Phase-shift calculation with realistic nuclear forces

--- Bridging bound (discrete) and continuum states ---

Y. Suzuki (Niigata)

Most of the present talk is based on

Y.S., W.Horiuchi, M.Orabi, K.Arai, FBS 42 (2008)
Detailed formulation with Correlated Gaussian basis
W.Horiuchi,Y.S., PRC78 (2008)
Application to ^{4}He levels with CG basis
Y.S., W.Horiuchi,**K.Arai**., arXiv:0812.4875 (submitted to NPA)
Phase-shift calculation in L^2-basis expansion method

Motivation

- NN interaction is characterized by strong short-range repulsion and long-range tensor force
  Interesting to analyze how nuclear spectrum evolves
- Accurate solution is possible for bound states of FBS

$$\text{square-integrable } (\mathcal{L}^2) \text{ basis functions}$$

- Scattering and reaction calculations with realistic NN forces are still difficult because of continuum states and boundary conditions

The aim is to apply $\mathcal{L}^2$ basis expansion method to problems of both discrete and continuum states with an emphasis on quantifying the role of central, tensor, … forces.

Variational Solution

$$\Phi(A,u,\alpha) = \mathcal{A}\Big\{\Big[\psi_L^{(\mathrm{orbital})}(A,u)\psi_S^{(\mathrm{spin})}(S_{12},S_{123},\ldots)\Big]_{JM} \times\psi_{TM_T}^{(\mathrm{isospin})}(T_{12},T_{123},\ldots)\Big\}$$

$$\alpha = (L,S,S_{12},\ldots,T_{12},\ldots)$$

$$\Psi_{JMTM_T} = \sum_{i=1}^{K} C_i\Phi(A_i,u_i,\alpha_i)$$

$$H_{ij} = \langle\Phi(A_i,u_i,\alpha_i)|H|\Phi(A_j,u_j,\alpha_j)\rangle$$

$$B_{ii} = \langle\Phi(A_i,u_i,\alpha_i)|\Phi(A_j,u_j,\alpha_j)\rangle$$

$$\sum_{j=1}^{K}(H_{ij}-EB_{ij})C_j = 0$$

Fulfillment of symmetry requirement: permutation, parity, translation, rotation

Explicitly correlated Gaussian (ECB) with angular function specified with global vectors

$$\Phi_{(LS)JM_JTM_T} = \mathcal{A}\left\{ e^{-\frac{1}{2}\tilde{\boldsymbol{x}}A\boldsymbol{x}} \left[\left[\mathcal{Y}_{L_1}(\widetilde{u}_1\boldsymbol{x})\mathcal{Y}_{L_2}(\widetilde{u}_2\boldsymbol{x}) \right]_L \chi_S \right]_{JM_J} \eta_{TM_T} \right\}$$

($\mathbf{x}_1,\ldots,\mathbf{x}_{N-1}$ Set of Jacobi coordinates but its choice is arbitrary)

$$\tilde{\boldsymbol{x}}A\boldsymbol{x} = \sum_{i,j=1}^{N-1} A_{ij}\boldsymbol{x}_i \cdot \boldsymbol{x}_j \qquad A_{ij} \neq 0$$

$$\mathcal{Y}_{LM}(\widetilde{u_1}\boldsymbol{x}) = |\widetilde{u_1}\boldsymbol{x}|^L Y_{LM}(\widehat{\widetilde{u_1}\boldsymbol{x}}) \qquad \widetilde{u_1}\boldsymbol{x} = \sum_{i=1}^{N-1} u_{1_i}\boldsymbol{x}_i$$

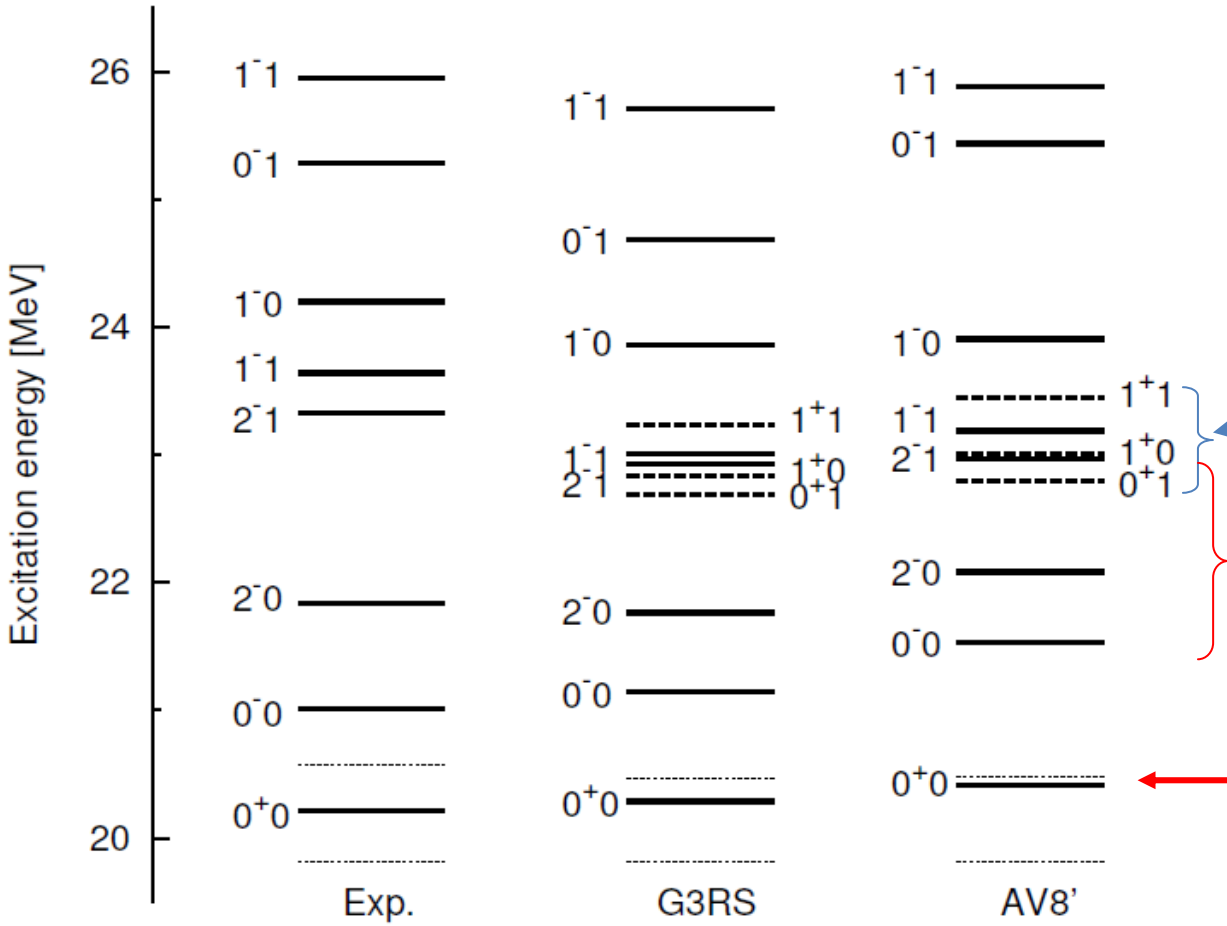
Parity=(-1)**(L_1+L_2) (Note: L=0, π =- needs three global vectors)

Elements of A, u_1, u_2 are variational parameters
and they are determined by a trial and error search
Variational solutions are obtained by SVM which consists of
enlargement of basis dimension and refinement of the bases

K.Varga, Y.S., PRC52(1995)
Y.S., K.Varga, Lecture Notes 54 (Springer, 1998)

Energy levels of ^{4}He

Lightest nucleus exhibiting the coexistence of different types of excitations



Role of tenor force in 0^-0 and 0^-1 spacing

$(J^\pi T=0^+1, 1^+0, 1^+1)$

P-wave cluster structure

(t+p)+(h+n) S-wave cluster structure

$J^\pi T=0^+0$

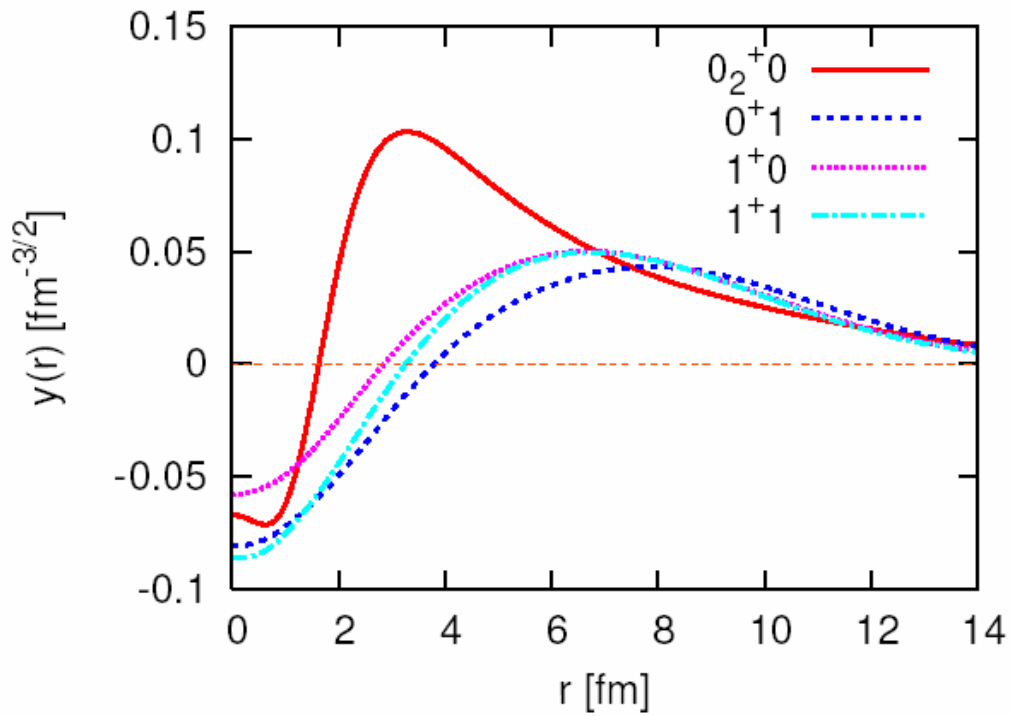
W.Horiuchi, Y.S., PRC78 (2008)

Spectroscopic amplitude (SA)

Useful to discuss clustering

$$A \leftrightarrow B + C \qquad y(r) = \langle \Psi(B)\Psi(C)|\Psi(A)\rangle$$

SAs of the quartet for the S-wave $^3\mathrm{He} + n$ decay

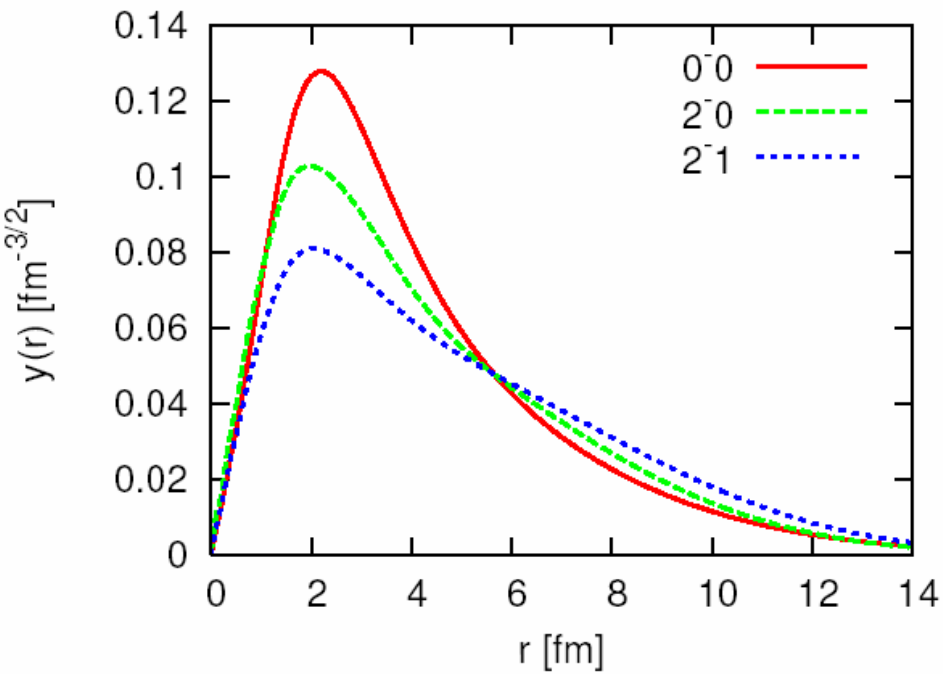


$3N$ radius ~ 2.3 fm

Only 0_2^+0 has a peak near 3N surface, indicating a resonance

Negative parity partners

SAs of the three lowest negative parity states for the P-wave ^{3}He+n decay with I=1



Peak position
Centrifugal barrier

Width of 0^- : 0.61 MeV (Cal)
0.84 MeV (Exp)

3N+N cluster structure → **Inversion doublet**

Energy contents of the negative parity states

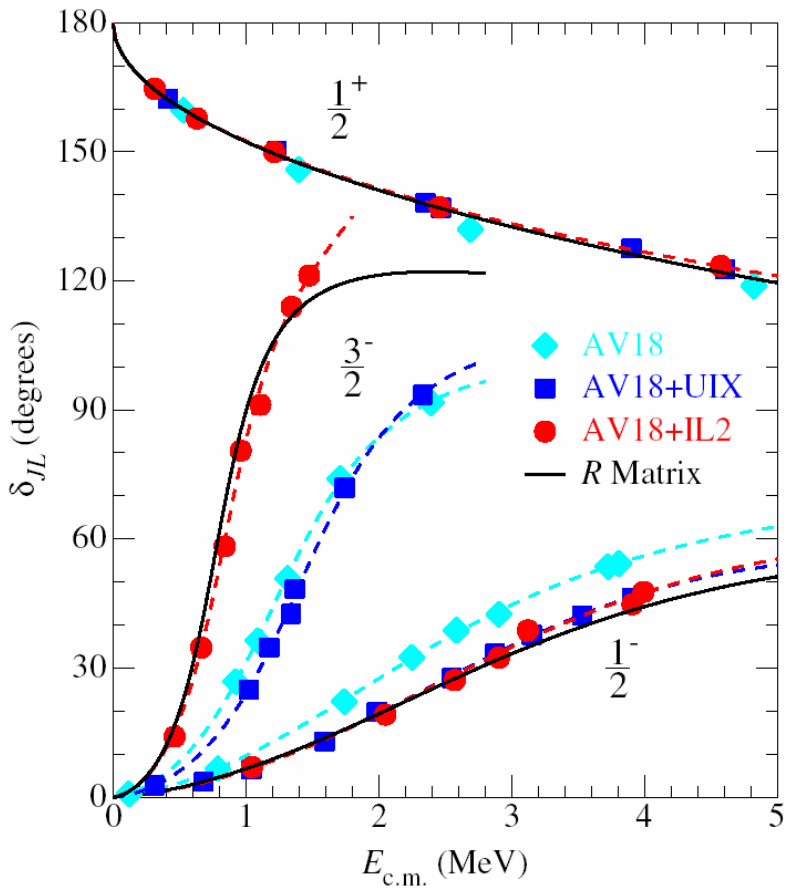
(MeV)

	$\langle T \rangle$	$\langle V_{\rm c} \rangle$	$\langle V_{\rm Coul} \rangle$	$\langle V_{\rm t} \rangle$	$\langle V_{\rm b} \rangle$
0^-0	48.38	−28.92	0.48	−26.63	0.29
0^-1	39.10	−24.79	0.44	−17.75	0.14
2^-0	41.08	−25.71	0.42	−21.39	−0.18
2^-1	40.25	−25.82	0.43	−19.30	−0.18
1^-0	37.72	−23.50	0.40	−18.32	0.006
1_1^-1	39.30	−25.14	0.43	−19.13	0.005
1_2^-1	32.48	−22.01	0.42	−12.67	−0.06

$|0^-0\rangle = a\,|L=1^-\ S=1\rangle + b\,|L=2^-,\ S=2\rangle$ $\quad a^2=0.95 \quad b^2=0.05$

Barrett (1967) Sakai et al. (1974)

Quantum Monte Carlo calculation for α +n phase shifts



K.M. Nollett et al. PRL99 (2007)

Effects of three-body forces in α +n scattering phase shifts

Formulation with Green's function

Phase shift is determined from the asymptotic behavior of **spectroscopic amplitude** (SA)

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

Test function for channel c=(I_1,I_2,I,l)

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

Equation of motion for exact y(r)

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

$$H = H_{\alpha_1} + H_{\alpha_2} + T_c + V_c \qquad (V_c\text{: 2BF+3BF+…})$$

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

$$z(r) = \langle \Phi_{cJM}(r) \mid V_c - U \mid \Psi_{JM} \rangle \qquad \text{(U(r): an arbitrary local potential)}$$

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

$$E_{\alpha_i} = \langle \psi_{I_i M_i} | H_{\alpha_i} | \psi_{I_i M_i} \rangle \qquad k = \sqrt{2\mu(E - E_{\alpha_1} - E_{\alpha_2})/\hbar^2}$$

A general form of SA: apparently correct asymptotics

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

$$\tan \delta_\ell = \tan \delta_\ell^{(0)} - \frac{2\mu k}{\hbar^2 \lambda} p(\infty)$$

$$p(r) = \int_0^r v(r')[z(r') + w(r')] r'^2 dr'$$

Suppose we have continuum-discretized states which are expected to be accurate in interaction region

$H \Psi_{JM} = E \Psi_{JM}$ ⟶ Calculate y(r): $\mathbf{y^{SA}(r)}$

Asymptotics of this y(r) is not good enough to obtain δ

z(r) can be accurate even though Ψ_{JM} has a bad tail
if U(r) is chosen to make V-U(r) vanish for large r ⟶ p(∞) accurate

$y^{SAGF}(r)$

$$y(r) = \left[\lambda + \frac{2\mu k}{\hbar^2} q(r)\right] v(r) + \frac{2\mu k}{\hbar^2} p(r) h(r)$$

$$q(r) = \int_r^\infty h(r')[z(r') + w(r')] r'^2 dr'$$

Determination of λ

(1) minimize over λ : $\sum_{i\,(r_0 \le r_i \le r_1)} [y^{\mathrm{SAGF}}(r_i) - y^{\mathrm{SA}}(r_i)]^2$

(2) Wronskian $W(y, h)$ minimize over λ : $\sum_{i\,(r_0 \le r_i \le r_1)} [\lambda(r_i) - \lambda]^2$

$W(y^{\mathrm{SAGF}}, h) = (\lambda / k r^2) + (2\mu/\hbar^2 r^2) q(r)$

$W(y^{\mathrm{SA}}, h)$

Check of the insensitivity of λ to [r_0, r_1]

Example 1. $^3S_1$ phase shifts of n+p scattering

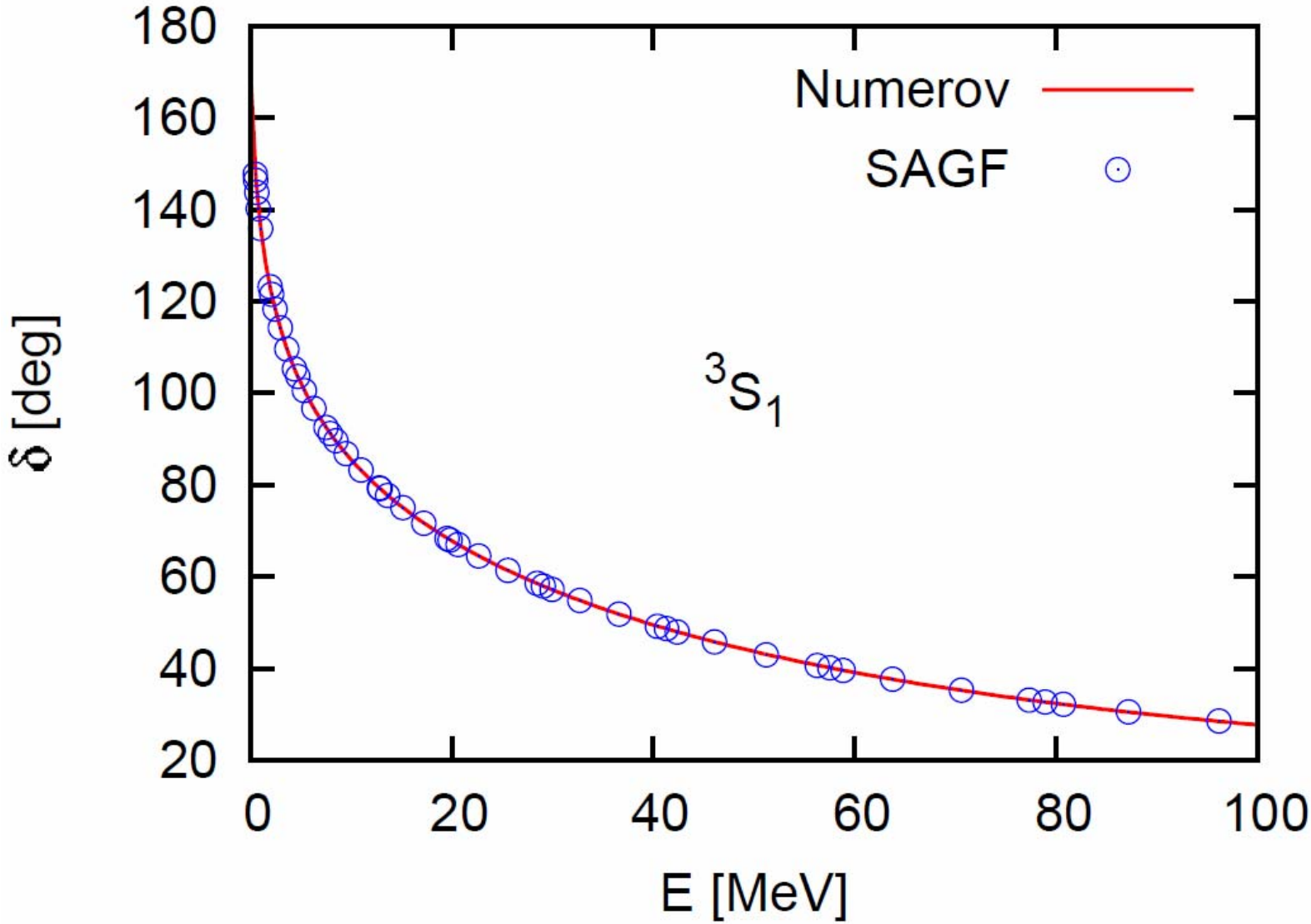
Minnesota potential

Diagonalizing the n+p Hamiltonian in Gaussians produces continuum-discretized states as well as the deuteron ground state

$$y^{\mathrm{SA}}(r) = \sum_{i=1}^{K} C_i(E)\, \mathrm{e}^{-\frac{1}{2}\beta_i r^2}$$

U(r)=0

E	Numerov	Method 1			Method 2
[MeV]		[0, 5]	[1, 6]	[2, 6]	[2, 6]
0.4986	147.7	147.7	147.8	147.7	147.7
1.959	123.2	123.3	123.2	123.2	123.3
4.395	105.3	105.2	105.3	105.3	105.3
7.948	91.2	91.4	91.2	91.2	91.1
12.87	79.2	79.0	79.2	79.2	79.4
19.54	68.5	68.7	68.5	68.5	68.3
28.49	58.5	58.2	58.6	58.6	58.8
40.42	49.3	49.6	49.3	49.3	49.1
56.28	40.8	40.4	40.8	40.8	40.8
77.31	33.2	33.6	33.1	33.2	33.3


180
160
140
120
100
80
60
40
20
δ [deg]
0
20
40
60
80
100
E [MeV]
Numerov
SAGF
$^3S_1$

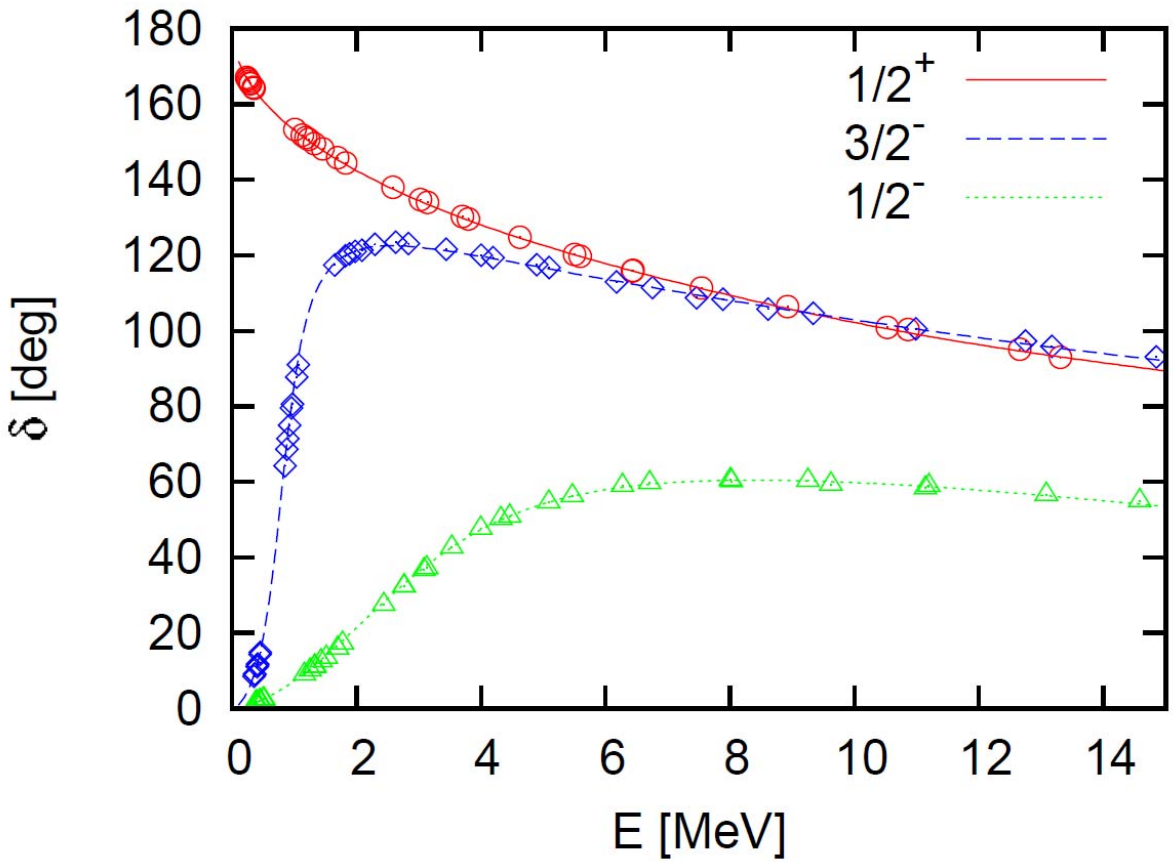
Example 2. α +n scattering with effective force

Minnesota force (Central + LS)

Single-channel calculation
Choice of A, u_1, u_2

$$\Psi_{cJM} = \int_0^\infty u_\ell(r)\mathcal{A}\Phi_{cJM}(r)r^2 dr$$

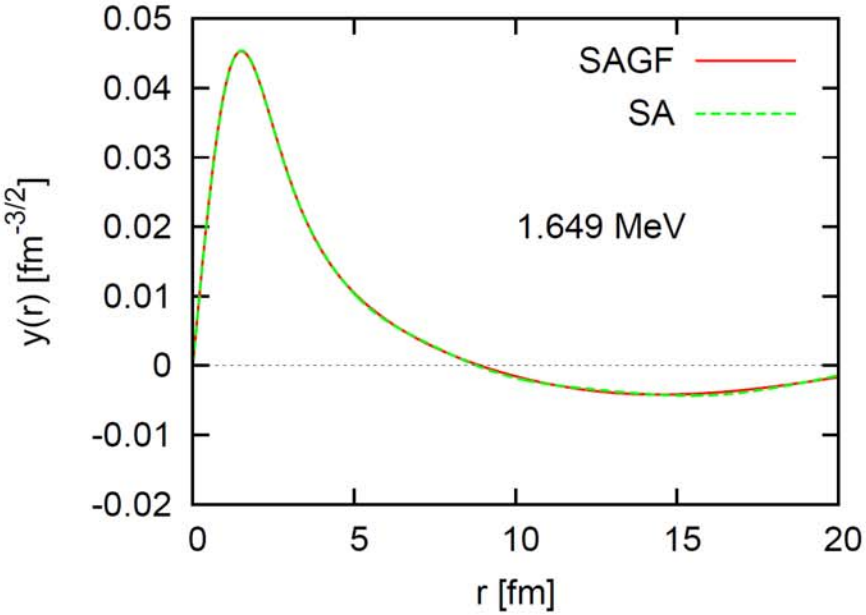
$$u_\ell(r) = \sum_{i=1}^{K} C_i\, r^\ell\, \mathrm{e}^{-\frac{1}{2}\beta_i r^2}$$

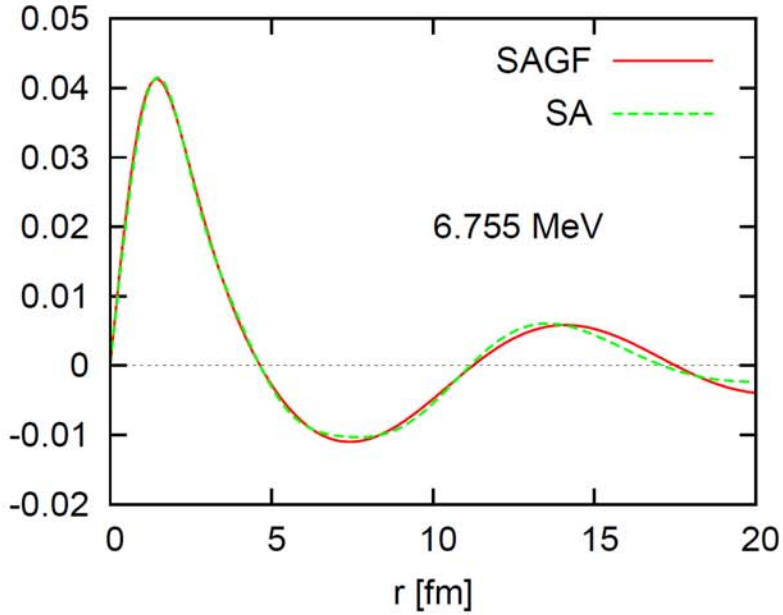


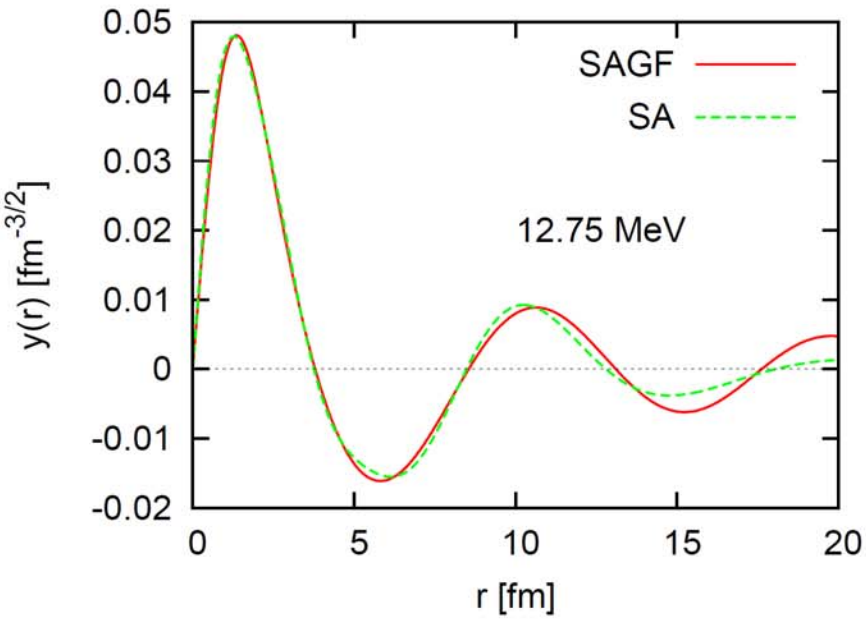
U(r)=0

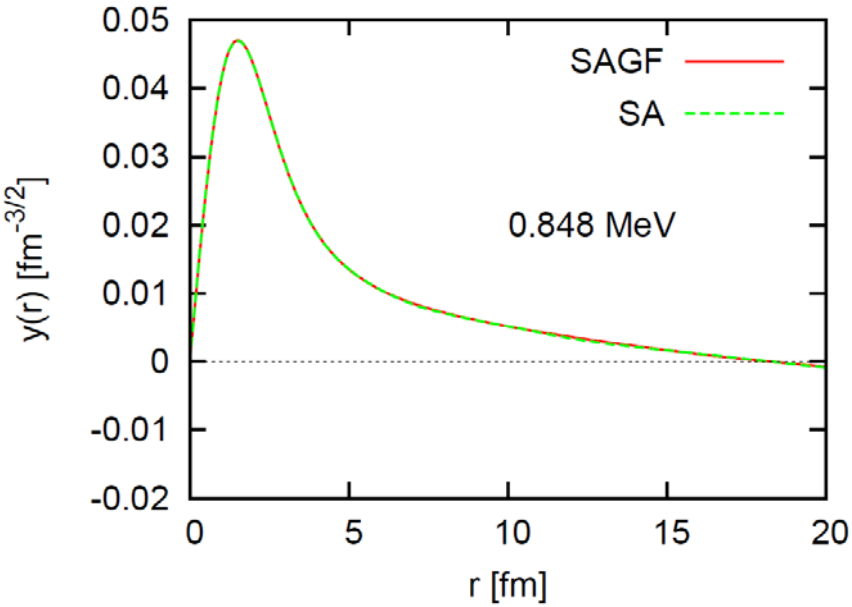
Good agreement with R-matrix calculation

Comparison between SA and SAGF for 3/2- states



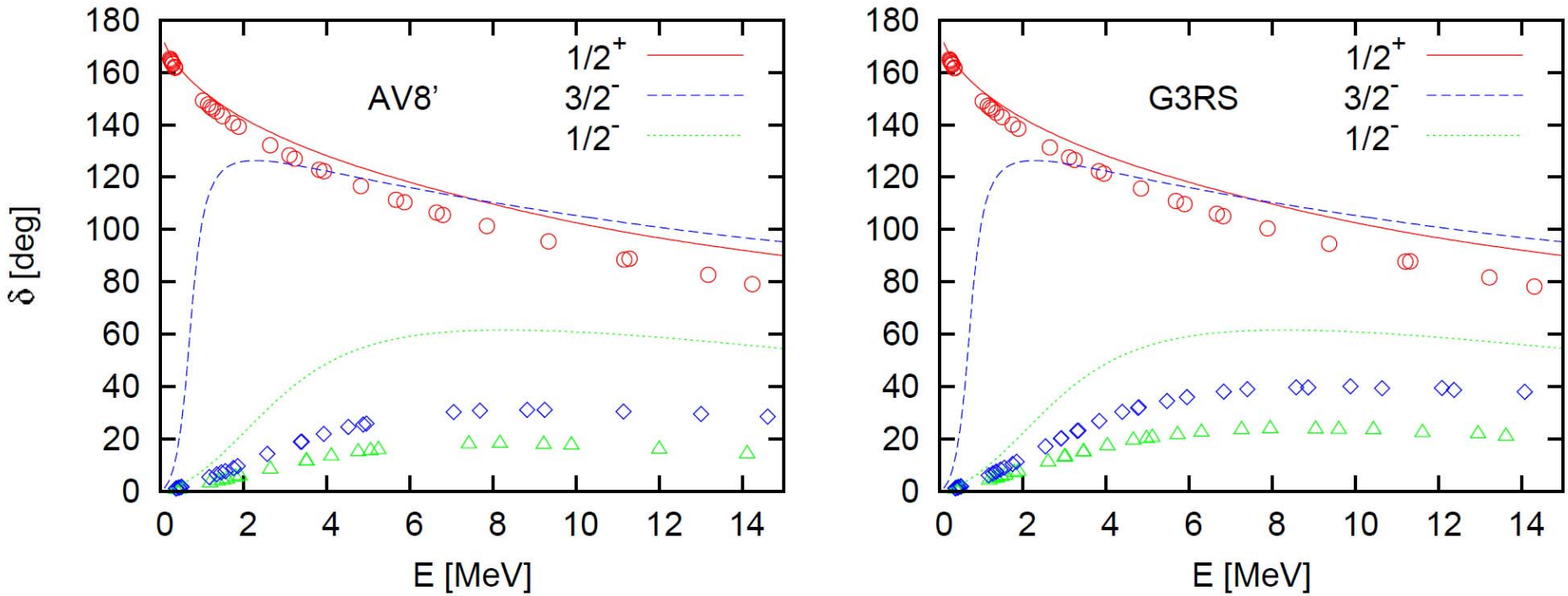






Example 3. α +n scattering with realistic forces

Microscopic five-body calculation with single channel
Use of α wave function solved accurately



S-wave phase-shifts are reasonable. P-wave phase-shifts are too small.

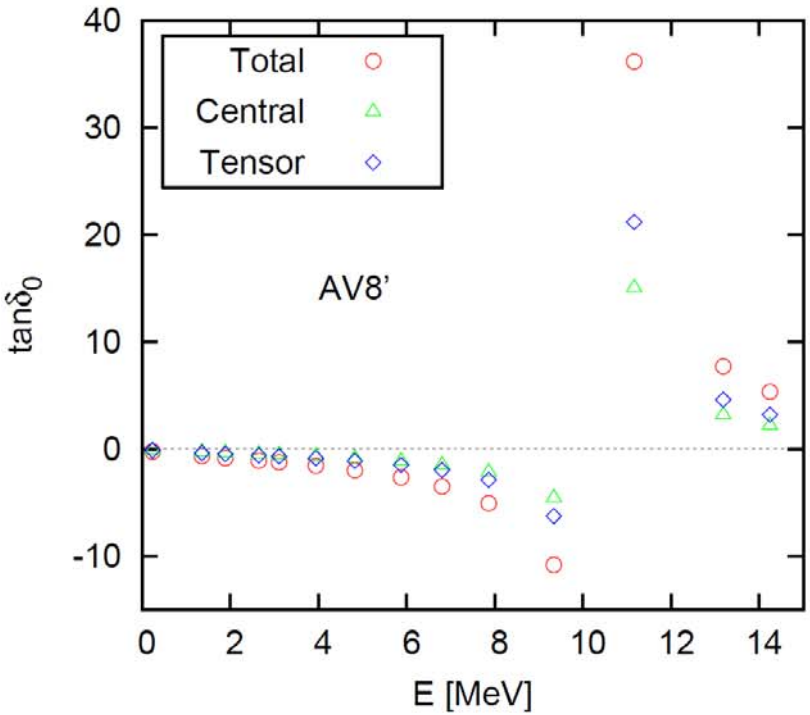
Our S-wave phase-shifts are similat to QMC results with AV18

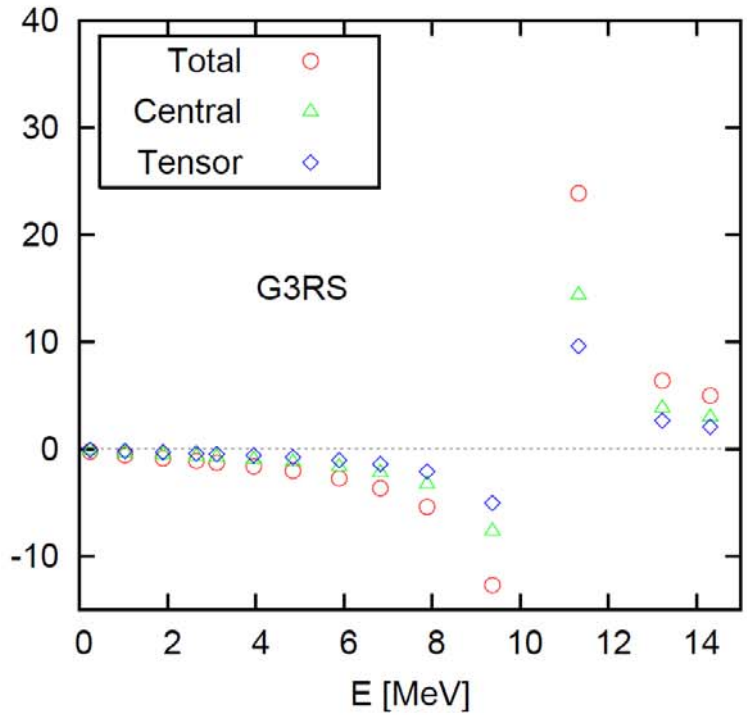
Decomposition of central, tensor, etc. contributions into tan δ

$$\tan\delta_\ell = \tan\delta_\ell^{(0)} - \frac{2\mu k}{\hbar^2\lambda} p(\infty)$$

$$p(r) = \int_0^r v(r')[z(r') + w(r')]r'^2 dr'$$

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





Tensor contribution is important in both bound and scattering states

Discussion on α +n phase shifts

P-wave phase shifts a sharp resonance for $3/2^-$
a broad resonance for $1/2^-$

S-wave phase shifts repulsive behavior in $1/2^+$

Understandable from Pauli principle

P-wave neutron can penetrate into α
S-wave neutron is repelled by Pauli exclusion

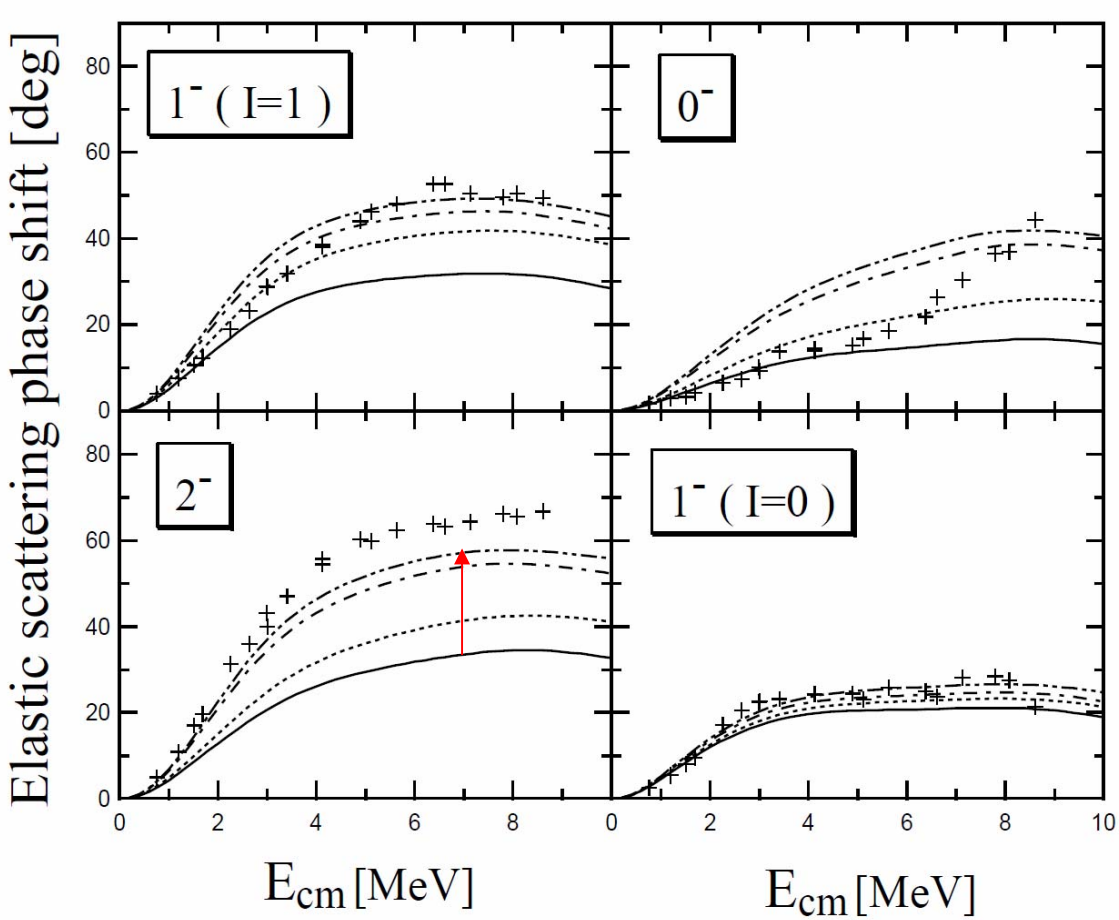
α can be distorted or excited in P-wave scattering
particularly through tensor forces

Similar phenomena occur in ^{3}He+p scattering

K.Arai, S.Aoyama, Y.S., arXiv:0812.4732

Microscopic four-body R-matrix calculation

^{3}He+p P-wave phase shifts



G3RS potential

Channel spin I=0, 1

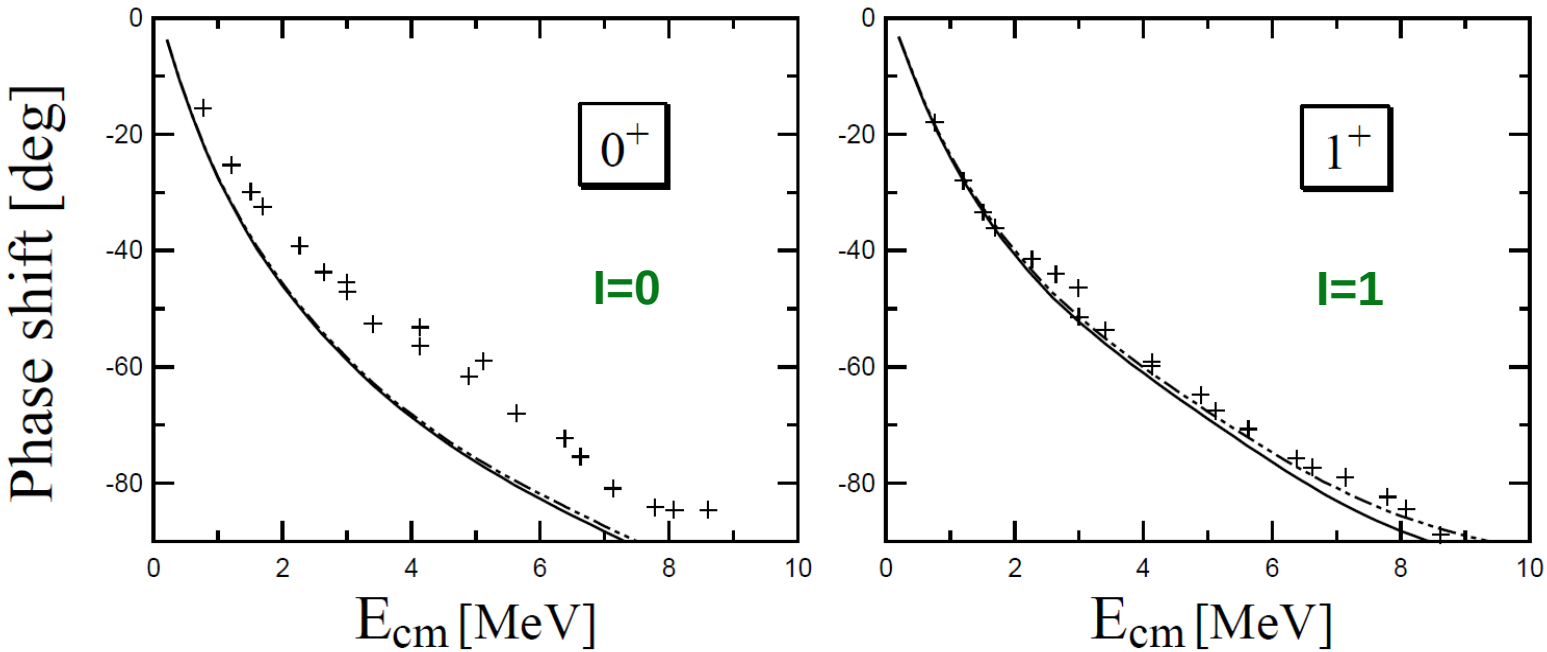
Single channel (Solid line)

$$^3\mathrm{He}(1/2^+)+p$$

Cluster distortion and coupled channels (Dash-dot-dot line)

$$^3\mathrm{He}(1/2^\pm, 3/2^\pm, 5/2^\pm)+p$$
$$+$$
$$d(0^+,1^+)+2p(0^+)$$

^{3}He+p S-wave phase shifts



Effects of cluster distortion and channel-coupling are small

Summary

- Ab initio type structure study with realistic forces in correlated basis
  - ^{4}He spectrum, Unified description of cluster like states and other negative parity states
- Green's function approach to phase-shift calculations using continuum-discretized states
  - Simplicity and accuracy
  - Decomposition of tan δ into contributions from potential components
  - ^{4}He+n phase shifts, Different nature of S, P-waves

- Extension to larger systems (in CG approach)
  - Tamed effective interactions determined model-space independently are desirable
  - e.g. UCOM (effects of higher order terms, effective operators other than Hamiltonian)
  - SRG
  - Transcorrelated method (elimination of short-ranged repulsion) is unexplored

Test of GVR

Alpha-particle

Potential	MN	G3RS		AV8′	
Method	GVR	GVR	PWE	GVR	PWE
$^4\mathrm{He}(0^+)$					
E	-29.94	-25.29	-25.29	-25.09	-25.05
$\langle T\rangle$	58.08	86.93	86.90	101.62	101.41
$\langle V_\mathrm{c}\rangle$	-88.86	-66.24	-66.19	-54.93	-54.76
$\langle V_\mathrm{Coul}\rangle$	0.83	0.76	0.76	0.77	0.77
$\langle V_\mathrm{t}\rangle$	–	-46.62	-46.65	-67.89	-67.82
$\langle V_\mathrm{b}\rangle$	–	-0.13	-0.12	-4.66	-4.66
$\sqrt{\langle r^2\rangle}$	1.41	1.51	1.51	1.49	1.49
$P(0,0)$	100	88.46	88.45	85.76	85.79
$P(2,2)$	–	11.30	11.30	13.88	13.85
$P(1,1)$	–	0.25	0.24	0.36	0.36

Most dramatic case: 0^-

Ex=-7.29 MeV
(1.20 MeV above t+p)
Γ =0.84 MeV

-6.07 MeV
(1.63 MeV above t+p)

Total

0_1^-	(1,1)	(2,2)	$P(L,S)$
(1,1)	1.137	−13.85	0.954
(2,2)		6.644	0.046

Kinetic

$\langle T \rangle$	(1,1)	(2,2)
(1,1)	41.87 (43.89)	
(2,2)		7.385 (160.2)

Central

$\langle V_c \rangle$	(1,1)	(2,2)
(1,1)	−27.98 (−29.33)	
(2,2)		−1.129 (−24.49)

Tensor

$\langle V_t \rangle$	(1,1)	(2,2)
(1,1)	−13.55 (−14.21)	−13.86 (−66.09)
(2,2)		0.367 (7.955)

Spin-orbit

$\langle V_b \rangle$	(1,1)	(2,2)
(1,1)	0.327 (0.343)	0.010 (0.050)
(2,2)		0.000 (0.006)

Coulomb

$\langle V_{\mathrm{Coul.}} \rangle$	(1,1)	(2,2)
(1,1)	0.469 (0.492)	
(2,2)		0.021 (0.454)

Bases with $L^\pi = 0^-$, S=0 are not included, but their role is expected to be minor.