Continuum and bound states

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Great progress in ab initio approach to bound states starting from realistic interactions

Predictability

Problems involving continuum states are still difficult esp. with realistic interactions

Application of bound state technique to continuum problem

Reducing the continuum problem to a class of bound-state problems in which L^2 basis functions are employed

References:

Y.S., W.Horiuchi, K.Arai, NPA823(2009) scattering

Y.S., W.Horiuchi, D.Baye, PTP123(2010) strength function

Y.S., D.Baye, A.Kievsky, NPA838(2010) coupled-channels scattering

Various problems including continuum states

Decay of resonance

A* ⟶ B+b, C+d+e

- Strength (response) function due to perturbation W

  A+W ⟶ A*, B+b, C+d+e

Radiative capture reactions

A+a ⟶ C+W(gamma)

(Inverse process: C+W ⟶ A+a)

- Two-body scattering and reactions

  A+a ⟶ B+b

I. Methods of strength function calculation

$$S(E) = \sum_{\nu} |\langle \Psi_\nu | W | \Psi_0 \rangle|^2 \delta(E_\nu - E)$$

$$= \langle \Psi_0 | W^\dagger \delta(H - E) W | \Psi_0 \rangle$$

$$= -\frac{1}{\pi} \mathrm{Im} \langle \Psi_0 | W^\dagger \mathcal{G}(E + i\epsilon) W | \Psi_0 \rangle$$

Ψ_0 ground state

Resolvent

$$\mathcal{G}(E) = \frac{1}{E - H}$$

This formulation is known for many years to include continuum effects
Shlomo & Bertsch, Recently Matsuo, Khan et al., others
It is limited to the case of single-particle in continuum,
based on a mean field theory

Extension to more general case is desired

Driven equation of motion method

$$S(E) = -\frac{1}{\pi}\mathrm{Im}\langle \Psi_0 | W^\dagger \underline{\mathcal{G}(E+i\epsilon) W | \Psi_0\rangle}$$

$$\Psi = \mathcal{G}(E+i\epsilon) W \Psi_0$$

$$S(E) = \frac{1}{\pi}\mathrm{Im}\langle \Psi | W | \Psi_0\rangle$$

$$\boxed{(H - E)\Psi = -W\Psi_0}$$

Outgoing-wave boundary condition

Double photoionization of two-electron atom
Exterior complex scaling
No application yet so far in nuclear physics

Complex scaling method

$$U(\theta) \qquad \boldsymbol{x} \to e^{i\theta}\boldsymbol{x}$$

Continuum is made
to damp asymptotically

$$S(E) = -\frac{1}{\pi}\mathrm{Im}\langle\Psi_0|W^\dagger U^{-1}(\theta)R(\theta)U(\theta)W|\Psi_0\rangle$$

$$R(\theta) = U(\theta)\mathcal{G}(E+i\epsilon)U^{-1}(\theta) = 1/(E - H(\theta) + i\epsilon)$$

$$H(\theta)\Psi^\lambda(\theta) = E^\lambda(\theta)\Psi^\lambda(\theta)$$

Non-Hermitian, but can be diagonalized in L^2 basis
Stability of S(E) wrt θis examined

Lorentz integral transform method

$$\mathcal{L}(z) = \int_{E_{\min}}^{\infty} \frac{S(E)}{(E-z)(E-z^*)} dE = \int_{E_{\min}}^{\infty} \frac{S(E)}{(E-E_R)^2 + E_I^2} dE$$

$$z = E_R + iE_I$$

$$\mathcal{L}(z) = \langle \Psi_0 | W^\dagger \mathcal{G}(z^*) \underline{\mathcal{G}(z) W | \Psi_0 \rangle}$$

$$= \langle \Psi(z) | \Psi(z) \rangle \qquad \Psi(z) = \mathcal{G}(z) W \Psi_0$$

$$\boxed{(H - z)\Psi(z) = -W\Psi_0}$$

L(z) is finite, hence the norm of Ψ(z) is finite, so that
Ψ(z) can be obtained in L^2 basis
L(z) has to be computed for many z values (E_R varied, E_I fixed)
to make the inversion possible

The inversion from L(z) to S(E) demands professional skill

Test in Solvable three-body problem

Hyperscalar potential $V(\rho) = V_0 \exp(-\kappa\rho^2)$

$$\rho^2 = \sum_{i=1}^{3} A_i(\boldsymbol{r}_i - \boldsymbol{x}_3)^2 = (1/A)\sum_{i<j} A_i A_j(\boldsymbol{r}_i - \boldsymbol{r}_j)^2$$

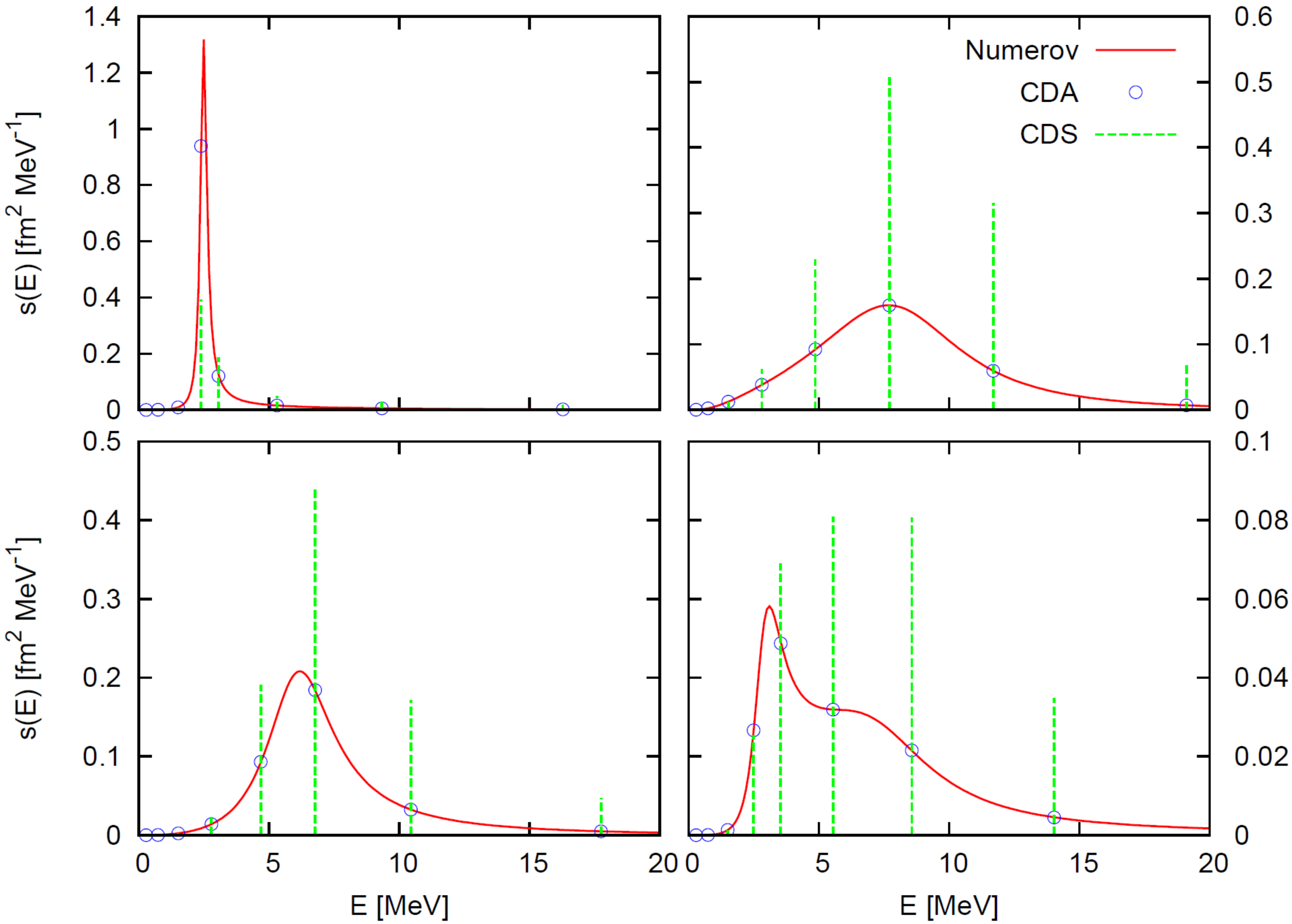
One charged particle, two neutral particles

(Numerically) Exactly solvable in Hyperspherical harmonics method

Set	V_0	κ	E_0	$\sqrt{\langle\rho^2\rangle}$
1	-110	0.16	-17.6	1.39
2	-90	0.16	-8.95	1.57
3	-75	0.16	-3.49	1.84
4	-610	0.25	-38.4	0.938
	570	0.16		
	-200	0.10		

Electric dipole strength

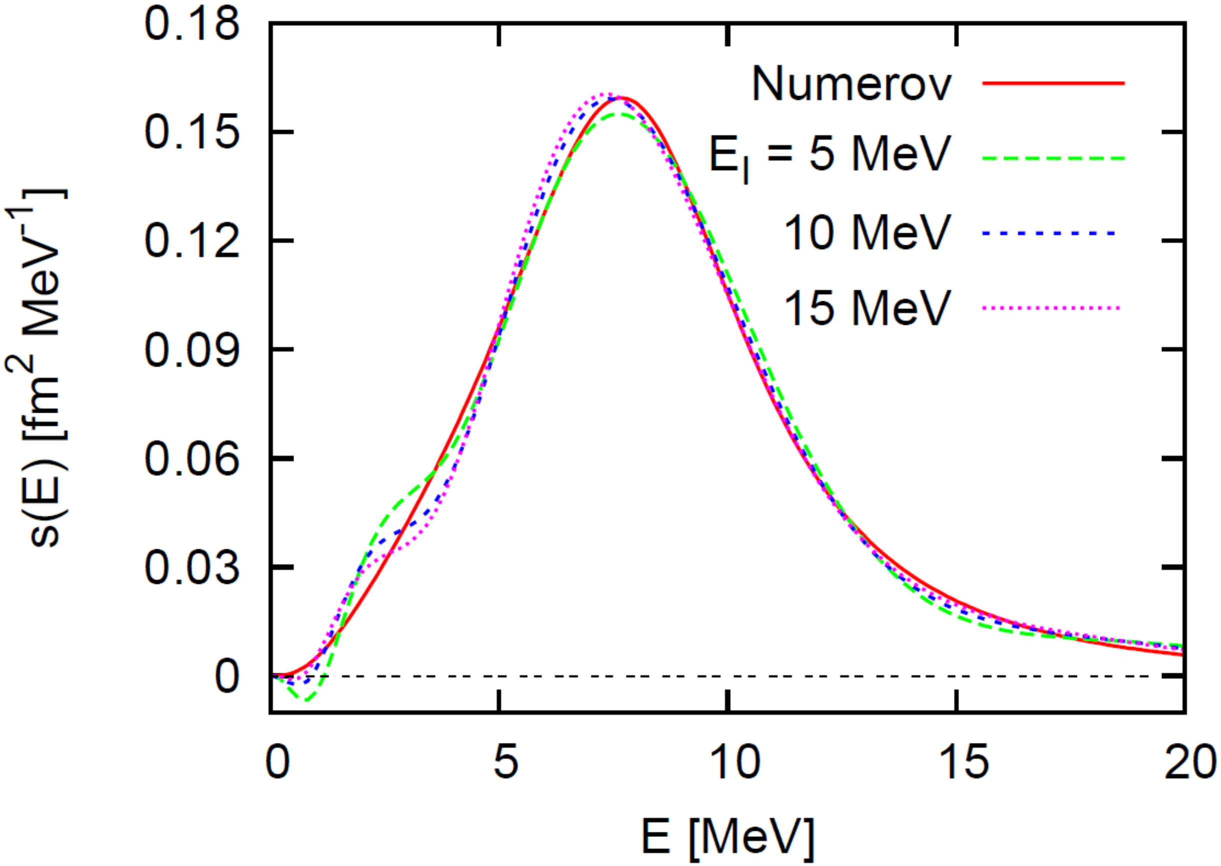
CDS: calculated from continuum discretized states
CDA: calculated from CDS with tail corrected



Set 1 (Left upper), Set 2 (Left lower), Set 3 (Right upper), Set 4 (Right lower)

Electric dipole strength

Lorentz integral transform method

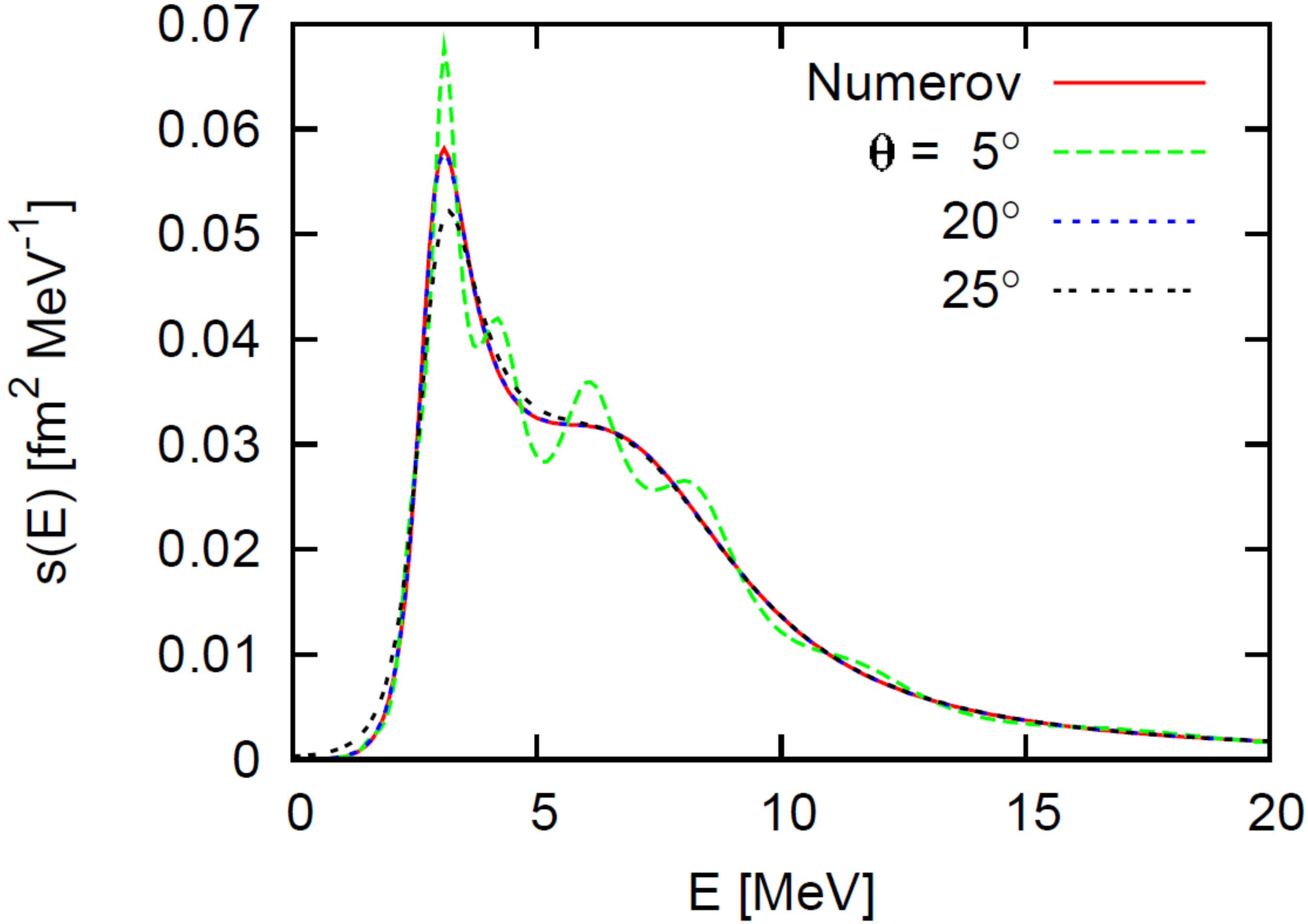


Set 3

Electric dipole strength

Complex scaling method

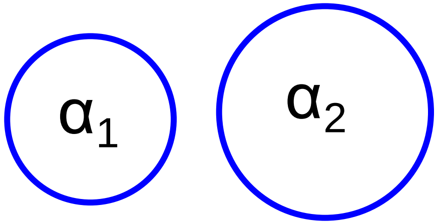
Set 4



For a fully-fledged application of complex scaling method
Next talk by W. Horiuchi

Strength functions of ^{4}He
using realistic nuclear interaction

II. Scattering problem



A single-channel case

$$H\Psi_{JM} = E\Psi_{JM}$$

with appropriate boundary condition

To make use of bound-state technique, we define **spectroscopic amplitude** (SA)

$$y(r) = \langle \Phi_{cJM}(r) | \Psi_{JM} \rangle$$

$$\Phi_{cJM}(r) = [[\psi_{I_1}(\alpha_1)\psi_{I_2}(\alpha_2)]_I Y_\ell(\hat{\boldsymbol{r}}_c)]_{JM} \frac{\delta(r_c - r)}{r_c r}$$

Phase shift is determined from the asymptotics of SA

Equation of motion for y(r)

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{\ell(\ell+1)}{r^2}-\frac{2\mu}{\hbar^2}U(r)+k^2\right]y(r)=\frac{2\mu}{\hbar^2}[z(r)+w(r)]$$

$$z(r)=\langle\Phi_{cJM}(r)\mid V_c-U\mid\Psi_{JM}\rangle \qquad V_c=\sum_{i\in\alpha_1,j\in\alpha_2}v_{ij}$$

U(r) : a local potential chosen to make V_c-U vanish for large r

$$w(r)=\langle\Phi_{cJM}(r)\mid H_{\alpha_1}-E_{\alpha_1}+H_{\alpha_2}-E_{\alpha_2}\mid\Psi_{JM}\rangle$$

Formal solution for y(r) with a proper asymptotics

$$y(r)=\lambda v(r)+\frac{2\mu}{\hbar^2}\int_0^\infty G(r,r')[z(r')+w(r')]r'^2dr'$$

Exact!

Green's function v(r) is a regular solution. λ is a constant to be determined

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{\ell(\ell+1)}{r^2}-\frac{2\mu}{\hbar^2}U(r)+k^2\right]G(r,r')=\frac{1}{rr'}\delta(r-r')$$

$$H\Psi_{JM} = E\Psi_{JM}$$

Diagonalize in L^2 basis set to obtain dicretized energies and approximate wave functions

$$\Psi_k = \mathcal{A}\{[[\psi_{I_1}(\alpha_1)\psi_{I_2}(\alpha_2)]_I Y_\ell(\mathbf{r})]_{JM} u_k(r)\} \quad k = 1, 2, \ldots$$

$$\Psi_{JM} \sim \sum_k C_k \Psi_k \qquad \sum_{k'} (H_{kk'} - EB_{kk'}) C_{k'} = 0$$

These ‘CDCC’ solutions are expected to be good in the interaction region but have bad asymptotics
Phase shifts are calculated at the discretized energies

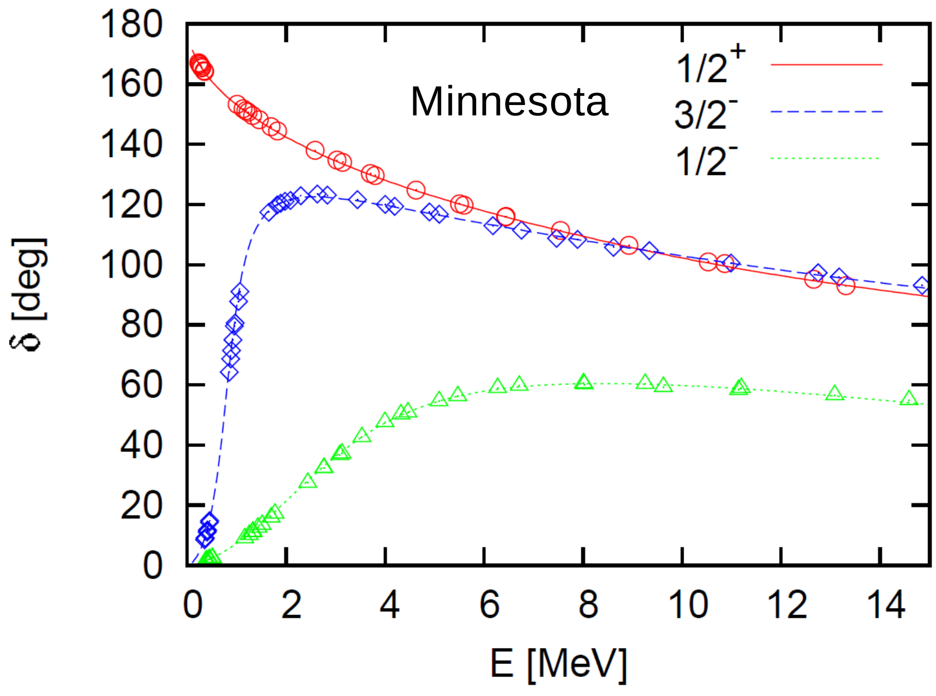
$$z(r) = \langle \Phi_{cJM}(r) \mid V_c - U \mid \Psi_{JM} \rangle \qquad y(r) = \langle \Phi_{cJM}(r) | \Psi_{JM} \rangle$$

z(r) is short-ranged, hence the exact wave function can be replaced with the approximate one in evaluating z(r)
λ is determined by comparing, at short distances, to the approximate y(r) calculated from this replacement

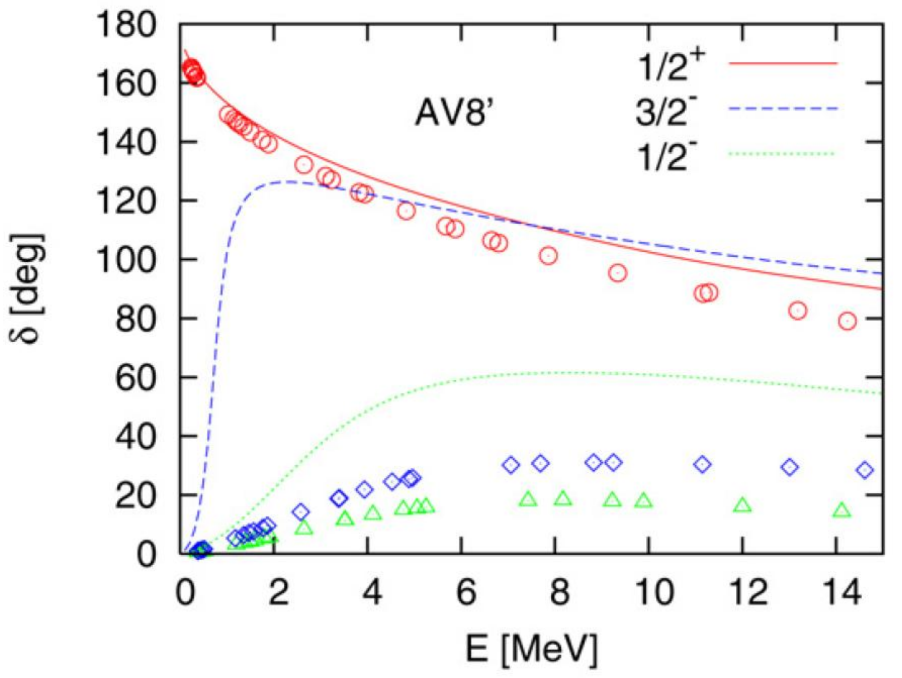
Green’s function assures correct asymptotics (GFM) α+n scattering in a single-channel calculation

- microscopic, full antisymmetrization
- use of elaborated α wave function
- Comparison with R-matrix or empirical p.s.

Effective force (C+LS)



Realistic force (C+T+LS)



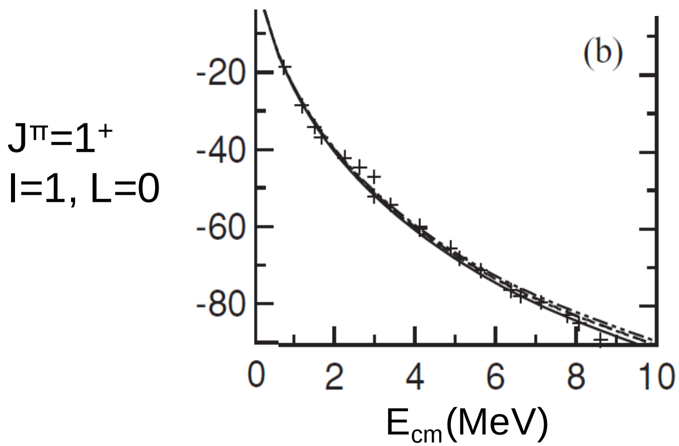
Discussion on α+n phase shifts

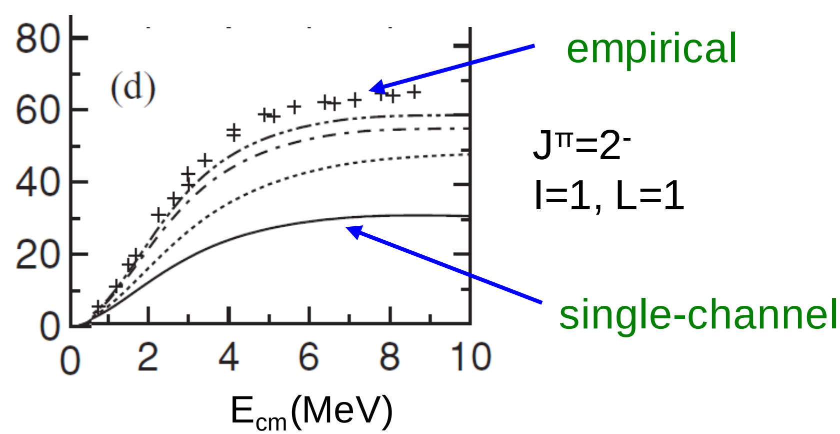
S-wave phase shifts are reasonable
P-wave phase shifts are too small
Understandable from Pauli principle

α: S-wave dominant, D-wave (< 15%)
P-wave neutron can penetrate into α
S-wave neutron is repelled by Pauli exclusion

αcan be distorted or excited by P-wave neutron particularly through tensor force
This effect cannot be accounted for in a single-channel RGM (Quaglioni & Navratil)

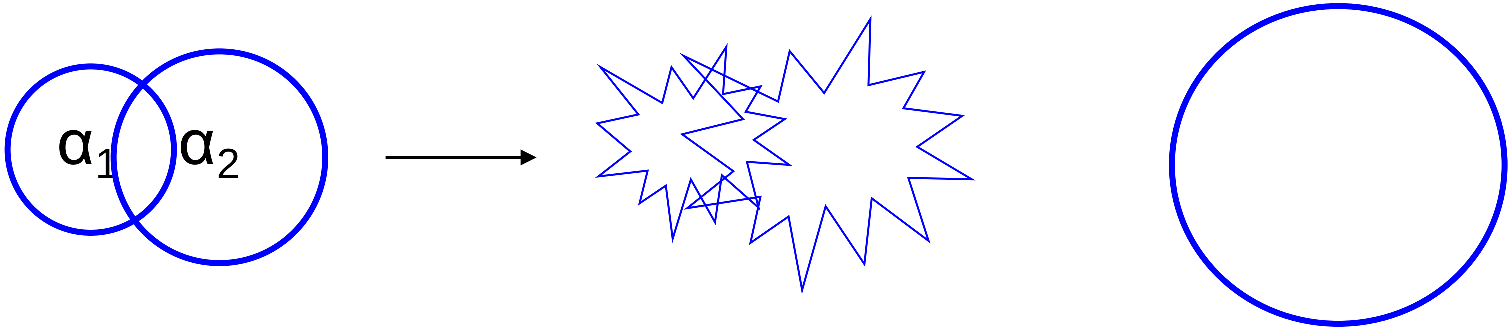
Similar phenomena in ^{3}He+p scattering: K.Arai, S.Aoyama, Y.S.,PRC81(2010)





Improving the solution in the interaction region is needed esp. for realistic interactions

1. To add many more channels (standard approach)
2. To solve A-body Schroedinger eq. more accurately in a confined region



For detailed analysis for d+d scattering including many distorted channels (method 1)

Talk by S. Aoyama
Cluster breaking effects in four nucleons scattering

Two problems remain:

1. Phase shifts are obtained only at discretized energies
   Scattering energy is not under control
2. Discretized solution is not degenerate, so that
   coupled-channels problems cannot be solved

To fix the problems:

Enclose the system within a set of walls and
adjust their strength to scattering energy

Only bound state solutions are needed

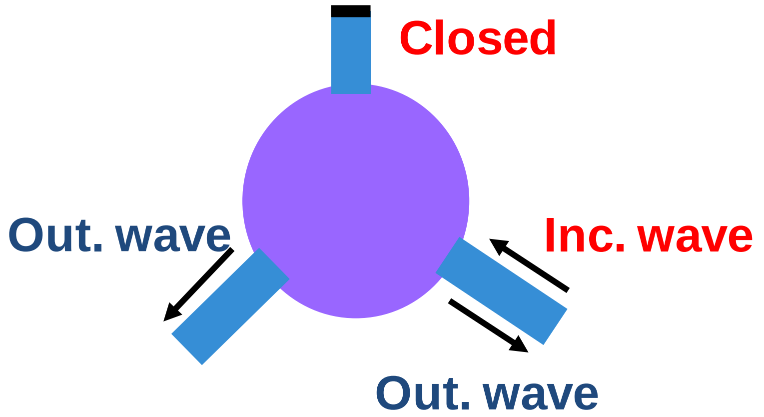
Coupled-channels case

$$-\frac{\hbar^2}{2\mu_c}\left(\frac{d^2}{dr^2}-\frac{\ell_c(\ell_c+1)}{r^2}+k_c^2\right)u_c(r)+\sum_{c'}\int_0^\infty V_{cc'}(r,r')u_{c'}(r')\,dr'=0$$

$$V_{cc'}(r,r')=V_{c'c}(r',r)$$

$$V_{cc'}(r,r')=0 \quad \text{for } r\geqslant a_c \text{ or } r'\geqslant a_{c'}$$

$$u_c(r)\to h_c^-(r)\delta_{c,c_0}-S_{cc_0}h_c^+(r)$$



$$\left(\frac{d^2}{dr^2}-\frac{\ell_c(\ell_c+1)}{r^2}+k_c^2\right)u_c(r)=\frac{2\mu_c}{\hbar^2}F_c(r)$$

$$F_c(r)=\sum_{c'}\int_0^\infty V_{cc'}(r,r')u_{c'}(r')\,dr'$$

$$u_c^k(r) = \lambda_c^k v_c(r) + \frac{2\mu_c}{\hbar^2} \int_0^\infty G_c(r, r') F_c^k(r') \, dr'$$

λ_c^k has to be determined $\qquad$ F_c^k has to be given

To reduce to a bound-state problem, add a confining potential

$$W_c(r) = 0 \quad \text{for } r \leqslant d_c \qquad\qquad W_c(r) \to \infty \quad \text{for } r \to \infty$$

$$a_c \leqslant d_c$$

Solution in the confining potential

$$-\frac{\hbar^2}{2\mu_c}\left(\frac{d^2}{dr^2} - \frac{\ell_c(\ell_c+1)}{r^2} + k_c^2\right) w_c(r) + \sum_{c'} \int_0^\infty V_{cc'}(r, r') w_{c'}(r') \, dr' + \underline{W_c(r) w_c(r)} = 0$$

- All the solutions become discrete bound states
- Both w_c and u_c satisfy the same eq. in the interaction region
- Tuning the strength of the confining potential in each channel generates the needed number of solutions with the same energy
- $V_{cc'}$ is short-ranged, u_c can be replaced with w_c in evaluating F_c

S-matrix calculation

$$u_c^k(r) = \lambda_c^k v_c(r) + \frac{2\mu_c}{\hbar^2} \int_0^\infty G_c(r,r') F_c^k(r')\, dr'$$

λ_c^k can be determined in the same way as before

A combination of $u_c^k(r)$ is a desired scattering solution

$$\sum_k \underline{X_{kc_0}} u_c^k(r) \rightarrow h_c^-(r)\delta_{c,c_0} - S_{cc_0} h_c^+(r)$$

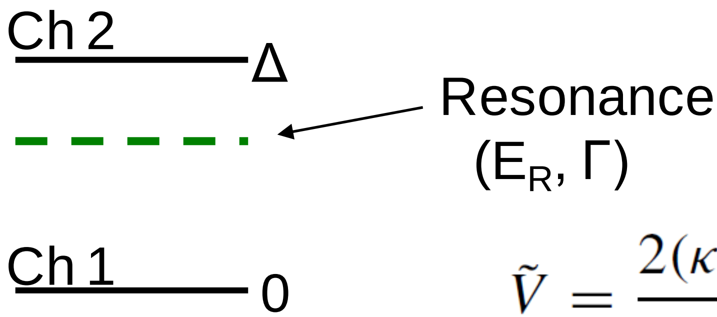
An example of the confining potential

$$W_c(r) = V_c\,(r - d_c)^2 \;\; H(r - d_c)$$

Adjust V_c to obtain the required energy

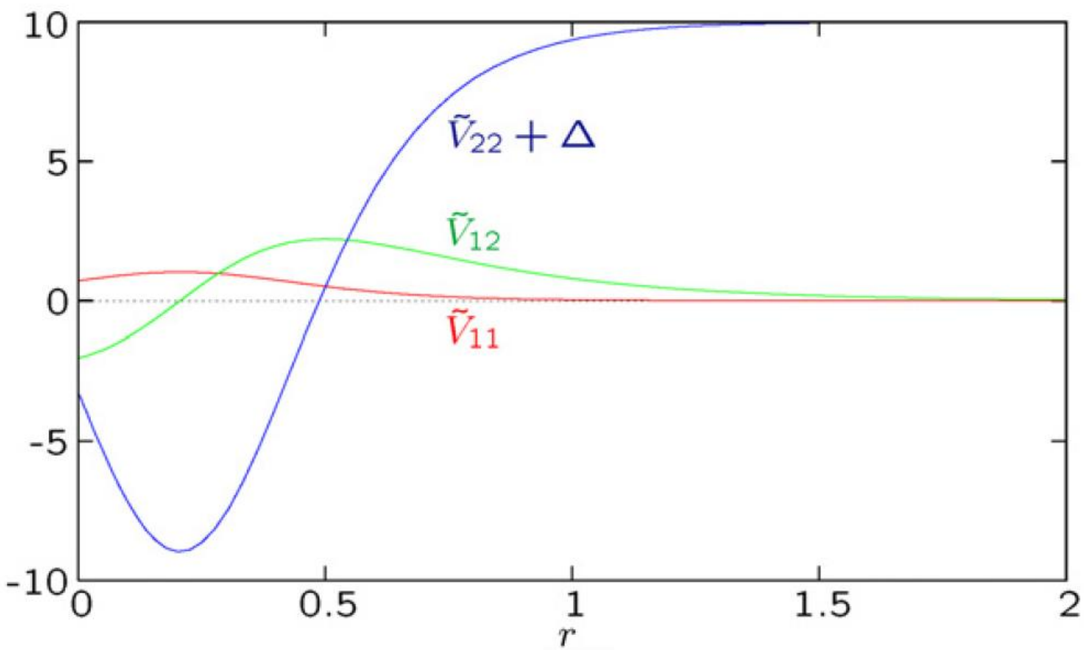
Exactly solvable 2-channel model with a Feshbach resonance

J.-M.Sparenberg et al., J.Phys.A39(2006)



$$\tilde{V} = \frac{2(\kappa_2 - \kappa_1)}{\cosh^2 y} \begin{pmatrix} \kappa_1 & \sqrt{\kappa_1 \kappa_2} \sinh y \\ \sqrt{\kappa_1 \kappa_2} \sinh y & -\kappa_2 \end{pmatrix}$$

$$y = (\kappa_2 - \kappa_1) r - \operatorname{arccosh} \sqrt{\kappa_1 \kappa_2 / \beta^2}$$

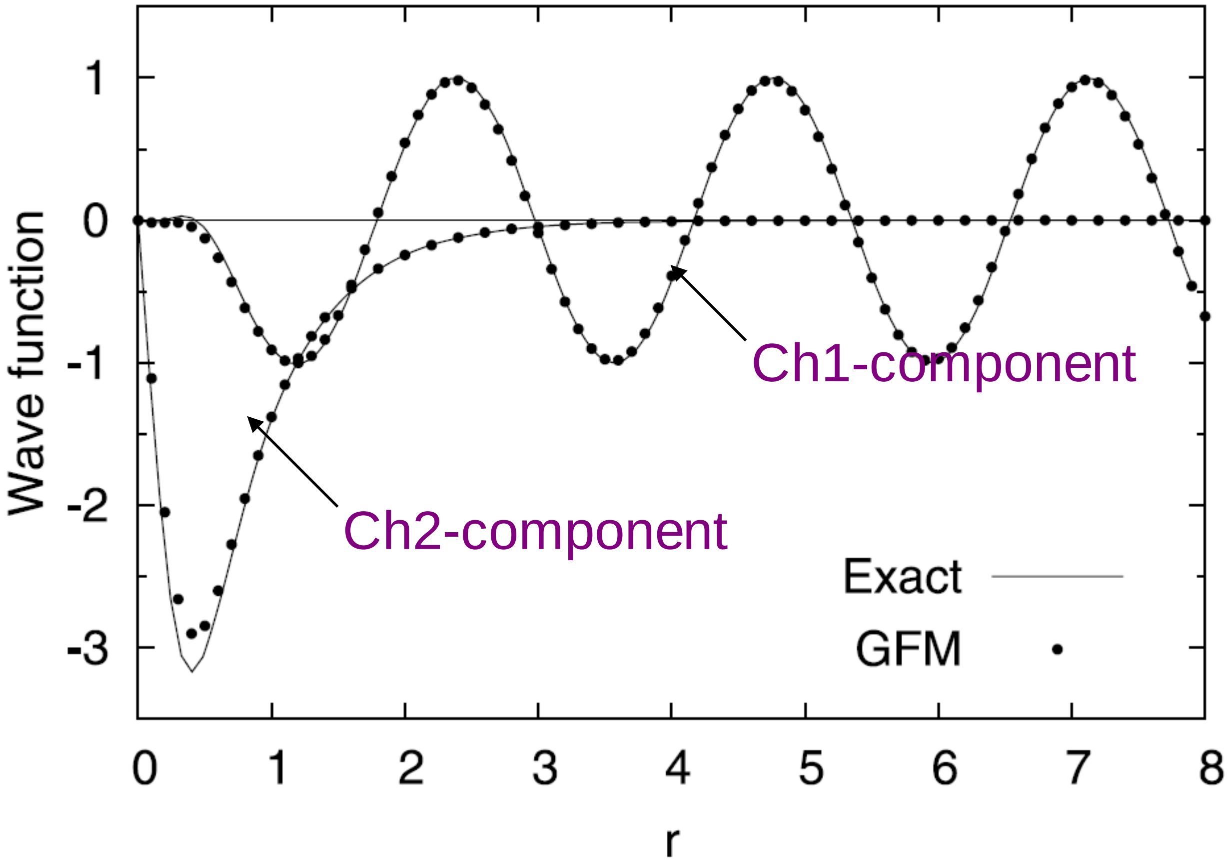


S-wave scattering

Δ=10
E_R=7
Γ=1

Comparison between the exact and GFM wave functions

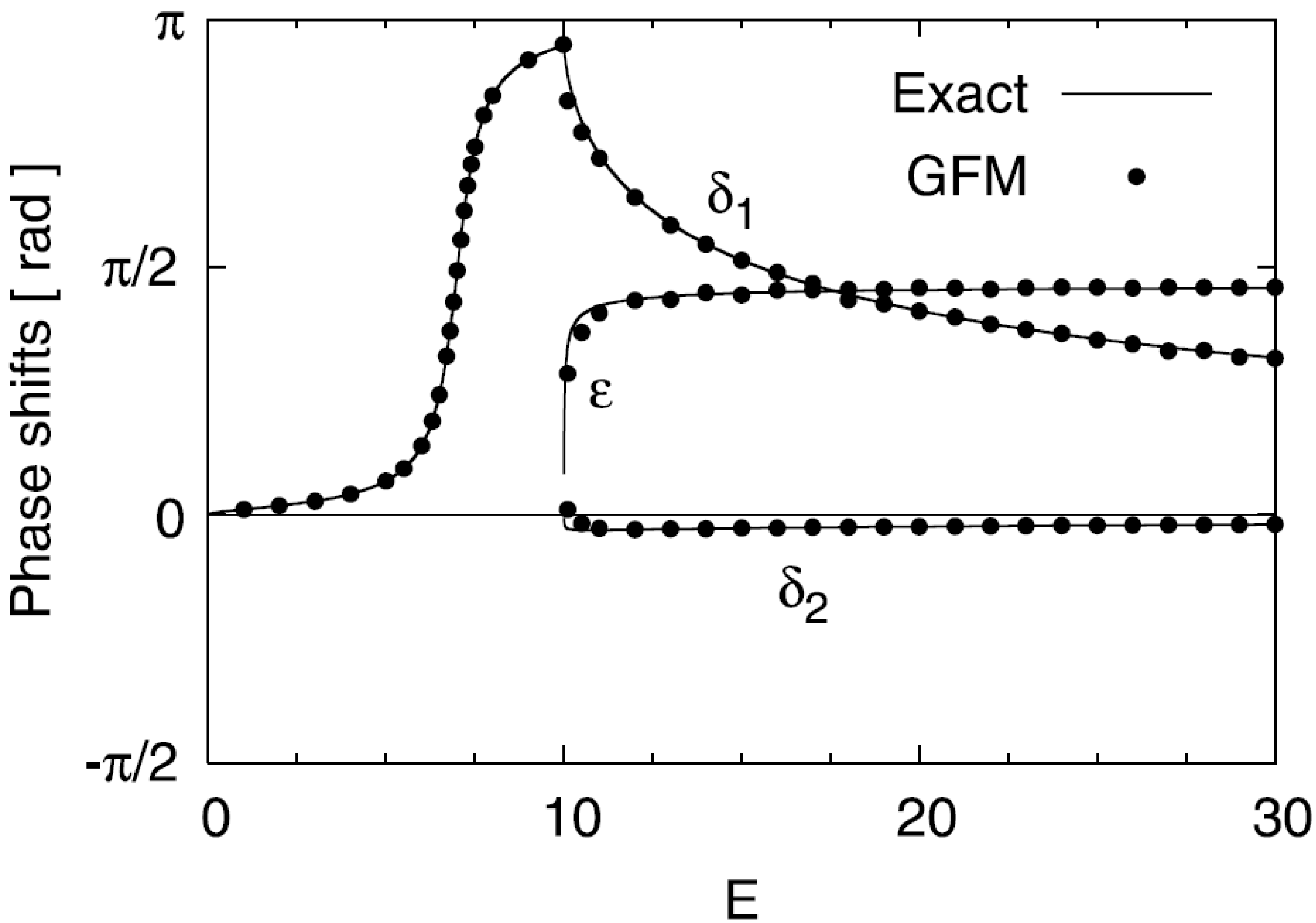
$$w_c(r) = \sum_{i=1}^{N_B} C_i^{(c)} \phi_{\ell_c}(a_i^{(c)}, r)$$



E = 7

Eigenphase rep.

$$S = \begin{pmatrix} \cos\varepsilon & -\sin\varepsilon \\ \sin\varepsilon & \cos\varepsilon \end{pmatrix} \begin{pmatrix} \exp(2i\delta_1) & 0 \\ 0 & \exp(2i\delta_2) \end{pmatrix} \begin{pmatrix} \cos\varepsilon & \sin\varepsilon \\ -\sin\varepsilon & \cos\varepsilon \end{pmatrix}$$



Conclusion

- Reducing continuum problems to a type of bound-state problems is discussed

- Complex scaling method appears versatile

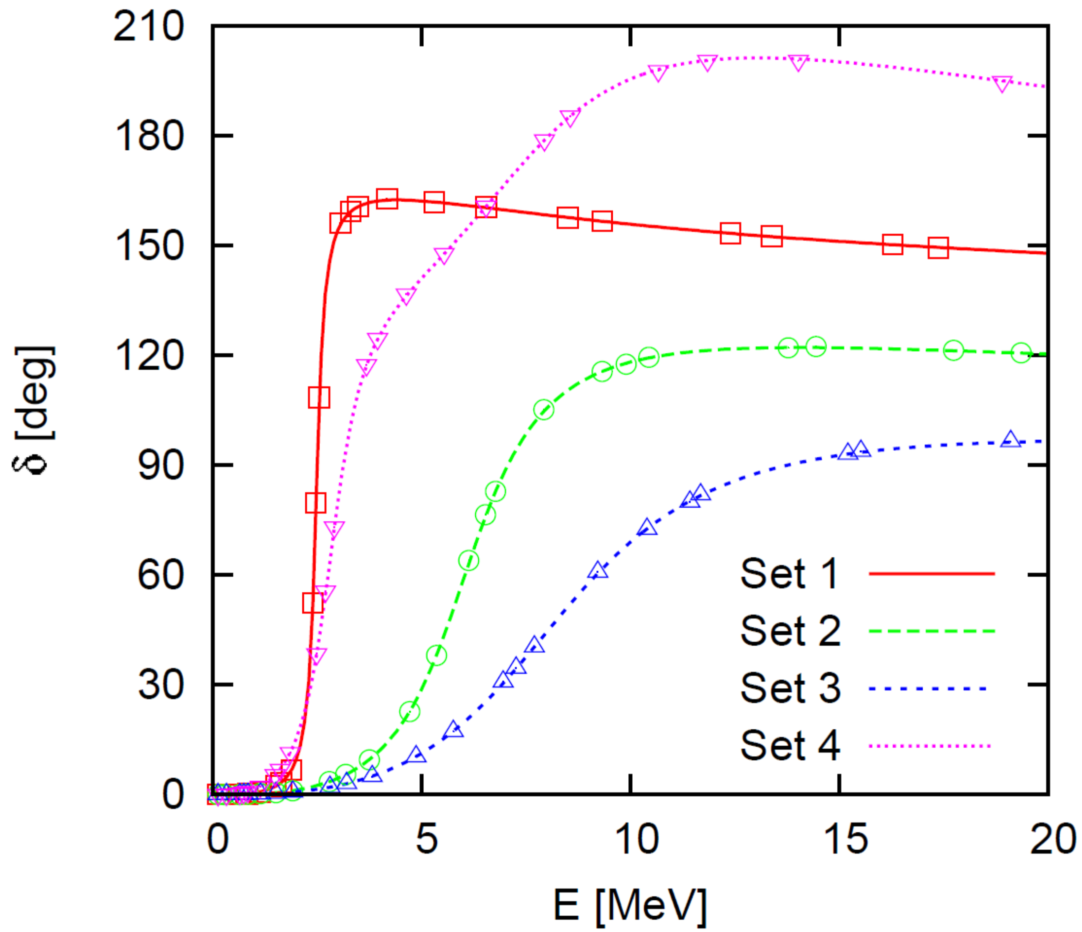
- Both wave functions and S-matrix for coupled-channels scattering problems can be obtained using bound-state codes
    real confining potentials acting only in external region

- Correct tail behavior is ensured with Green's function

- Application to real problems

P-wave (K=1) phase shifts
Numerov vs CDA
(continuum-discretized approximation)

Asymptotics corrected
with Green's function

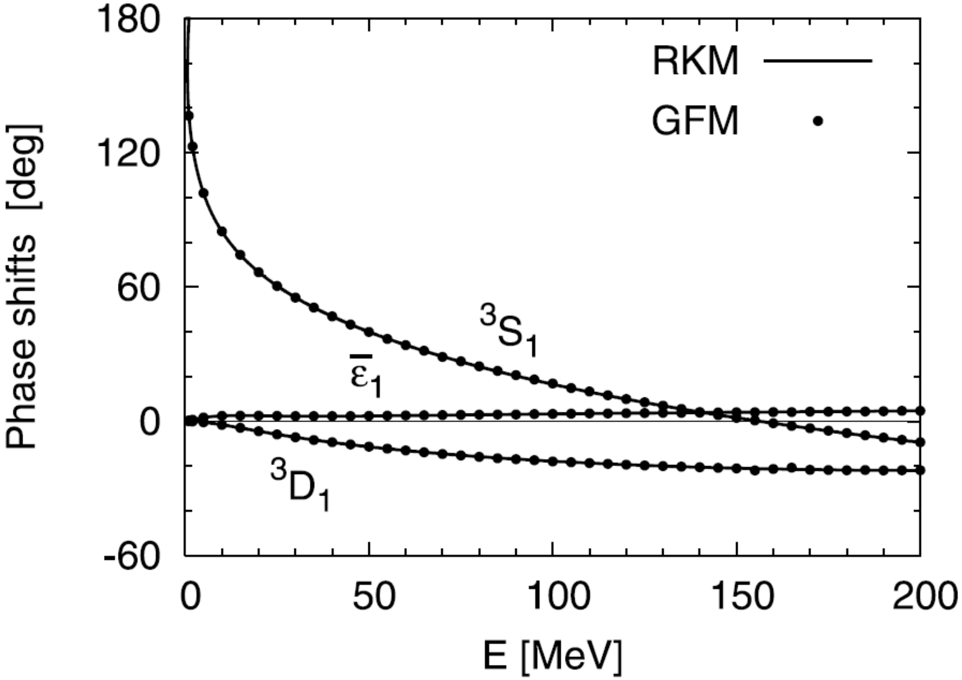


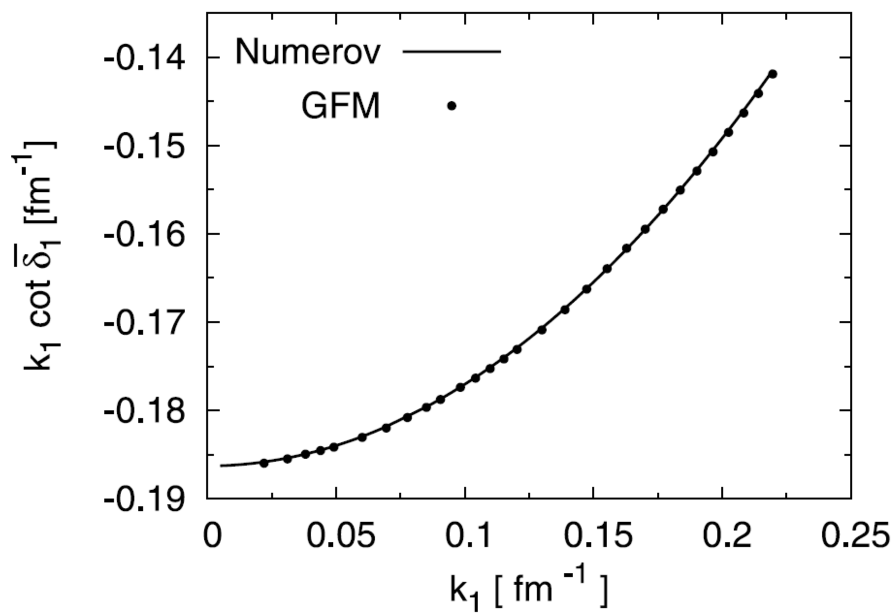
Nucleon-nucleon scattering

G3RS potential
Comparison with
numerical solutions

$^3S_1 + {}^3D_1$ pn scattering

$$S = \begin{pmatrix} \exp(i\bar{\delta}_1) & 0 \\ 0 & \exp(i\bar{\delta}_2) \end{pmatrix} \begin{pmatrix} \cos 2\bar{\varepsilon}_J & i \sin 2\bar{\varepsilon}_J \\ i \sin 2\bar{\varepsilon}_J & \cos 2\bar{\varepsilon}_J \end{pmatrix} \begin{pmatrix} \exp(i\bar{\delta}_1) & 0 \\ 0 & \exp(i\bar{\delta}_2) \end{pmatrix}$$





Good agreement in wide energy region

$^3P_2$ + $^3F_2$ pp scattering

G3RS potential
with Coulomb potential