Toward a description of nuclear scattering with the no-core shell model basis

Perspective of the Ab Initio No-Core Shell Model
February 10-12, 2011
TRIUMF, Vancouver, BC, Canada

Wataru Horiuchi (GSI)

Introduction

- Accurate solution with realistic interactions
  - Realistic interaction (short-range repulsion, tensor)
- Unifying nuclear structures and reactions
  - Continuum description

    → much more difficult (boundary conditions etc.)
  - Use of a square integrable (L^2) basis
    - Easy to handle
    - Ill behavior of the asymptotics

Outline

- Green's function method

  Collaborators: Y. Suzuki (Niigata, RIKEN), K. Arai (Nagaoka)

  – N-^{4}He scattering

- NCSM/RGM approach

  Collaborators: P. Navratil (TRIUMF), S. Quaglioni (LLNL)

  – Three-particle projectile (^{3}H, ^{3}He)

Formalism(1)

The wave function of the system with E $\Psi_{JM} = \sum_c \Psi_{cJM} + \cdots,$

Key quantity: Spectroscopic amplitude (SA) $y(r) = \langle \Phi_{cJM}(r) | \Psi_{JM} \rangle$

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

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

$$H = H_{\alpha_1} + H_{\alpha_2} + T_c + V_c \qquad V_c = \sum_{i \in \alpha_1, j \in \alpha_2} v_{ij}$$

Inhomogeneous equation for y(r)

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

U(r): arbitrary local potential (cf. Coulomb)

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

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

Formalism(2)

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

G(r, r'): Green's function

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

$$G(r,r') = \begin{cases} kv(r)h(r') & r \le r' \\ kh(r)v(r') & r \ge r' \end{cases}$$

v(r): regular solution
h(r): irregular solution

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

The asymptotics is corrected by the Green's function

$$p(r) = \int_0^r v(r')[z(r')+w(r')]r'^2 dr', \qquad q(r) = \int_r^\infty h(r')[z(r')+w(r')]r'^2 dr'$$

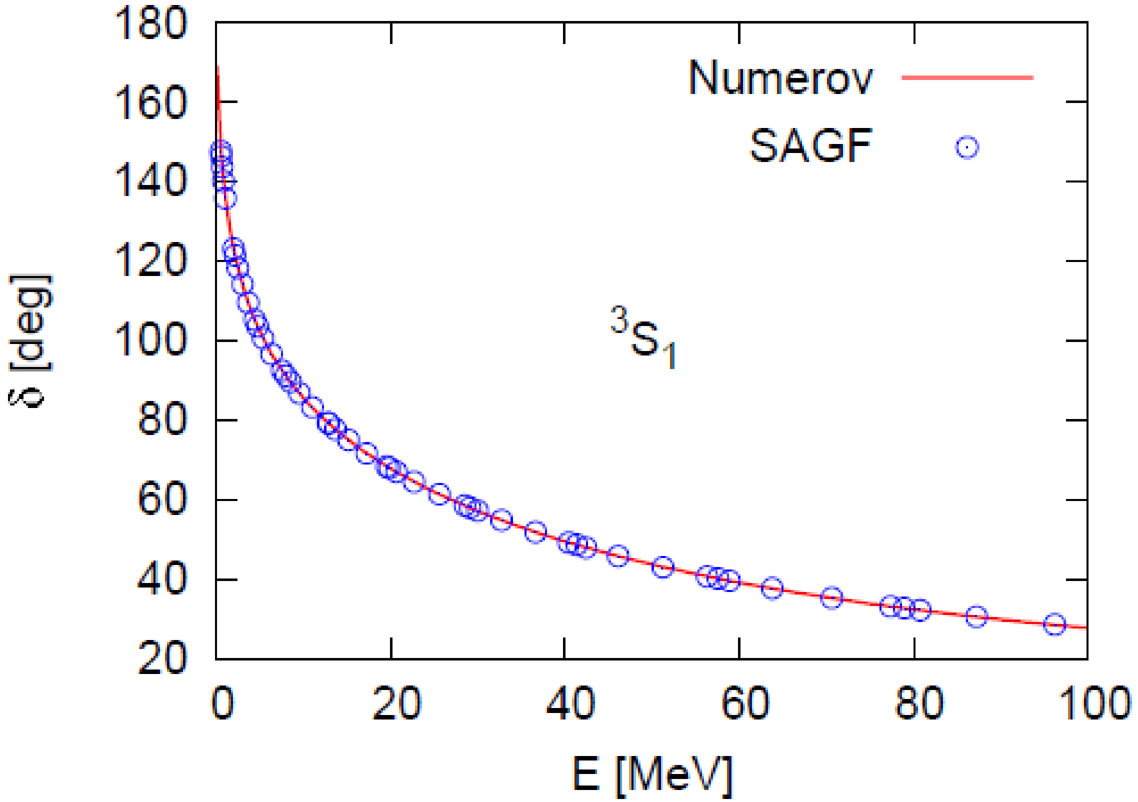
Phase shift:
$$\tan(\delta_\ell - \delta_\ell^{(0)}) = -\frac{2\mu k}{\hbar^2 \underline{\lambda}} p(\infty)$$

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

Test calculation (1)

Neutron-proton phase shift with Minnesota potential (Central)
Comparison with Numerov ("exact") method

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



Perfect agreement

N-^{4}He phase shift calculation

- Input (Local): $y(r)$, $z(r)$
- Nuclear wave function
  - Explicitly correlated basis

Variational calculation for many-body systems

Hamiltonian

$$H = \sum_{i=1}^{A} T_i - T_{\rm cm} + \sum_{i<j}^{A} v_{ij} + \left(\sum_{i<j<k}^{A} v_{ijk} \right)$$

$$v_{12} = V_c(r) + V_{\rm Coul.}(r) P_{1\pi} P_{2\pi} + V_t(r) S_{12} + V_b(r) \boldsymbol{L} \cdot \boldsymbol{S}$$

Argonne V8 type potential: central, tensor, spin-orbit

Generalized eigenvalue problem

$$\Psi_{JM_J} = \sum_{i=1}^{K} c_i \Psi(\alpha_i)$$

$$\sum_{j=1}^{K} (H_{ij} - E B_{ij}) c_j = 0 \quad (i = 1, \ldots, K)$$

$$\begin{pmatrix} H_{ij} \\ B_{ij} \end{pmatrix} = \langle \Psi(\alpha_i) | \begin{pmatrix} H \\ 1 \end{pmatrix} | \Psi(\alpha_j) \rangle$$

Basis function

$$\Psi_{(LS)JM_JTM_T} = \mathcal{A} \left\{ \left[\psi_L^{\rm (space)} \psi_S^{\rm (spin)} \right]_{JM_J} \psi_{TM_T}^{\rm (isospin)} \right\}$$

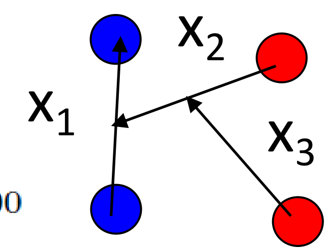
$$\psi_{SM_S}^{\rm (spin)} = \left| [\cdots [[[\tfrac{1}{2} \tfrac{1}{2}]_{S_{12}} \tfrac{1}{2}]_{S_{123}}] \cdots]_{SM_S} \right\rangle$$

Correlated Gaussian and global vector

Correlated Gaussian

$$\exp\left(-\frac{1}{2}ar^2\right) \rightarrow \exp\left(-\frac{1}{2}\tilde{\boldsymbol{x}}A\boldsymbol{x}\right) = \exp\left(-\frac{1}{2}\sum_{i,j=1}^{A-1} A_{ij}\boldsymbol{x}_i \cdot \boldsymbol{x}_j\right)$$

$$\exp\left(A_{ij}\boldsymbol{x}_i \cdot \boldsymbol{x}_j\right) \sim \sum_n (\boldsymbol{x}_i \cdot \boldsymbol{x}_j)^n \sim \sum_{\ell=n,n-2,\dots} [\mathcal{Y}_\ell(\boldsymbol{x}_i)\mathcal{Y}_\ell(\boldsymbol{x}_j)]_{00}$$



Global vector

$$r^l Y_{lm}(\hat{\boldsymbol{r}}) \equiv \mathcal{Y}_{lm}(\boldsymbol{r}) \rightarrow \mathcal{Y}_{LM_L}(\tilde{u}\boldsymbol{x}) = \mathcal{Y}_{LM_L}\left(\sum_{i=1}^{A-1} u_i \boldsymbol{x}_i\right)$$

$$\mathcal{Y}_{LM_L}(u_1\boldsymbol{x}_1 + u_2\boldsymbol{x}_2) = \sum_{\ell=0}^{L}\sqrt{\frac{4\pi(2L+1)!}{(2\ell+1)!(2L-2\ell+1)!}}\; u_1^\ell u_2^{L-\ell}[\mathcal{Y}_\ell(\boldsymbol{x}_1)\mathcal{Y}_{L-\ell}(\boldsymbol{x}_2)]_{LM_L}$$

Global Vector Representation (GVR) Parity $(-1)^{L_1+L_2}$

$$F_{(L_1L_2)LM}(u_1, u_2, A, \boldsymbol{x}) = \exp\left(-\frac{1}{2}\tilde{\boldsymbol{x}}A\boldsymbol{x}\right)[\mathcal{Y}_{L_1}(\widetilde{u_1}\boldsymbol{x})\mathcal{Y}_{L_2}(\widetilde{u_2}\boldsymbol{x})]_{LM}$$

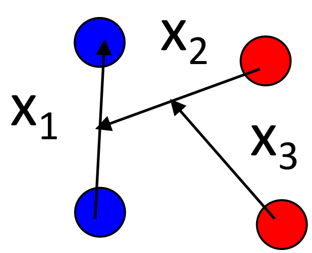
Advantages of GVR

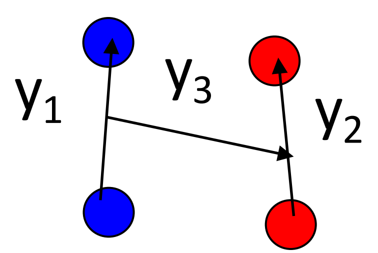
Variational parameters A, u

→ Stochastic Variational Method (SVM)

K. Varga, Y. Suzuki, PRC52, 2885 (1995).

- No need to specify intermediate angular momenta.
  – Specify total angular momentum L
- Nice property for coordinate transformations
  – Antisymmetrization, rearrangement channels





$$y = Tx \quad \Longrightarrow \quad \tilde{y}By = \tilde{x}\tilde{T}BTx \qquad\qquad \tilde{v}y = \widetilde{\tilde{T}v}x$$

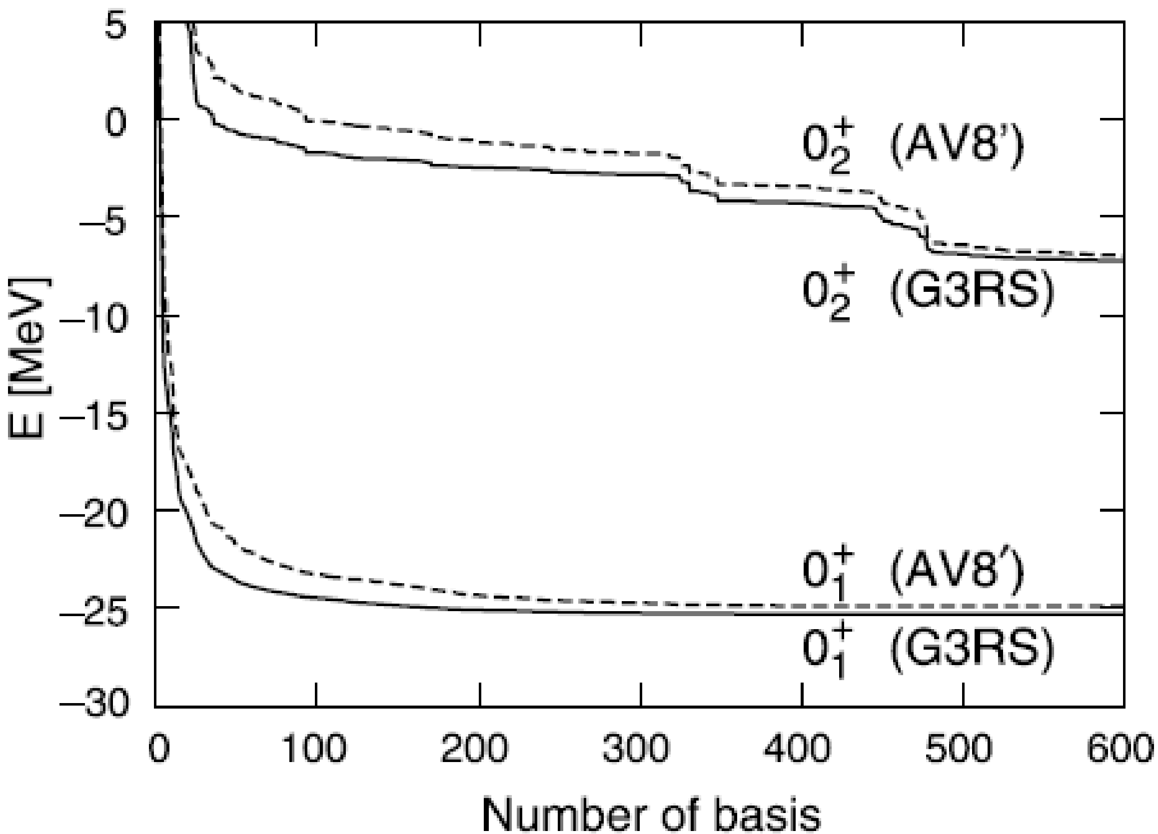
Algorithm of the SVM

Possibility of the stochastic optimization
1. increase the basis dimension one by one
2. set up an optimal basis by trial and error procedures
3. fine tune the chosen parameters until convergence

1. **Generate** $(A_k^1, A_k^2, \cdots\cdots, A_k^m)$ **randomly**
2. **Get the eigenvalues** $(E_k^1, E_k^2, \cdots\cdots, E_k^m)$
3. **Select** A_k^n corresponding to the lowest E_k^n and **Include** it in a basis set
4. **k → k+1**

Y. Suzuki and K. Varga, Stochastic variational approach to quantum-mechanical few-body problems, LNP 54 (Springer, 1998).
K. Varga and Y. Suzuki, Phys. Rev. C52, 2885 (1995).

Energy convergence of ^{4}He



V8 type interactions:
AV8', G3RS
Central, tensor, LS

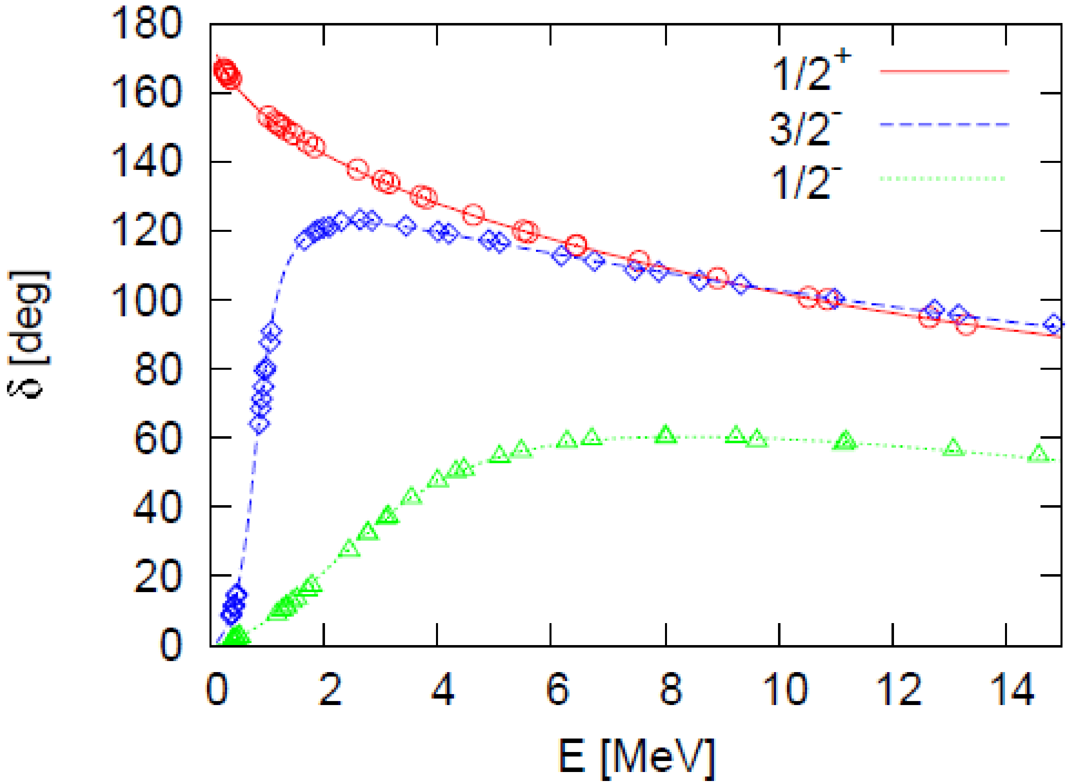
Convergence is reached in 600 basis states
Ground state energy -25.09 MeV in good agreement with other accurate method (within 60 keV)

Test calculation (2)

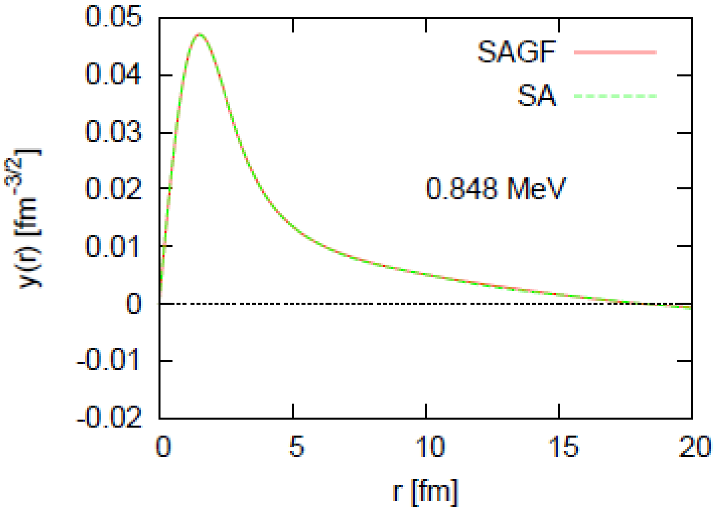
Neutron-alpha phase shift with Minnesota potential + spin-orbit

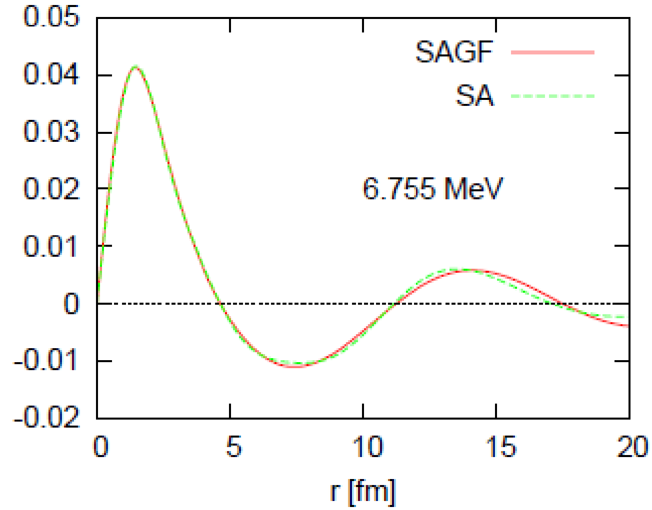
Alpha particle → four-body cal.

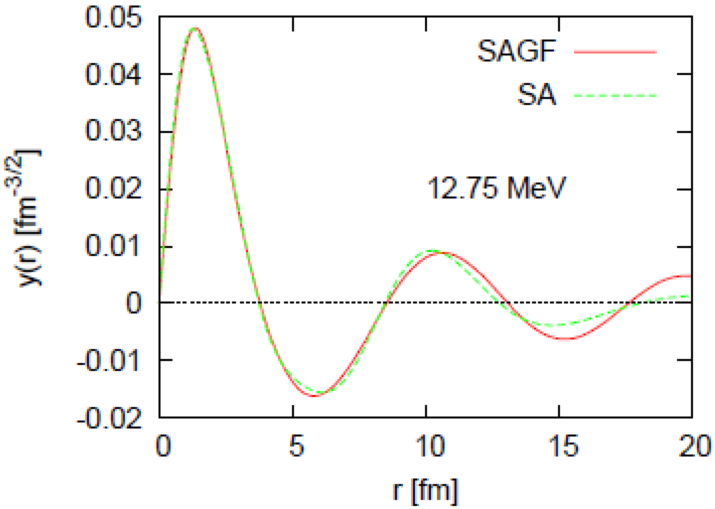
Comparison with the R-matrix method



Improvement of the asymptotics







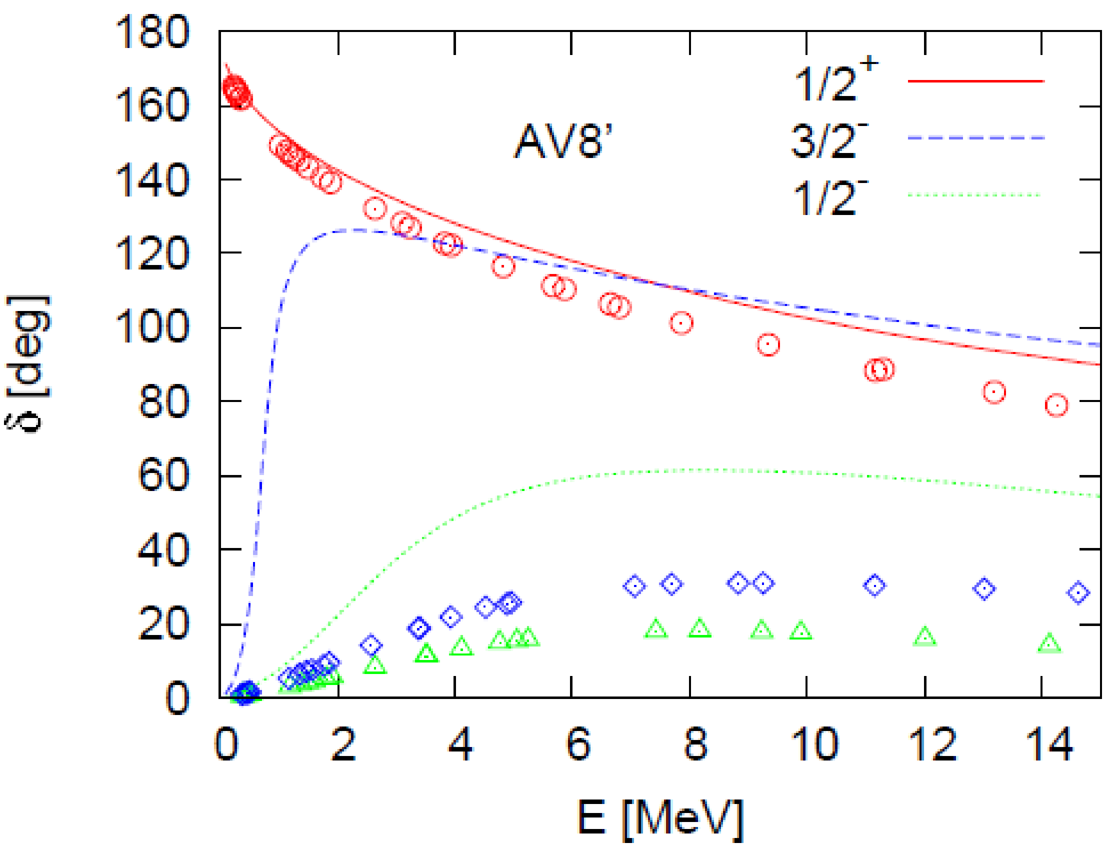
Wrong asymptotics is corrected by the Green's function

n+^{4}He scattering

Interaction: AV8' (Central, Tensor, Spin-orbit)

Alpha particle → four-body cal.

Single channel calculation with α+n



1/2$^+$ → fair agreement

1/2$^-$, 3/2$^-$ → fail to reproduce

- distorted configurations
- three-body force

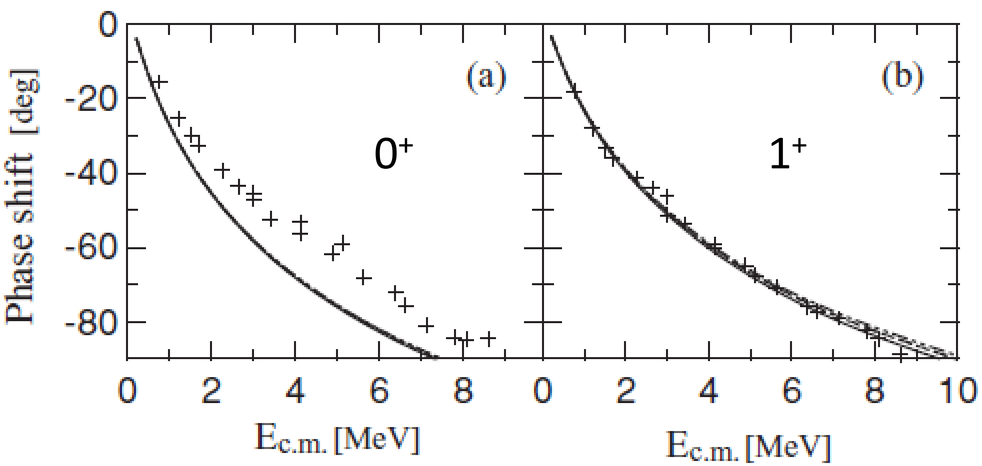
p-^{3}He scattering

Interaction: AV8′

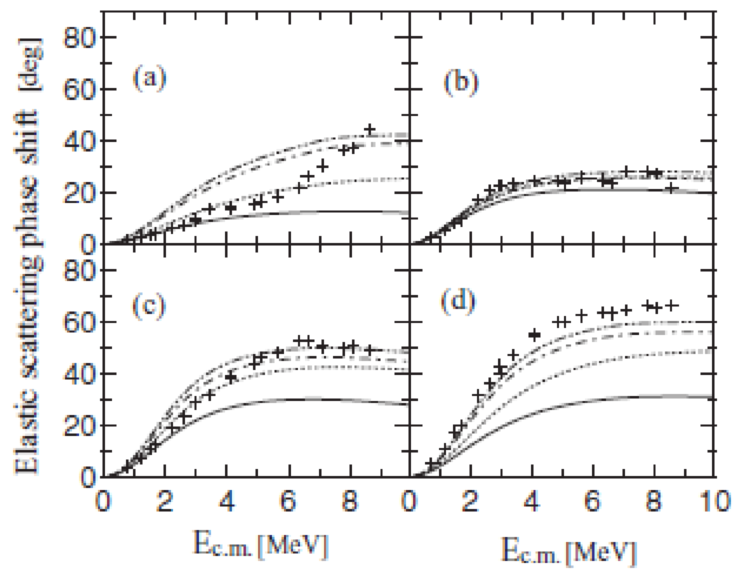
Dynamics: R-matrix method

K. Arai, S. Aoyama, Y. Suzuki, PRC81, 037301 (2010).

S-wave



P-wave



Minnesota (central), P-wave

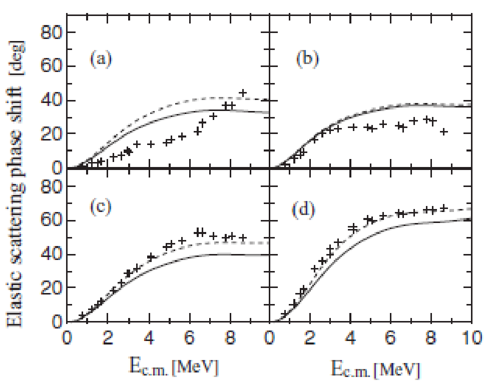
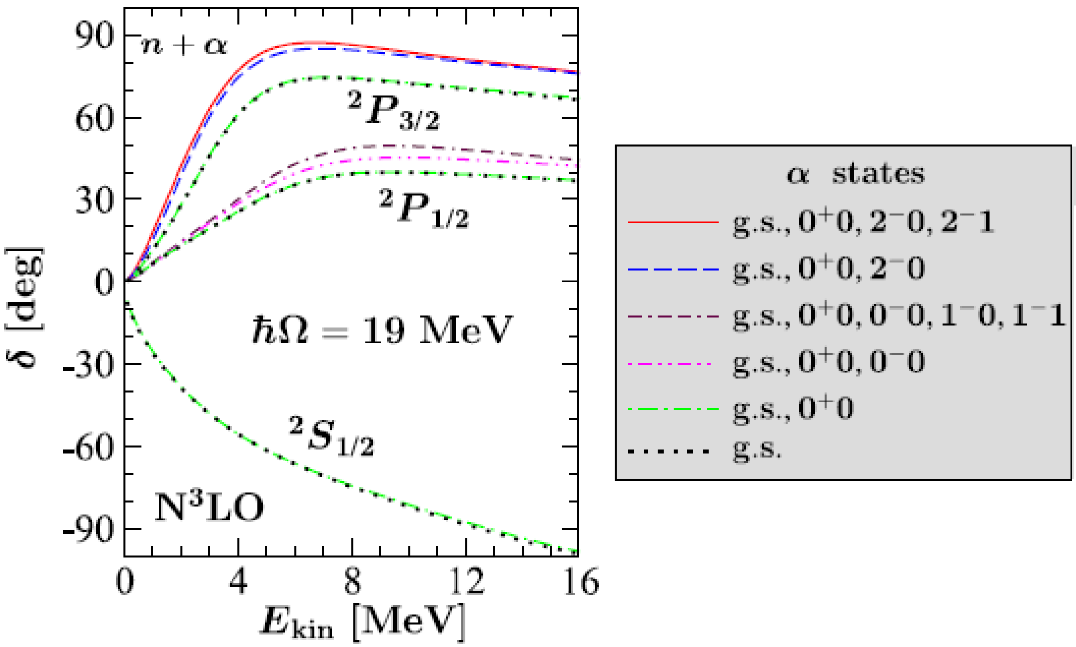
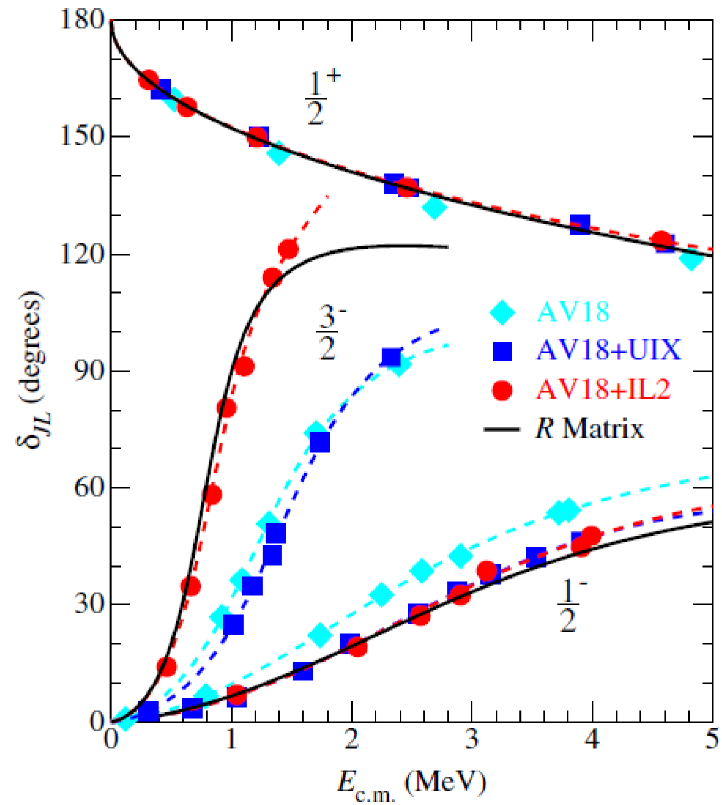


FIG. 3. The ^{3}He + p P-wave elastic scattering phase shifts of (a) 0^-, (b) $1^-(I=0)$, (c) $1^-(I=1)$, and (d) 2^- states calculated with the AV8′ potential. The lines denote the results obtained including the following configurations: solid, ^{3}He$(1/2^+) + p$; dotted, ^{3}He$(1/2^\pm, 3/2^\pm, 5/2^\pm) + p$; dash-dotted, $[^3\mathrm{He}(1/2^+) + p] + [d(0^+, 1^+) + 2p(0^+)]$; dash-dot-dotted $[^3\mathrm{He}(1/2^\pm, 3/2^\pm, 5/2^\pm) + p] + [d(0^+, 1^+) + 2p(0^+)]$. The crosses denote the experimental data [21] and the error bars of the data are omitted.

n-^{4}He scattering





S. Quaglioni, P. Navratil,
PRL101, 092501 (2008)
NCSM/RGM

K. M. Nollett et al.
PRL99, 022502 (2007)
Green's function
Monte Carlo

Summary (1)

- SA solved with the Green's function (SAGF) method

  Y. Suzuki, W.H., K. Arai, NPA823, 1 (2009)

  - Easy and good accuracy
  - Difficulty to control an incident energy

    -> use of confinement pot. Y. Suzuki, D. Baye, A. Kievsky, NPA838, 20 (2010)
  - N-^{4}He: fail to reproduce p-wave resonances
    - Distorted configurations (n-^{4}He*, d-^{3}H)
    - Three-body force
- Global vector representation (GVR)
  - A flexible basis: Easy to transform a coordinate set
  - Applicable only for very light nuclei

    -> NCSM basis (A<16)

NCSM/RGM calculation

- Consistent description of bound and scattering states
  - No core shell model (NCSM)
    - Effective interaction starting from realistic force
    - Applicable A<16
  - Resonating Group Method (RGM)
    - Fully microscopic
    - Proper treatment of continuum states

- Single-particle projectile (N-^{3}H, N-^{4}He, N-^{10}Be)

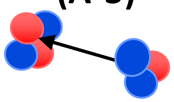
  S. Quaglioni, P. Navratil, PRC79, 044606 (2009).
- Combined with IT-NCSM (N-^{7}Li, N-^{7}Be, N-^{12}C, N-^{16}O)

  P. Navratil, R. Roth, S. Quaglioni, PRC82, 034609 (2010).
- Two-particle projectile (d-^{3}H->n-^{4}He) -> underway
- Three-particle projectile (^{3}H-^{3}H, ^{3}He-^{4}He, …)

Formalism

Scattering wave function

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



Translationally invariant basis function

$$\left|\Phi_{\nu r}^{J^\pi T}\right\rangle = \left[\left(\left|A-3\,\alpha_1 I_1^{\pi_1} T_1\right\rangle \left|a=3\,\alpha_2 I_2^{\pi_2} T_2\right\rangle\right)^{(sT)} Y_\ell(\hat{r}_{A-3,3})\right]^{(J^\pi T)} \frac{\delta(r - r_{A-3,3})}{r r_{A-3,3}}$$

Schroedinger equation (RGM equation)

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

Non-local matrix elements

Norm kernel

$$\mathcal{N}_{\nu'\nu}^{J^\pi T}(r',r) = \left\langle \Phi_{\nu' r'}^{J^\pi T}\right| \hat{\mathcal{A}}_{\nu'} \hat{\mathcal{A}}_\nu \left|\Phi_{\nu r}^{J^\pi T}\right\rangle$$

Hamiltonian kernel

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

$$H = T_{\rm rel} + \mathcal{V}_{\rm rel} + V_C(r) + H_{A-3} + H_{a=3}$$

Calculation of RGM matrix elements

1. Basis: Combination of SD and Jacobi basis

$$\left|\Phi_{\nu n}^{J^\pi T}\right\rangle_{\rm SD} = \Big[\big(\underbrace{|A-3\,\alpha_1 I_1^{\pi_1} T_1\rangle_{\rm SD}}_{\text{SD basis}}\,\underbrace{|a=3\,\alpha_2 I_2^{\pi_2} T_2\rangle}_{\text{Jacobi basis}}\big)^{(sT)}\, Y_\ell(\hat{R}_{\rm cm}^{(a=3)})\Big]^{(J^\pi T)}\, R_{n\ell}(R_{\rm cm}^{(a=3)})$$

Slater determinant (SD) basis is computationally advantageous.

2. Write it down with single particle HO states
3. Calculate the Norm and Hamiltonian kernels
   – Expression: Sum of A-body (up to 4) density matrices
4. Get translationally invarient matrix elements

Spurious c.m. motion can be properly removed from the basis.

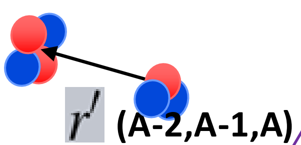
S. Quaglioni, P. Navratil, PRC79, 044606 (2009).

Norm kernel

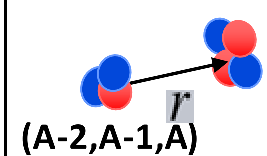
- Antisymmetrizer between two clusters

$$\mathcal{A}^{(A-3,3)} = \sqrt{\frac{6}{A(A-1)(A-2)}}\Bigg[1 - \sum_{i=1}^{A-3}\hat{P}_{i,A} - \sum_{i=1}^{A-3}\hat{P}_{i,A-1} - \sum_{i=1}^{A-3}\hat{P}_{i,A-2} + \frac{1}{2}\sum_{i\neq j}\left(\hat{P}_{i,A}\hat{P}_{j,A-1} + \hat{P}_{i,A-2}\hat{P}_{j,A} + \hat{P}_{i,A-1}\hat{P}_{j,A-2}\right) - \frac{1}{6}\sum_{i\neq j\neq k}\hat{P}_{i,A}\hat{P}_{j,A-1}\hat{P}_{k,A-2}\Bigg]$$

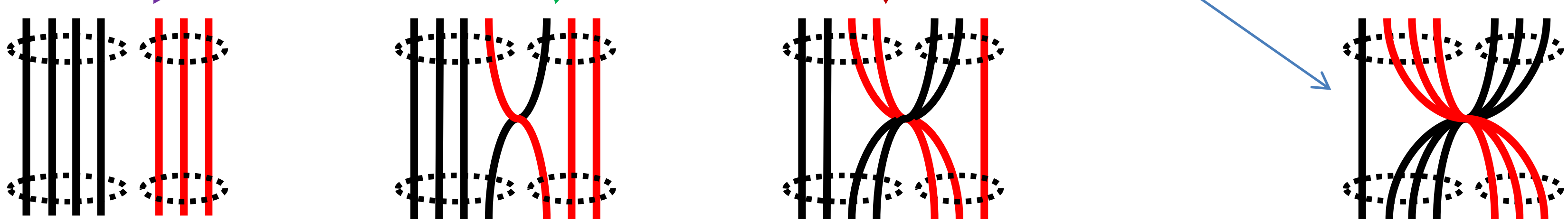
- Norm kernel $\mathcal{N}^{J^\pi T}_{\nu'\nu}(r',r) = \left\langle \Phi^{J^\pi T}_{\nu' r'} \right| \mathcal{A}^2 \left| \Phi^{J^\pi T}_{\nu r} \right\rangle$



$$\Bigg\langle \quad \Bigg| \; 1 - 3(A-3)\hat{P}_{A-4,A-3} + \frac{3}{2}(A-3)(A-4)\hat{P}_{A-4,A}\hat{P}_{A-5,A-1} - \frac{1}{6}(A-3)(A-4)(A-5)\hat{P}_{A-4,A}\hat{P}_{A-5,A-1}\hat{P}_{A-6,A-2} \; \Bigg| \quad \Bigg\rangle$$



"Direct" "Exchange"



$${}_{SD}\langle \psi^{A-3}_{\mu'} | a^\dagger a | \psi^{A-3}_{\mu} \rangle_{SD} \qquad {}_{SD}\langle \psi^{A-3}_{\mu'} | a^\dagger a^\dagger a a | \psi^{A-3}_{\mu} \rangle_{SD} \qquad {}_{SD}\langle \psi^{A-3}_{\mu'} | a^\dagger a^\dagger a^\dagger a a a | \psi^{A-3}_{\mu} \rangle_{SD}$$

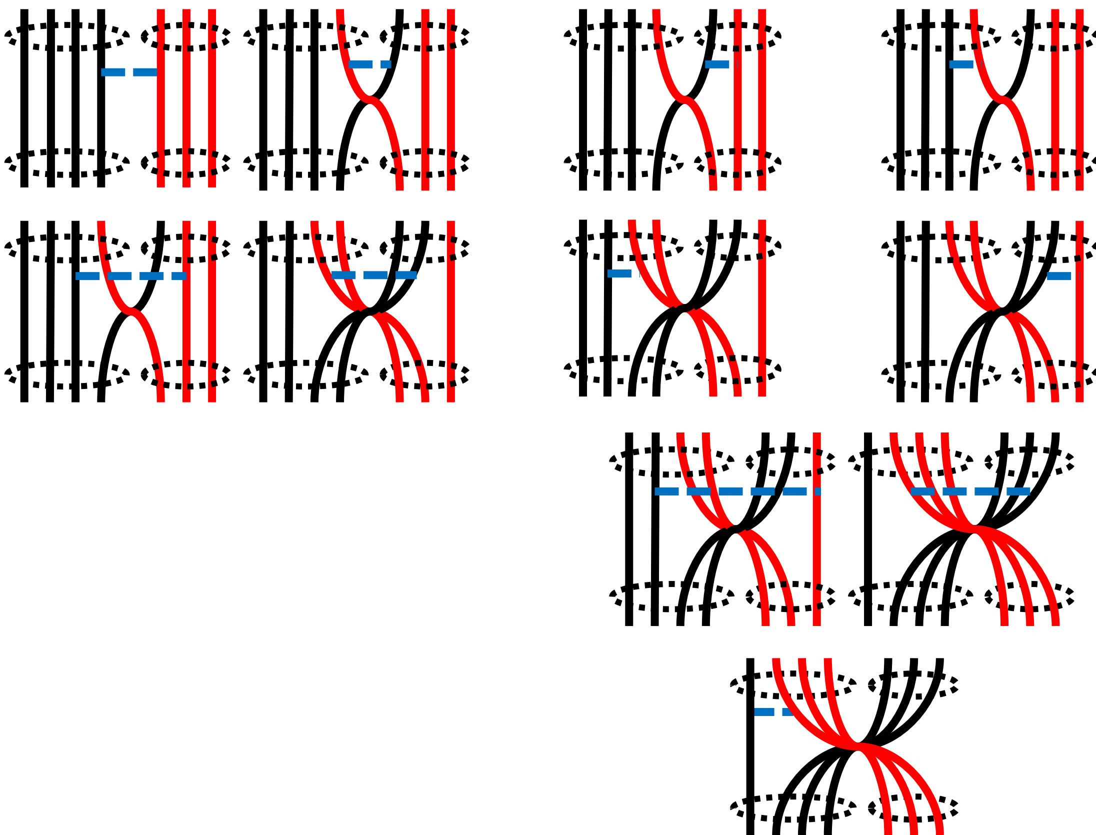
Hamiltonian kernel

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

$$\mathcal{V}_{\nu',\nu}(r',r) = \left\langle \Phi^{J^\pi T}_{\nu' r'} \right| \mathcal{V}_{\rm rel} \mathcal{A}^2 \left| \Phi^{J^\pi T}_{\nu r} \right\rangle$$

8 terms →

$$\begin{aligned} & 3(A-3)V_{A-3,A-2}(1-\hat{P}_{A-3,A-2}) - 6(A-3)V_{A-3,A-1}\hat{P}_{A-3,A-2} \\ & - 3(A-3)(A-4)V_{A-4,A-2}\hat{P}_{A-3,A-2} \\ & - 6(A-3)(A-4)V_{A-3,A}(1-\hat{P}_{A-3,A})\hat{P}_{A-4,A-1} \\ & + 3(A-3)(A-4)V_{A-3,A-2}\hat{P}_{A-3,A}\hat{P}_{A-4,A-1} \\ & + 3(A-3)(A-4)(A-5)V_{A-5,A}\hat{P}_{A-3,A}\hat{P}_{A-4,A-1} \\ & + \tfrac{3}{2}(A-3)(A-4)(A-5)V_{A-5,A-2}\hat{P}_{A-3,A}\hat{P}_{A-4,A-1}(1-\hat{P}_{A-5,A-2}) \\ & - \tfrac{1}{2}(A-3)(A-4)(A-5)(A-6)V_{A-6,A}\hat{P}_{A-3,A}\hat{P}_{A-4,A-1}\hat{P}_{A-5,A-2} \end{aligned}$$



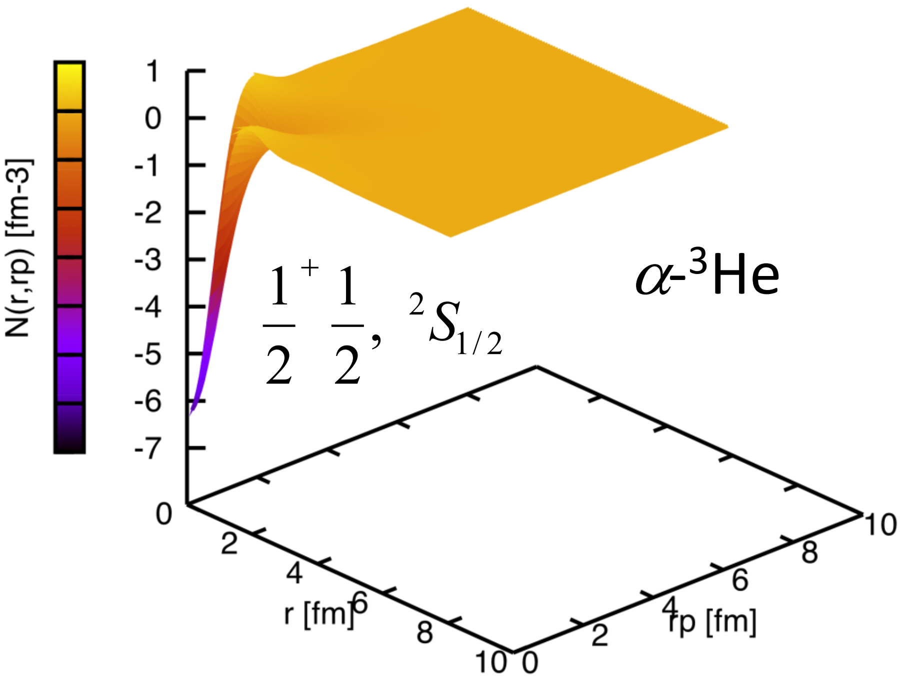
$${}_{\rm SD}\langle \psi^{A-3}_{\mu'} | a^\dagger a | \psi^{A-3}_{\mu} \rangle_{\rm SD}$$

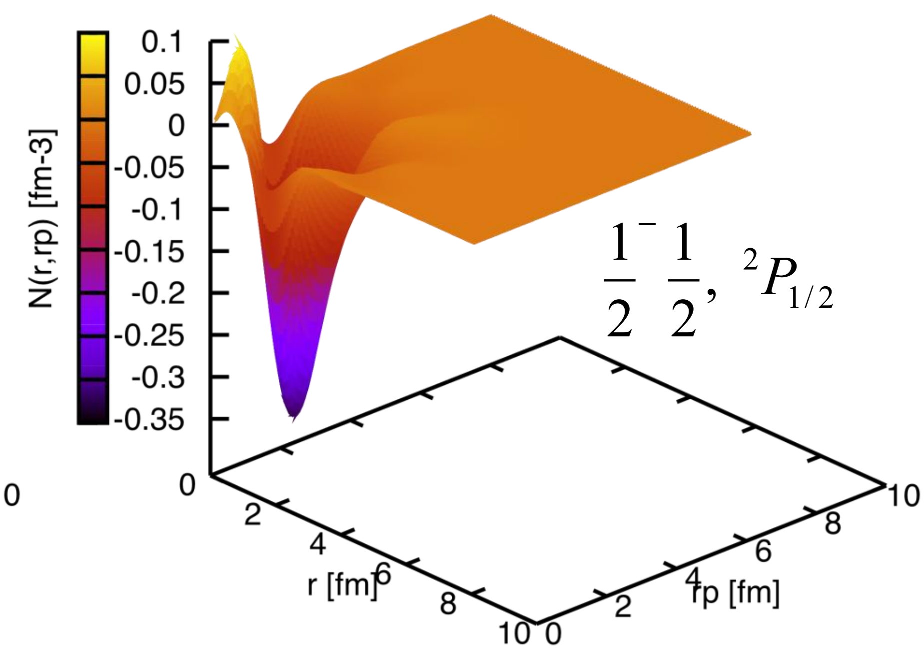
$${}_{\rm SD}\langle \psi^{A-3}_{\mu'} | a^\dagger a^\dagger a a | \psi^{A-3}_{\mu} \rangle_{\rm SD}$$

$${}_{\rm SD}\langle \psi^{A-3}_{\mu'} | a^\dagger a^\dagger a^\dagger a a a | \psi^{A-3}_{\mu} \rangle_{\rm SD}$$

$${}_{\rm SD}\langle \psi^{A-3}_{\mu'} | a^\dagger a^\dagger a^\dagger a^\dagger a a a a | \psi^{A-3}_{\mu} \rangle_{\rm SD}$$

Examples of the norm kernel





Progress so far

Norm kernel: completed!

Hamiltonian kernel: in progress

Algebraic derivations worked out, to be finished soon

Summary and future works

- NCSM/RGM with three-body projectile, underway

- Green's function method

  Recent progress

  - Coupled channel method

    Y. Suzuki, D. Baye, A. Kievsky, NPA838, 20 (2010)

  - Three-body continuum (HH formalism)

    Y. Suzuki, W.H., D. Baye, PTP123, 547 (2010)

- Possible applications
  - NCSM+Green's function method
  - High energy reaction calculations for neutron-rich isotopes