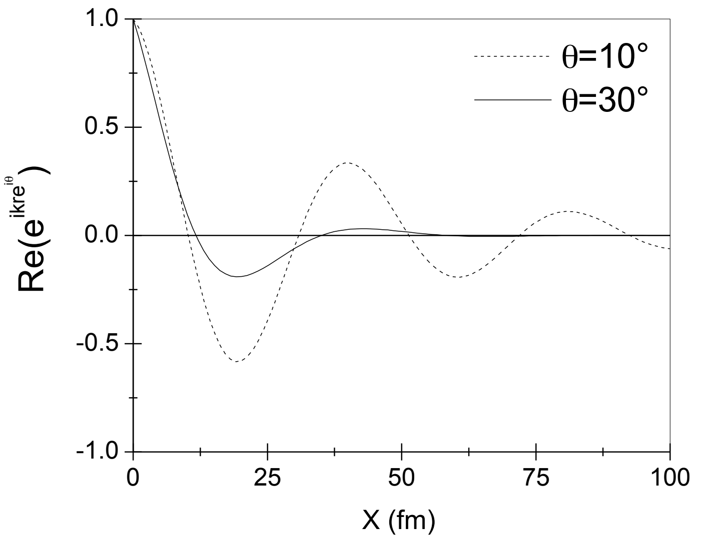


FIG. 1: (Color online) $^1S_0$ NN phaseshift at E_{cm}= … ly. Calculations
performed with cut-off imposed at r_{max}=50 and 1 … nes) and θ =30°
(solid line). Pure strong interaction result is prese… omb interaction
for pp-pair are presented in the right figure.



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Complex scaling method (2b scattering)

Solution obtained by imposing $\varphi(r_{max})=0$ condition at the border r_{max} of the finite grid.
Using spline discretization technique.

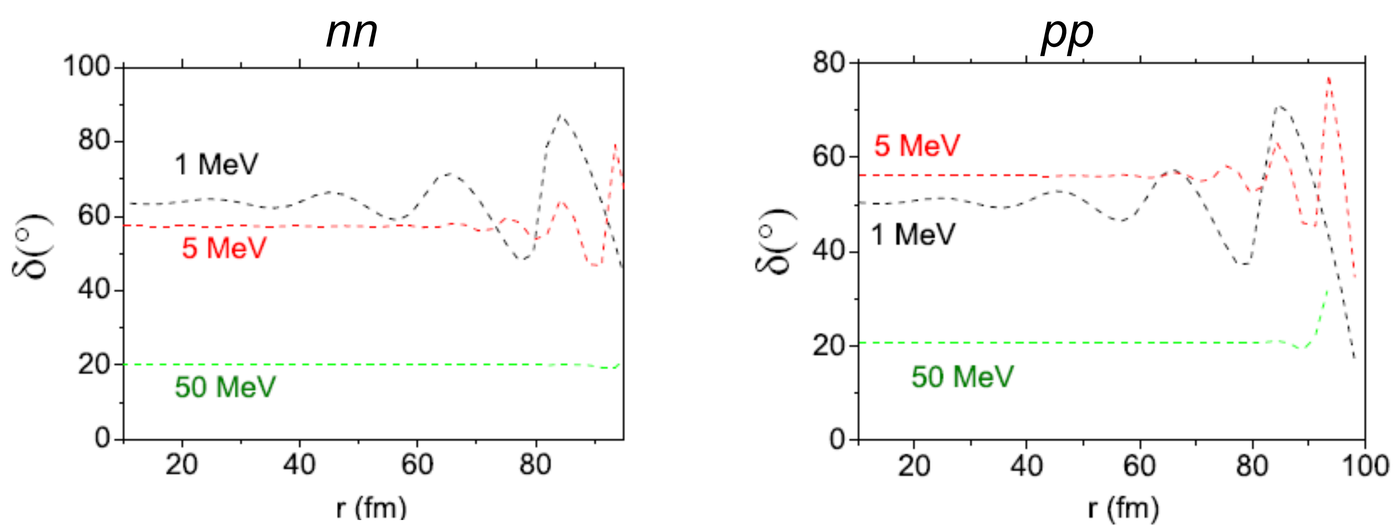
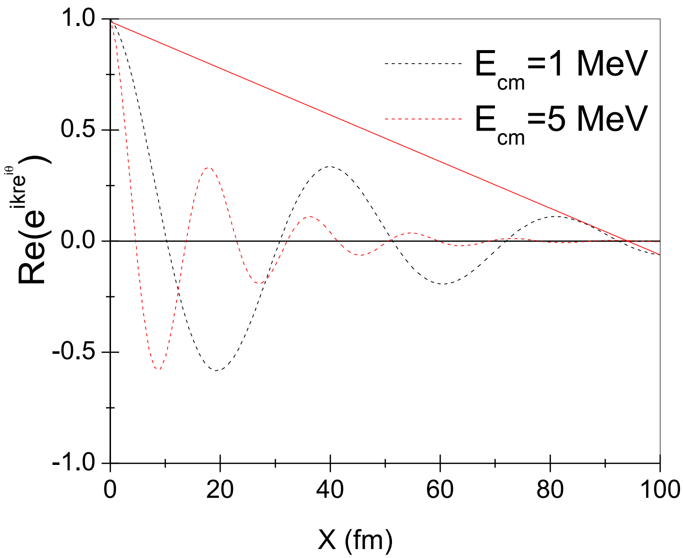


FIG. 2: (Color online) $^1S_0$ NN] … sing relations eq. 5-6 and 9-10
respectively. Calculations perforr … tion by the angle θ =10°. Pure
strong interaction result is prese … mb interaction for pp-pair are
presented in the right figure.



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Complex scaling method (2b scattering)

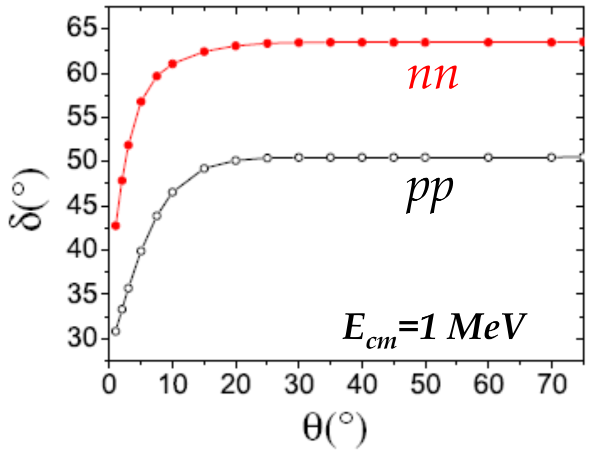
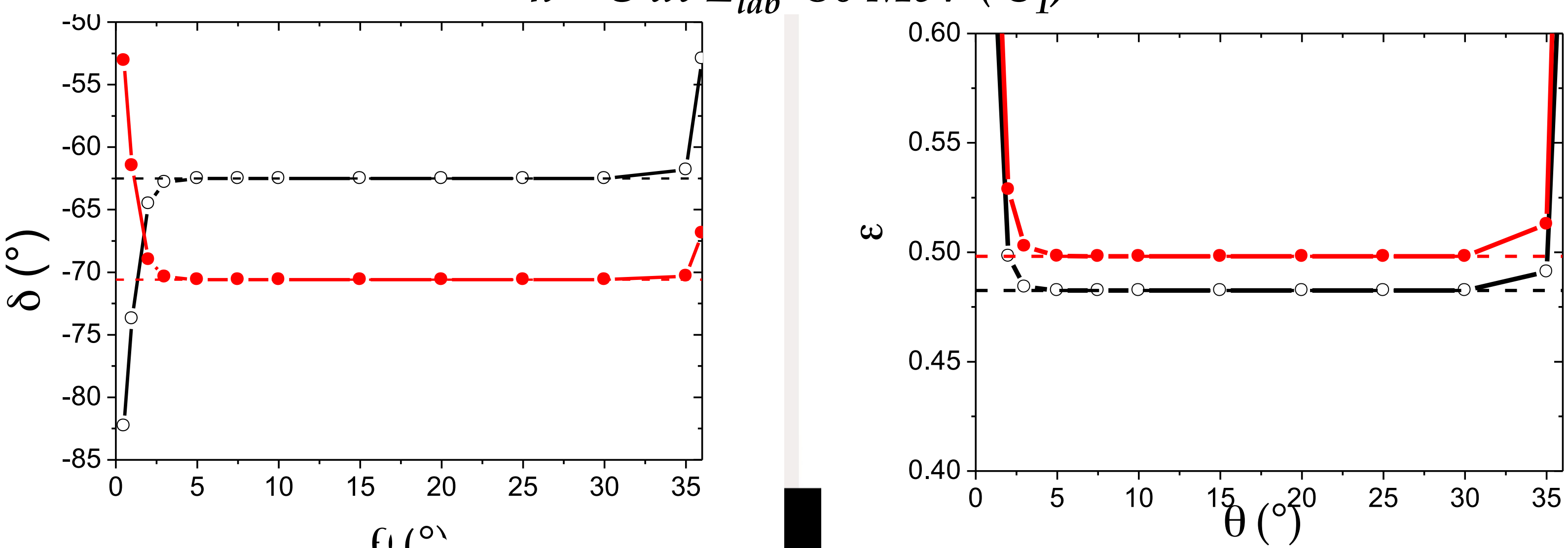


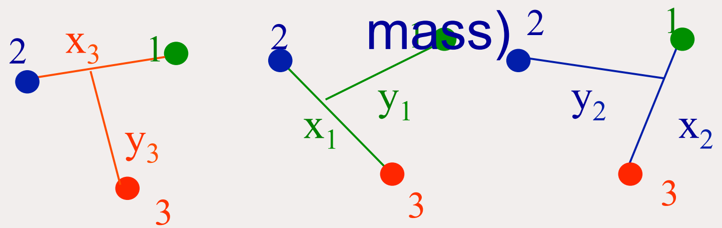
FIG. 3: (Color online) Dependence of the calculated NN $^1S_0$ phaseshift using integral expression as a function of the complex rotation angle. Grid was limited to r_{max}=100 fm. The upper curve correspond Coulomb-free case, the bottom one includes Coulomb.

n-^{12}C at E_{lab}=30 MeV ($^2S_1$)



Complex scaling method (3b scattering)

Faddeev eq. (particles of identical mass)



Jacobi coord :

$$\begin{cases} \vec{x}_k = \vec{r}_j - \vec{r}_i \\ \vec{y}_k = \sqrt{\frac{4}{3}}\left(\vec{r}_k - \frac{\vec{r}_j + \vec{r}_i}{2}\right) \end{cases}$$

Wave function

$$\Psi(\vec{x},\vec{y}) = \sum_{k=1}^{3} F_k(\vec{x}_k,\vec{y}_k)$$

Faddeev eq.:

$$\begin{cases} (E - V_1(x_1) - \hat{H}_0)F_1 - V_1(x_1)(F_2 + F_3) = 0 \\ (E - V_2(x_2) - \hat{H}_0)F_2 - V_2(x_2)(F_1 + F_3) = 0 \\ (E - V_3(x_3) - \hat{H}_0)F_3 - V_3(x_3)(F_1 + F_2) = 0 \end{cases}$$

Outgoing
2b or 3b wave

Driven Faddeev eq.:

$$F_1(\vec{x}_1,\vec{y}_1) = F_1^{in}(\vec{x}_1,\vec{y}_1) + F_1^{sc}(\vec{x}_1,\vec{y}_1)$$

$$F_1^{in}(\vec{x}_1,\vec{y}_1) = f_1^{l_x}(x_1)\hat{j}_{l_y}(qy_1)\left\{Y_{l_x}(\hat{x}) \otimes Y_{l_y}(\hat{y})\right\}_{LM}$$

$$\begin{cases} (E - V_1(x_1) - \hat{H}_0)F_1^{sc} - V_1(x_1)(F_2^{sc} + F_3^{sc}) = 0 \\ (E - V_2(x_2) - \hat{H}_0)F_2^{sc} - V_2(x_2)(F_1^{sc} + F_3^{sc}) = V_2(x_2)F_1^{in} \\ (E - V_3(x_3) - \hat{H}_0)F_3^{sc} - V_3(x_3)(F_1^{sc} + F_2^{sc}) = V_3(x_3)F_1^{in} \end{cases}$$

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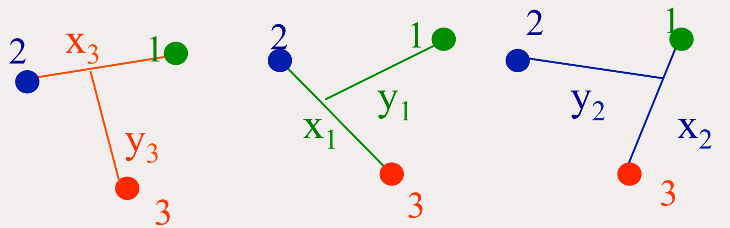
Complex scaling method (3b scattering)

Faddeev eq. (particles of identical mass)



Driven Faddeev eq.:

$$F_1(\vec{x}_1,\vec{y}_1) = F_1^{in}(\vec{x}_1,\vec{y}_1) + F_1^{sc}(\vec{x}_1,\vec{y}_1)$$

$$F_1^{in}(\vec{x}_1,\vec{y}_1) = f_1^{l_x}(x_1)\hat{j}_{l_y}(qy_1)\left\{Y_{l_x}(\hat{x})\otimes Y_{l_y}(\hat{y})\right\}_{LM}$$

Complex scaling $\quad x \longrightarrow xe^{i\theta}; \quad y \longrightarrow ye^{i\theta}$

Outgoing wave $F_1^{sc}(\vec{x}_1 e^{i\theta},\vec{y}_1 e^{i\theta})$ becomes exponentialy bound:

- 2-body plane out. waves

$$\sim \exp(-k_{bs}x)\exp(-qy\sin\theta) \qquad k_{bs} = \sqrt{\frac{m}{\hbar^2}|B_{bs}|}; \; q = \sqrt{\frac{2m}{3\hbar^2}E_{lab}}$$

- 3-body break-up out. wave

$$\sim \exp(-K\rho\sin\theta) \qquad K = \sqrt{\frac{m}{\hbar^2}\left(\frac{2}{3}E_{lab} - B_{bs}\right)}; \; \rho = \sqrt{x^2+y^2}$$

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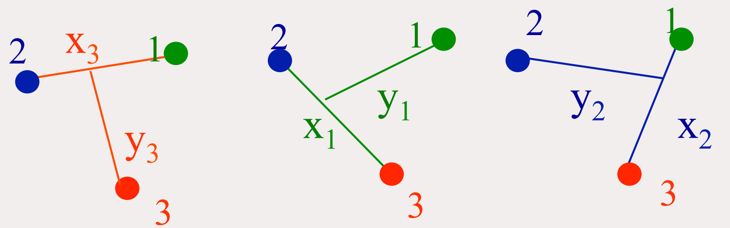
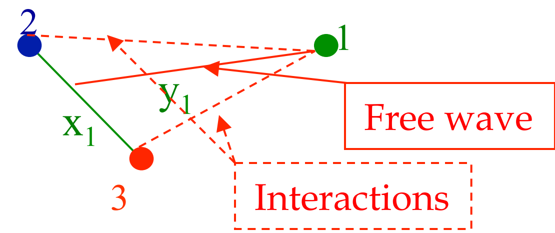
Complex scaling method (3b scattering)

Faddeev eq. (particles of identical mass)



$$\begin{cases} (E - V_1(x_1) - \hat{H}_0)F_1^{sc} - V_1(x_1)(F_2^{sc} + F_3^{sc}) = 0 \\ (E - V_2(x_2) - \hat{H}_0)F_2^{sc} - V_2(x_2)(F_1^{sc} + F_3^{sc}) = V_2(x_2)F_1^{in} \\ (E - V_3(x_3) - \hat{H}_0)F_3^{sc} - V_3(x_3)(F_1^{sc} + F_2^{sc}) = V_3(x_3)F_1^{in} \end{cases}$$



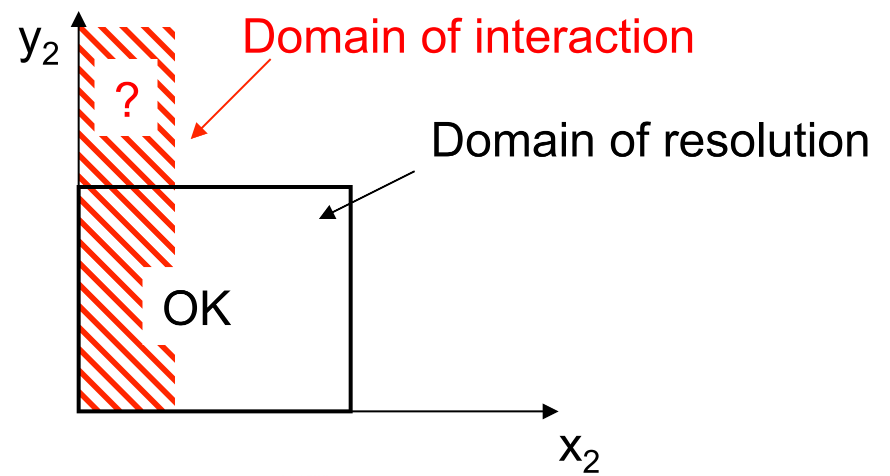
Complex scaling $\quad x \longrightarrow xe^{i\theta}; \quad y \longrightarrow ye^{i\theta}$

Ensure that the terms $V_2(x_2)F_1^{in}(\vec{x}_1 e^{i\theta}, \vec{y}_1 e^{i\theta})$ *and* $V_3(x_3)F_1^{in}(\vec{x}_1 e^{i\theta}, \vec{y}_1 e^{i\theta})$ are bound!!

$$\tan\theta < \frac{k\sqrt{3}}{q} = \frac{\sqrt{3B_{bs}}}{\sqrt{B_{bs} + \frac{2}{3}E_{lab}}}$$

Angle θ becomes small for large scattering energies E_{lab}

$V_2(x_2)F_1^{in}(\vec{x}_1 e^{i\theta}, \vec{y}_1 e^{i\theta})$



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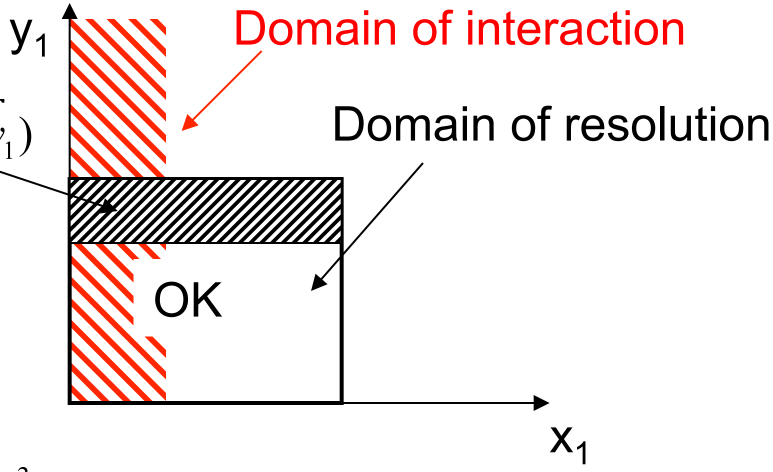
Complex scaling method (3b scattering)

Extraction of the scattering amplitudes:

- From the asymptote of the solution $\tilde{F}_1^{sc}(\vec{x}_1, \vec{y}_1)$

Cumbersome for break-up!!



- Using Green's theorem

$$A_l^{el}(q) \sim \iint \tilde{\Psi}_1^{in} \left[V_2^s(x_2 e^{i\theta}) + V_3^s(x_3 e^{i\theta}) \right] (\tilde{\Psi}^{sc} + \tilde{\Psi}_1^{in}) e^{6i\theta} d^3x d^3y$$

Solution: Faddeev equations+PW decomposition+spline discretization of xy

R. Lazauskas, PhD thesis, Université Joseph Fourier Grenoble (2003)

*R. Lazauskas and J. Carbonell, Phys. Rev. C **84 (2011)**, 034002*

Complex scaling method (3b scattering)

TABLE III: Neutron-deuteron scattering phaseshift and inelasticity parameter as a function of the complex rotation angle (
compared with benchmark results of [23, 24]. Our calculations has been performed by setting y_{max}=100 fm.

	3°	4°	5°	6°	7.5°	10°	12.5°	Ref. [23, 24]
				nd doublet at E_{lab}=14.1 MeV				
Re(δ)	105.00	105.43	105.50	105.50	105.50	105.49	105.48	105.49
η	0.4559	0.4638	0.4653	0.4654	0.4653	0.4650	0.4649	0.4649
				nd doublet at E_{lab}=42 MeV				
Re(δ)	41.71	41.63	41.55	41.51	41.45	41.04		41.35
η	0.5017	0.5015	0.5014	0.5014	0.5015	0.5048		0.5022
				nd quartet at E_{lab}=14.1 MeV				
Re(δ)	68.47	68.90	68.97	68.97	68.97	68.97	68.97	68.95
η	0.9661	0.9762	0.9782	0.9784	0.9783	0.9782	0.9780	0.9782
				nd quartet at E_{lab}=42 MeV				
Re(δ)	37.83	37.80	37.77	37.77	37.74	38.06	-	37.71
η	0.9038	0.9034	0.9032	0.9030	0.9029	0.8980	-	0.9033

Ref.[23] J. L. Friar et al.:, Phys. Rev. ***C 51*** *(1995) 2356.*
Ref.[24] A. Deltuva, A. C. Fonseca et al.:,, Phys. Rev. ***C 71*** *(2005) 064003.*

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Complex scaling method (3b scattering)

TABLE IV: Proton-deuteron scattering phaseshift and inelasticity parameter as a function of the complex rotation angle θ compared with benchmark values of [24]. Our calculations has been performed by setting y_{max}=150 fm.

	3°	4°	5°	6°	7.5°	10°	12.5°	Ref. [24]
				pd doublet at E_{lab}=14.1 MeV				
Re(δ)	108.46	108.43	108.43	108.43	108.43	108.43	108.42	108.41[3]
η	0.5003	0.4993	0.4990	0.4988	0.4986	0.4984	0.4981	0.4983[1]
				pd doublet at E_{lab}=42 MeV				
Re(δ)	43.98	43.92	43.87	43.82	43.78	44.83	-	43.68[2]
η	0.5066	0.5060	0.5056	0.5054	0.5052	0.5488	-	0.5056
				pd quartet at E_{lab}=14.1 MeV				
Re(δ)	72.70	72.65	72.65	72.64	72.64	72.63	72.62	72.60
η	0.9842	0.9827	0.9826	0.9826	0.9826	0.9828	0.9829	0.9795[1]
				pd quartet at E_{lab}=42 MeV				
Re(δ)	40.13	40.11	40.08	40.07	40.05	40.35	-	39.96[1]
η	0.9052	0.9044	0.9039	0.9036	0.9034	0.9026	-	0.9046

Ref.[24] A. Deltuva, A. C. Fonseca et al.:, Phys. Rev. ***C 71*** *(2005) 064003.*

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Complex scaling method (3b scattering)

TABLE V: Neutron-deuteron $^3S_1$ break-up amplitude calculated at E_{lab}=42 MeV as a function of the break-up angle ϑ.

	0°	10°	20°	30°	40°	50°	60°	70°	80°	90°
This work Re(^{3}S$_1$)	1.49[-2]	8.84[-4]	-3.40[-2]	-3.33[-2]	7.70[-2]	2.52[-1]	4.47[-1]	6.47[-1]	6.30[-1]	1.62[-1]
This work Im(^{3}S$_1$)	1.69[0]	1.74[0]	1.87[0]	1.92[0]	1.80[0]	1.68[0]	1.70[0]	1.96[0]	2.23[0]	3.17[0]
Ref. [23] Re(^{3}S$_1$)	1.48[-2]	9.22[-4]	-3.21[-2]	-3.09[-2]	7.70[-2]	2.52[-1]	4.51[-1]	6.53[-1]	6.93[-1]	1.05[-1]
Ref. [23] Im(^{3}S$_1$)	1.69[0]	1.74[0]	1.87[0]	1.92[0]	1.80[0]	1.67[0]	1.70[0]	1.95[0]	2.52[0]	3.06[0]

Ref.[23] J. L. Friar et al.:, Phys. Rev. C 51 (1995) 2356.

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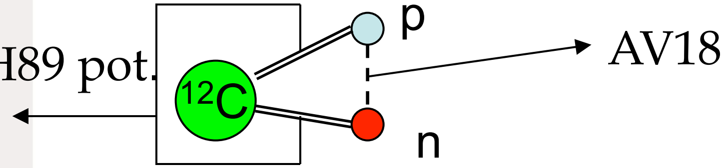
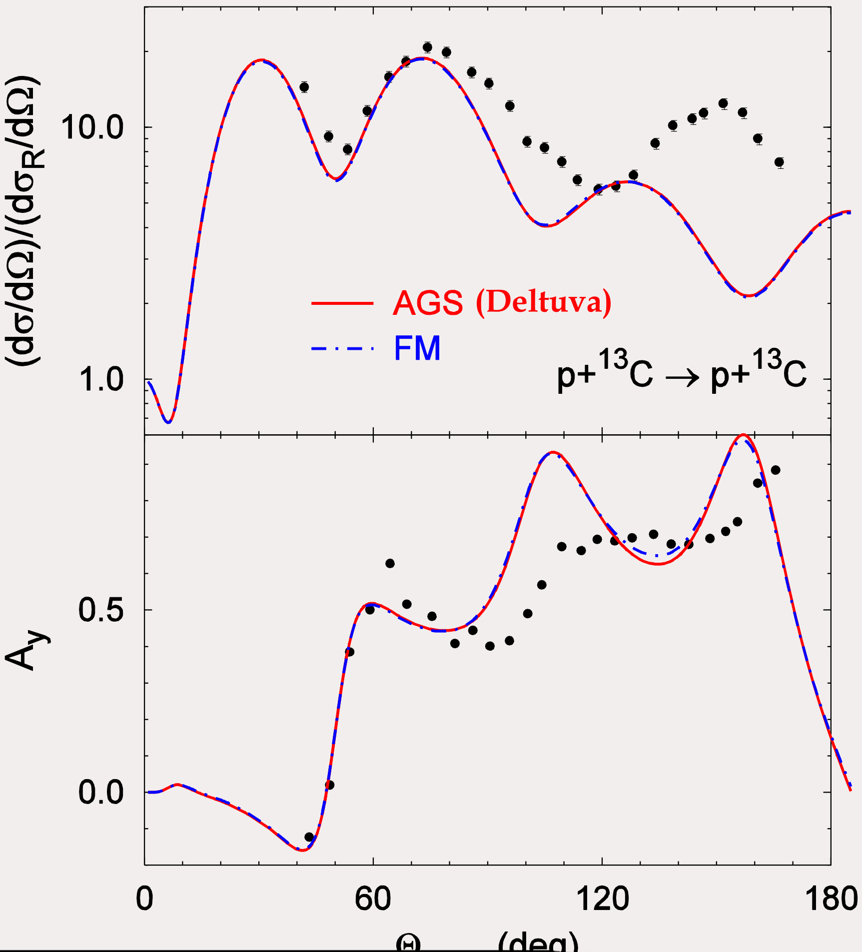
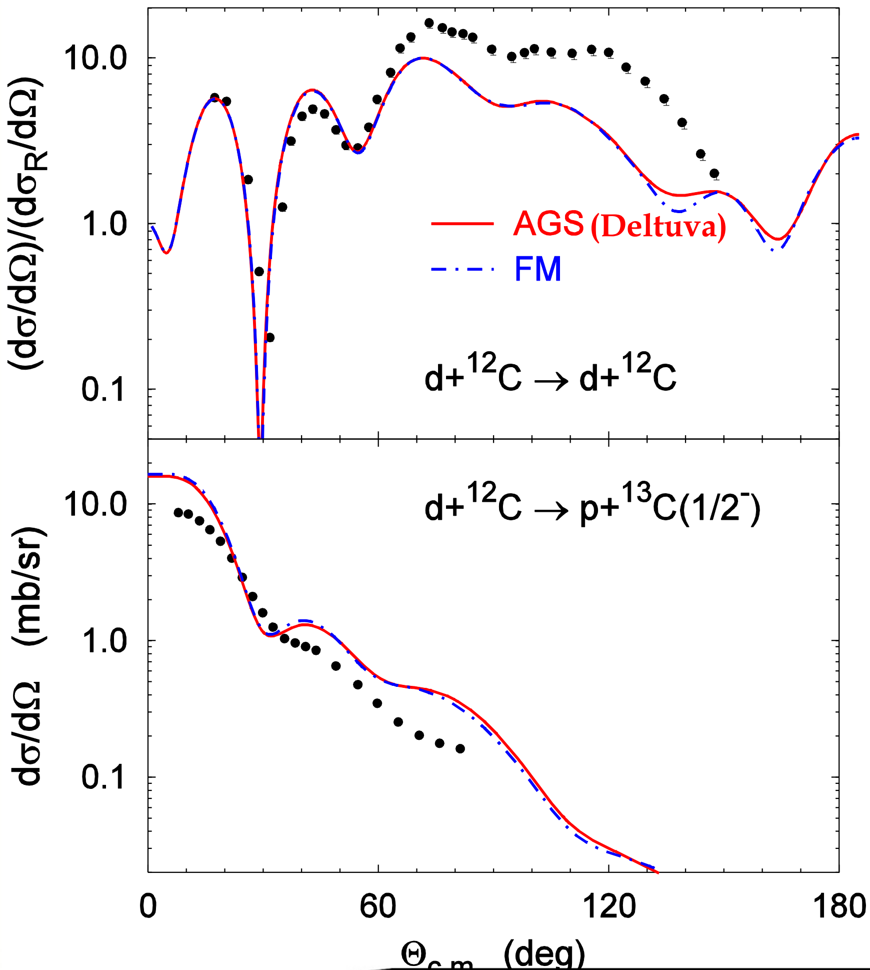
Complex scaling method (3-body system with optical pot.)

$$^{13}C + p \Leftrightarrow \begin{array}{l} ^{12}C + d \\ ^{13}C + p \\ ^{12}C + n + p \end{array}$$







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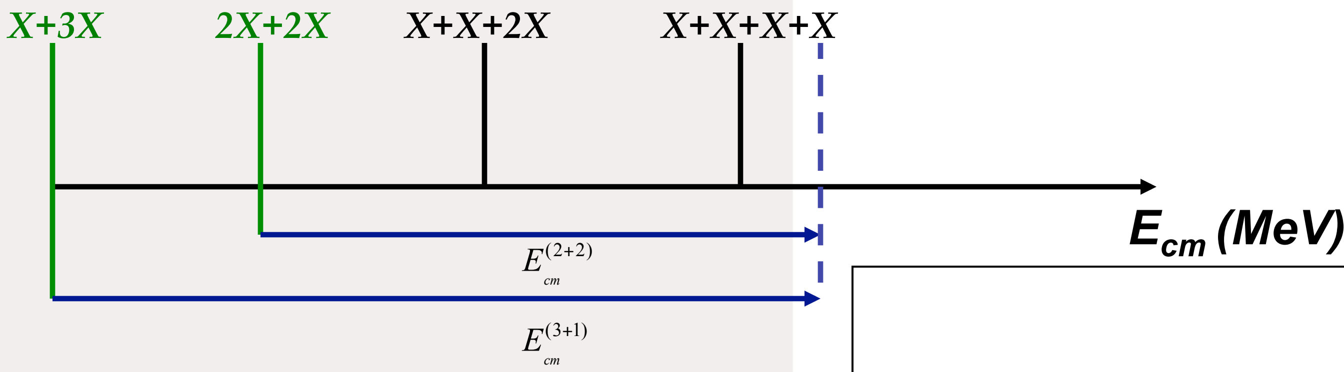
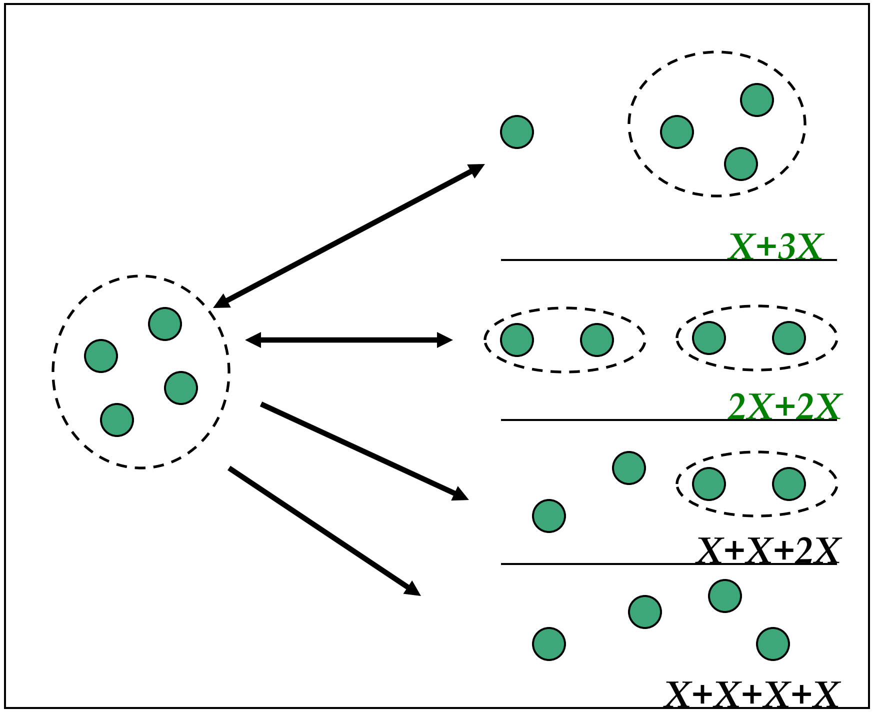
4-body system



Limitation for complex scaling angle:

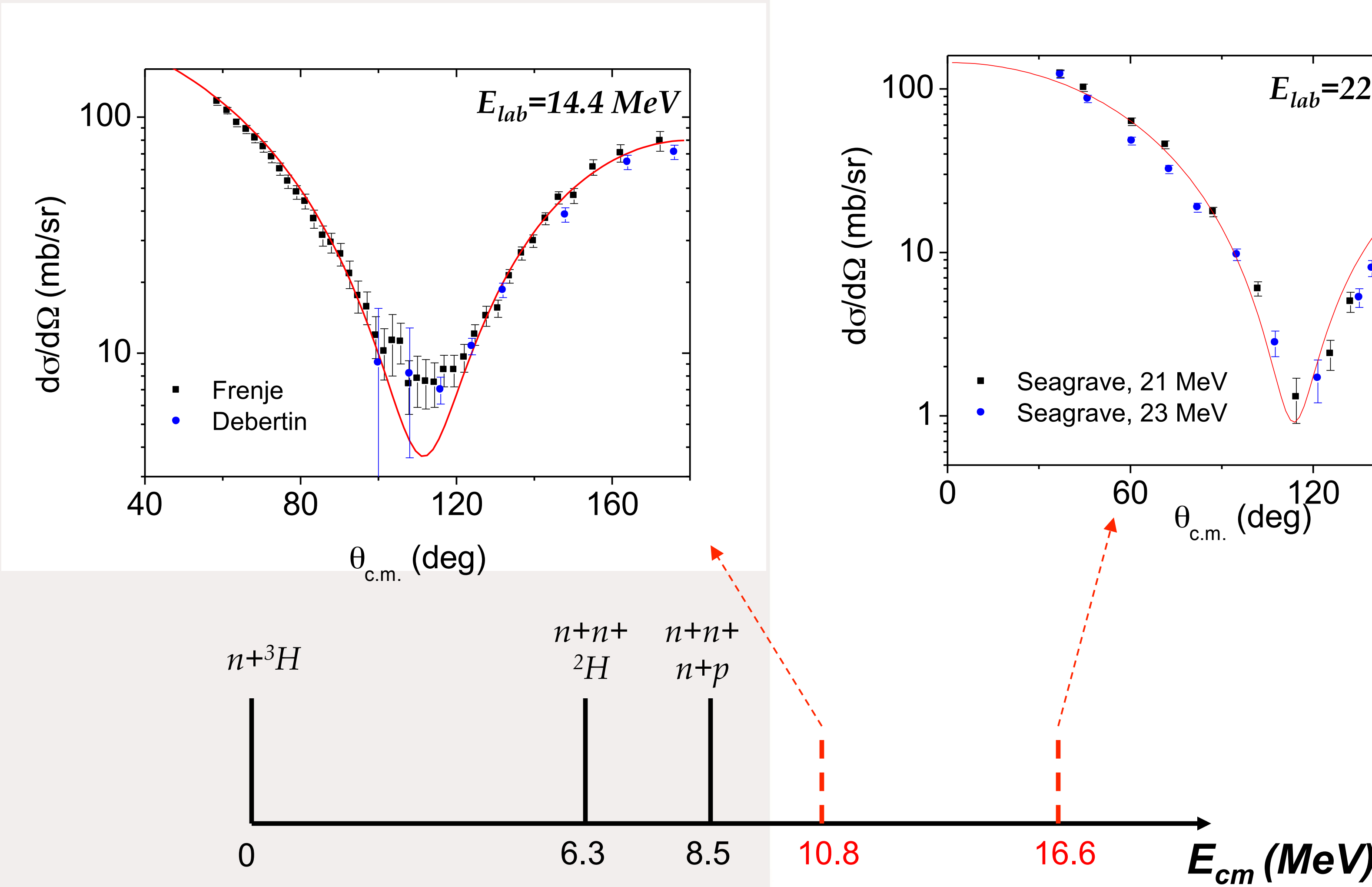
- 3+1 channels $\tan\theta < \dfrac{\sqrt{2B_3}}{\sqrt{E_{cm}^{(3+1)}}}$
- 2+2 channels $\tan\theta < \dfrac{\sqrt{2B_2}}{\sqrt{E_{cm}^{(2+2)}}}$



Solution: FY equations+PW decomposition+spline discretization of xyz

R. Lazauskas, PhD thesis, Université Joseph Fourier Grenoble (2003)

$n+^3H$ (T=1) scattering with MT I-III potential



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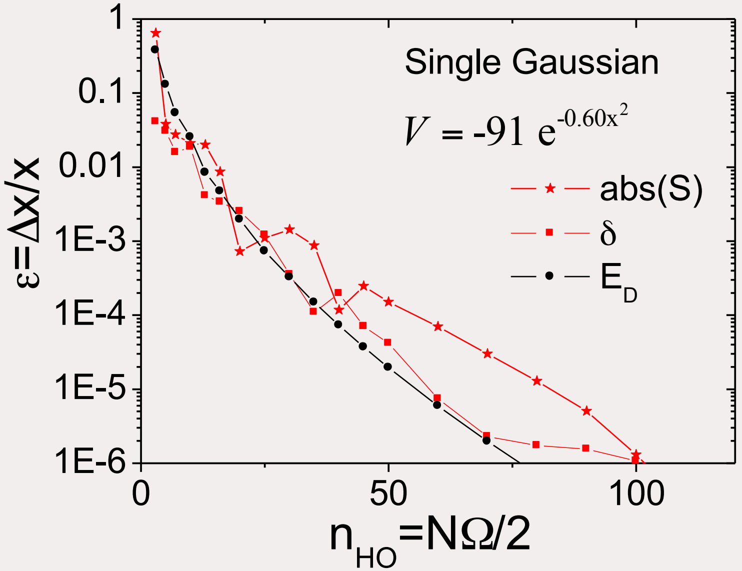
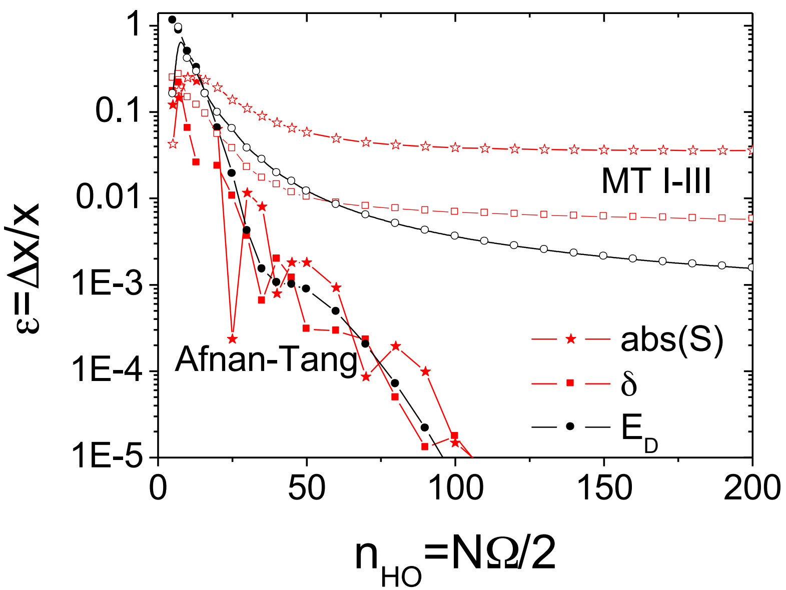
$n+^{3}H$ $(T=1)$ scattering with MT I-III potential

E_{lab} (MeV)	MT I-III (this work)			INOY (Deltuva)			Exp.
	σ_e (mb)	σ_b (mb)	σ_t (mb)	σ_e (mb)	σ_b (mb)	σ_t (mb)	σ_t (mb)
14.4	922	11	933	928	19	947	978 ± 70
18.0	690	25	715	697	41	738	750 ± 60
22.1	512	38	550	536	61	597	620 ± 24

NCSM application?

Deuteron binding energy calculation compared with np scattering calculation at 20 MeV for $^3S_1$ wave





$$Afnan-Tang: \quad V = 1000e^{-3x^2} - 326e^{-1.05x^2} - 43\ e^{-0.60x^2}$$

$$MT \quad I-III: \quad V = \frac{1438.72e^{-3.11x}}{x} - \frac{626.885e^{-1.55x}}{x}$$

- **Similar convergence (only less regular) as for the weakly bound state calculations**
- **Results for the soft potentials converge much faster**

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Method summary

👍 Trivial boundary conditions.
👍 Full information: elastic, inelastic and break-up amplitudes obtained after minimal modification of the bound state code
👍 Valid for any exponentially bound interaction, possible to include Coulomb. Inclusion of Coulomb for A>2 systems requires small improvable approximation - neglecting the action of the polarization terms on incoming wave.

😐 Problem solved in complex arithmetics.
😐 Potential must be analytical and remain short range after complex scaling (sets upper limit on θ)
😐 Additional limitation on θ for A>2 problem (sets upper limit on θ, this angle reduces when increasing scattering energy)

👎 Hamiltonian is not Hermitian anymore. It is more costly to ensure unitarity of the S-matrix. Nevertheless phases are obtained very accurately, convergence of inelasticity parameters if they are small (or close to 1) is slower.
👎 Difficulty to treat close to the threshold region (some of outgoing waves converge slowly)

Conclusion

- Complex scaling method is efficient tool to solve bound, resonant as well as continuum states problem without explicit treatment of the boundary conditions

- Scattering problem might be solved using bound state methods in complex arithmetic (almost by any config. space bound state technique and require very limited effort)

- Simple extension of the formalism to many-body scattering case

- Reliable results are already obtained for 3-body and 4-body elastic and break-up scattering, including long-range and optical potentials

"p+^{3}H" (T=0) scattering with MT I-III potential, (by ignoring Coulomb)

E_{cm}=20.5 MeV

		δ (°)	η
L=0	S=0	-56.6	0.650
	S=1	68.8	0.947
L=1	S=0	-85.3	0.945
	S=1	64.9	0.886
L=2	S=0	47.1	0.678
	S=1	1.09	0.896

E_{cm}=30. MeV

		δ (°)	η
L=0	S=0	-81.0	0.618
	S=1	56.9	0.882
L=1	S=0	78.9	0.918
	S=1	52.8	0.843
L=2	S=0	44.7	0.720
	S=1	4.49	0.851

$J^\pi=0^+$

E_{cm} (MeV)	MT I-III (this work)		Yamaguchi (Uzu)	
	δ (°)	η	δ (°)	η
7.3	-4.46	0.988	-5.51	0.899
20.5	-56.6	0.650	-61.7	0.746

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