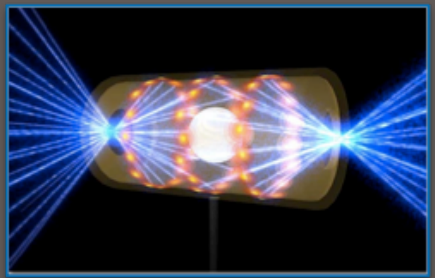
TRIUMF

Canada's national laboratory for particle and nuclear physics
Laboratoire national canadien pour la recherche en physique nucléaire et en physique des particules

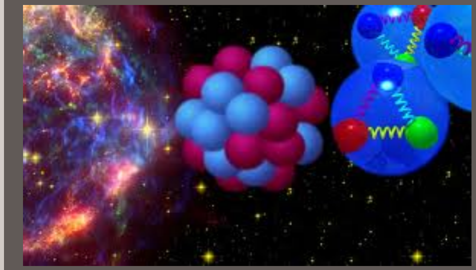
Nuclear structure and reaction calculations with chiral three-nucleon interactions



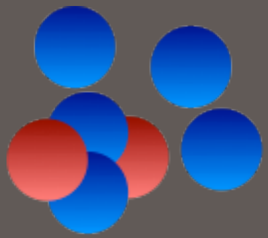
INT Workshop INT-13-1a

Computational and Theoretical Advances for Exotic Isotopes in the Medium Mass Region

27th March 2013, Institute for Nuclear Theory



Petr Navratil | TRIUMF



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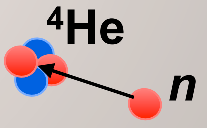
Outline

- Chiral 3N force
- No-core shell model
- Transformations of the 3N matrix elements in the HO basis
- Some results for bound states
- Including the continuum with the resonating group method
  - NCSM/RGM
    - n-^{4}He with the chiral 3N
  - NCSMC
- Outlook

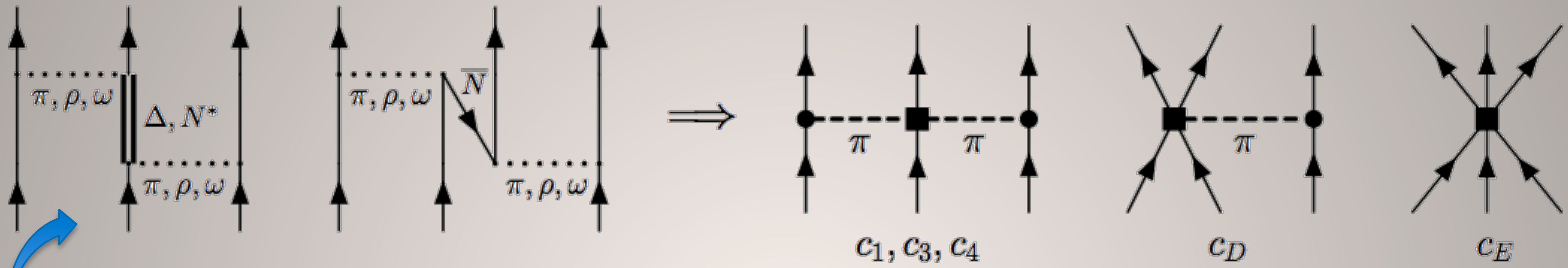


Chiral Effective Field Theory

- **First principles for Nuclear Physics:** **QCD**
  - Non-perturbative at low energies
  - Lattice QCD in the future
- ***For now a good place to start:***
- Inter-nucleon forces from chiral effective field theory
  - Based on the symmetries of QCD
    - Chiral symmetry of QCD ($m_u \approx m_d \approx 0$), spontaneously broken with pion as the Goldstone boson
    - Degrees of freedom: nucleons + pions
  - Systematic low-momentum expansion to a given order (Q/Λ_χ)
  - Hierarchy
  - Consistency
  - Low energy constants (LEC)
    - Fitted to data
    - Can be calculated by lattice QCD

Λ_χ~1 GeV :
Chiral symmetry breaking scale

Three-nucleon forces why?



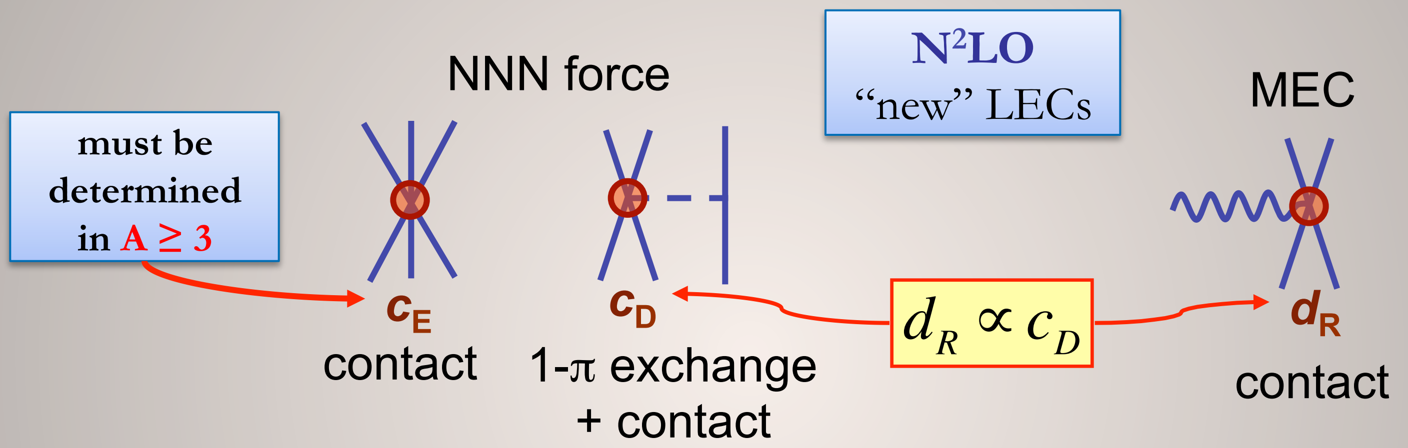
Eliminating degrees of freedom leads to three-body forces.

Two-pion exchange with **virtual Δ excitation** – Fujita Miyazawa (1957)

- Leading three-nucleon force terms
  - Long-range two-pion exchange
  - Medium-range one-pion exchange + two-nucleon contact
  - Short range three-nucleon contact

The question is not: Do three-body forces enter the description?
The only question is: How large are three-body forces?

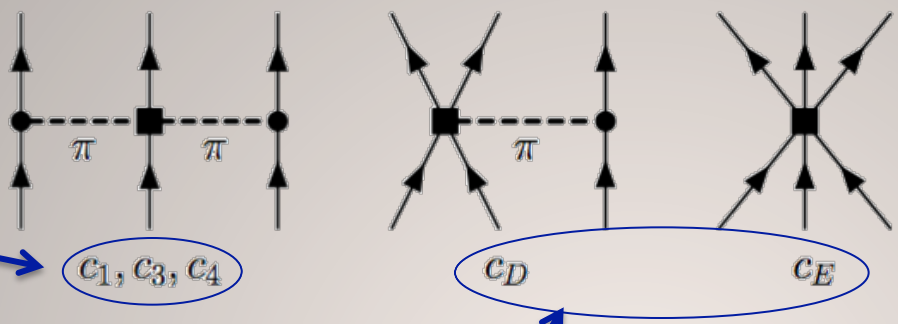
"New" low-energy constants of chiral NNN potential from fit to three-nucleon properties



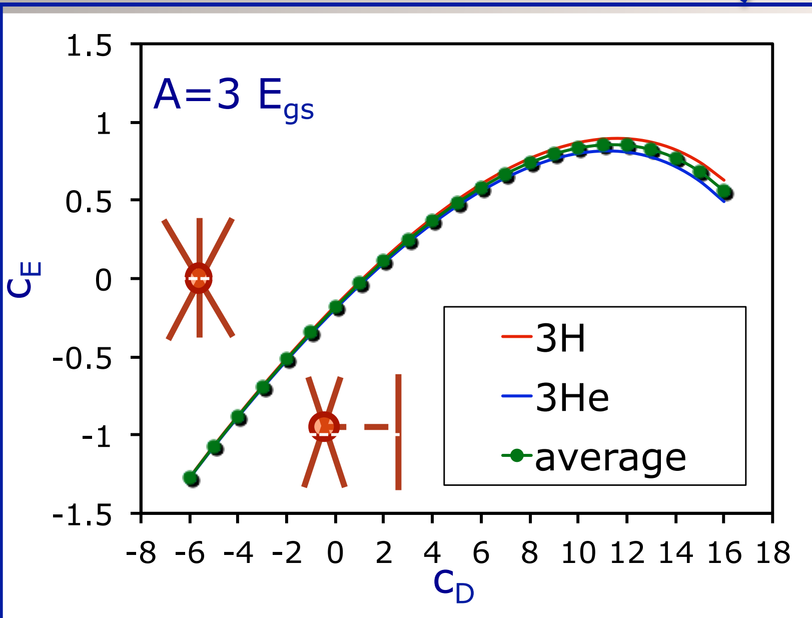
- Need two (hopefully uncorrelated) observables to fit the "new" low-energy constants. One could be the *A*=3 binding energy.
- There is a link between the medium-range (c_D term) NNN force and the meson-exchange current appearing in nuclear beta decay
  - A second observable could be the half life of tritium

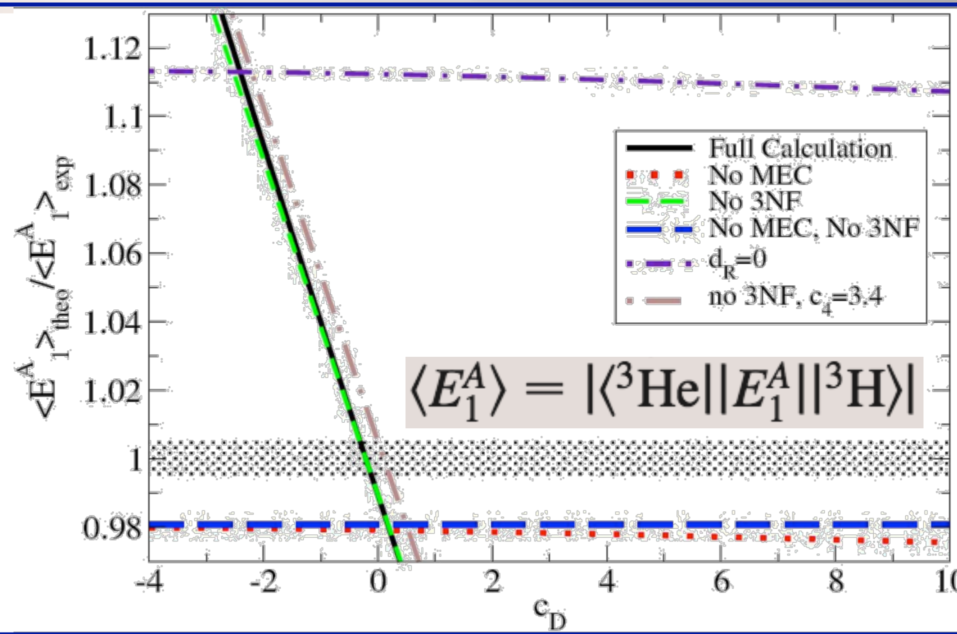
Leading terms of the chiral NNN force

From pion-nucleon scattering



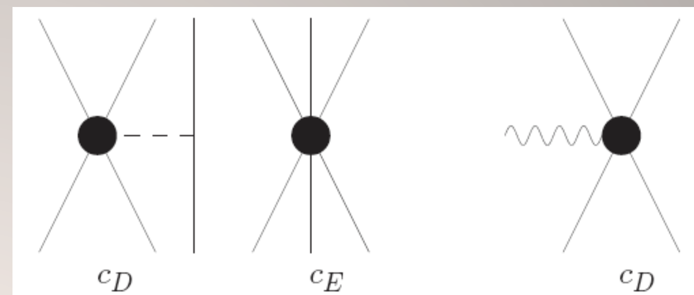
Ab initio calculations (NCSM, in this case) are needed not only to test nuclear interaction models, but also to constrain the interaction itself





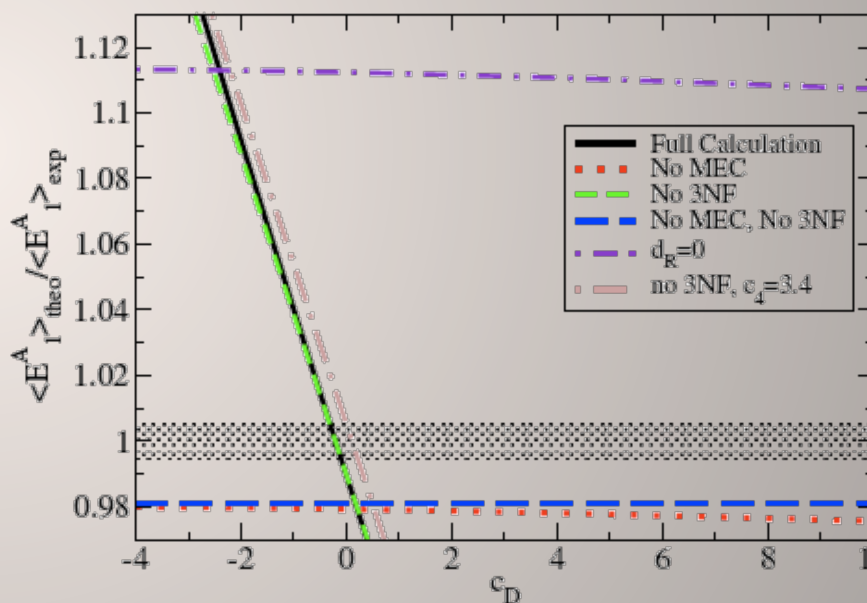
Determination of NNN constants c_D and c_E from the triton binding energy and the half life

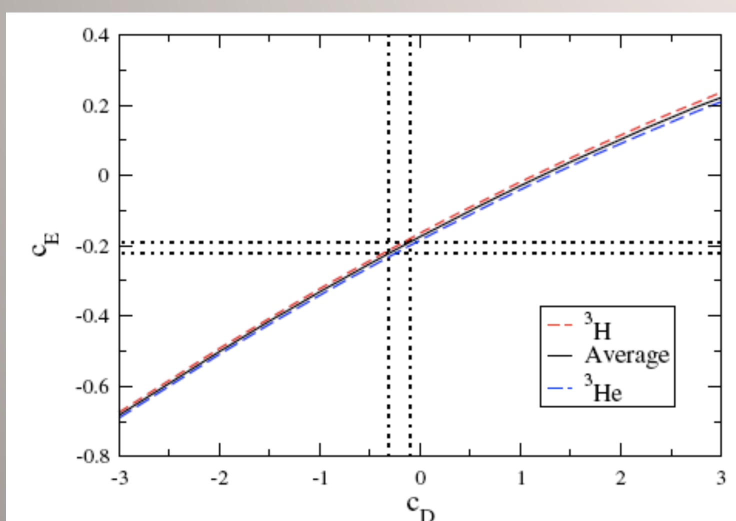
- **Chiral EFT**: c_D also in the two-nucleon contact vertex with an external probe
- Calculate $\langle E_1^A \rangle = |\langle {}^3\mathrm{He} || E_1^A || {}^3\mathrm{H} \rangle|$
  - Leading order GT
  - N^2LO: one-pion exchange plus contact



- *A*=3 binding energy constraint:

c_D=-0.2±0.1 c_E =-0.205±0.015





PRL 103, 102502 (2009) PHYSICAL REVIEW LETTERS week ending 4 SEPTEMBER 2009

Three-Nucleon Low-Energy Constants from the Consistency of Interactions and Currents in Chiral Effective Field Theory

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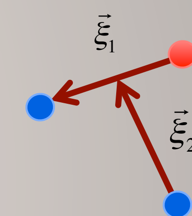
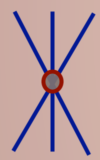
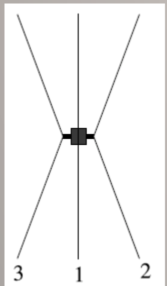
Local chiral N²LO NNN interaction

- Regulator depending on momentum transfer ⇒ local NNN interaction in coordinate space
  - Simpler to use, more like TM', UIX, IL
  - Different space-tensor structure (compared to regulation with nucleon momenta)
  - **Example:** Even the simplest, the contact term, gets involved…





$$
\begin{aligned}
W_1^{\rm cont} &= E\vec{\tau}_2\cdot\vec{\tau}_3\,\delta(\vec{r}_1-\vec{r}_2)\delta(\vec{r}_3-\vec{r}_1)\\
&= E\vec{\tau}_2\cdot\vec{\tau}_3\frac{1}{(2\pi)^6}\frac{1}{(\sqrt{3})^3}\int d\vec{\pi}_1 d\vec{\pi}_2 d\vec{\pi}_1' d\vec{\pi}_2' |\vec{\pi}_1\vec{\pi}_2\rangle\langle\vec{\pi}_1'\vec{\pi}_2'|
\end{aligned}
$$



$$
\begin{aligned}
W_1^{\rm cont,Q} &= E\vec{\tau}_2\cdot\vec{\tau}_3\frac{1}{(2\pi)^6}\frac{1}{(\sqrt{3})^3}\int d\vec{\pi}_1 d\vec{\pi}_2 d\vec{\pi}_1' d\vec{\pi}_2' |\vec{\pi}_1\vec{\pi}_2\rangle F(\vec{Q}^2;\Lambda)F(\vec{Q}'^2;\Lambda)\langle\vec{\pi}_1'\vec{\pi}_2'|\\
&= E\vec{\tau}_2\cdot\vec{\tau}_3\int d\vec{\xi}_1 d\vec{\xi}_2 |\vec{\xi}_1\vec{\xi}_2\rangle Z_0(\sqrt{2}\xi_1;\Lambda)Z_0(|\tfrac{1}{\sqrt{2}}\vec{\xi}_1+\sqrt{\tfrac{3}{2}}\vec{\xi}_2|;\Lambda)\langle\vec{\xi}_1\vec{\xi}_2|
\end{aligned}
$$

$$
\begin{aligned}
\vec{\xi}_1 &= \frac{1}{\sqrt{2}}(\vec{r}_1-\vec{r}_2)\\
\vec{\xi}_2 &= \sqrt{\frac{2}{3}}\left(\frac{1}{2}(\vec{r}_1+\vec{r}_2)-\vec{r}_3\right)\\
\vec{\pi}_1 &= \frac{1}{\sqrt{2}}(\vec{p}_1-\vec{p}_2)\\
\vec{\pi}_2 &= \sqrt{\frac{2}{3}}\left(\frac{1}{2}(\vec{p}_1+\vec{p}_2)-\vec{p}_3\right)
\end{aligned}
$$

$$
\begin{aligned}
\vec{Q} &= \vec{p}_2'-\vec{p}_2 = -\frac{1}{\sqrt{2}}(\vec{\pi}_1'-\vec{\pi}_1)+\frac{1}{\sqrt{6}}(\vec{\pi}_2'-\vec{\pi}_2)\\
\vec{Q}' &= \vec{p}_3'-\vec{p}_3 = \sqrt{\frac{2}{3}}(\vec{\pi}_2-\vec{\pi}_2')
\end{aligned}
$$

$$Z_0(r;\Lambda) = \frac{1}{2\pi^2}\int dq\, q^2 j_0(qr)F(q^2;\Lambda)$$

$$F(q^2;\Lambda) = \exp[-q^4/\Lambda^4]$$

- Technical details in

Few Body Syst (2007) 41: 117–140
DOI 10.1007/s00601-007-0193-3
Printed in The Netherlands

Few-Body Systems

Local three-nucleon interaction from chiral effective field theory

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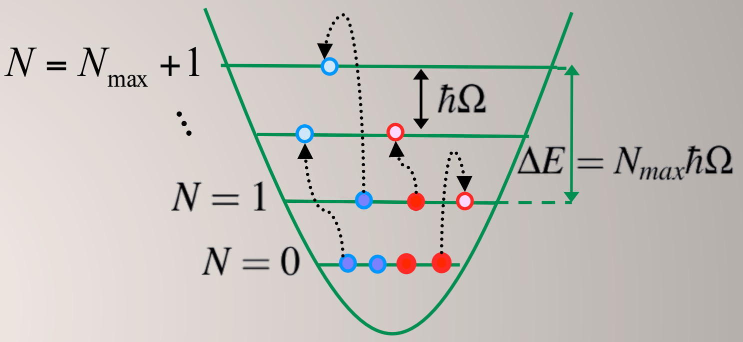
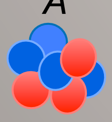
The *ab initio* no-core shell model (NCSM)

- The NCSM is a technique for the solution of the *A*-nucleon bound-state problem
- Realistic nuclear Hamiltonian
  - High-precision nucleon-nucleon potentials
  - Three-nucleon interactions



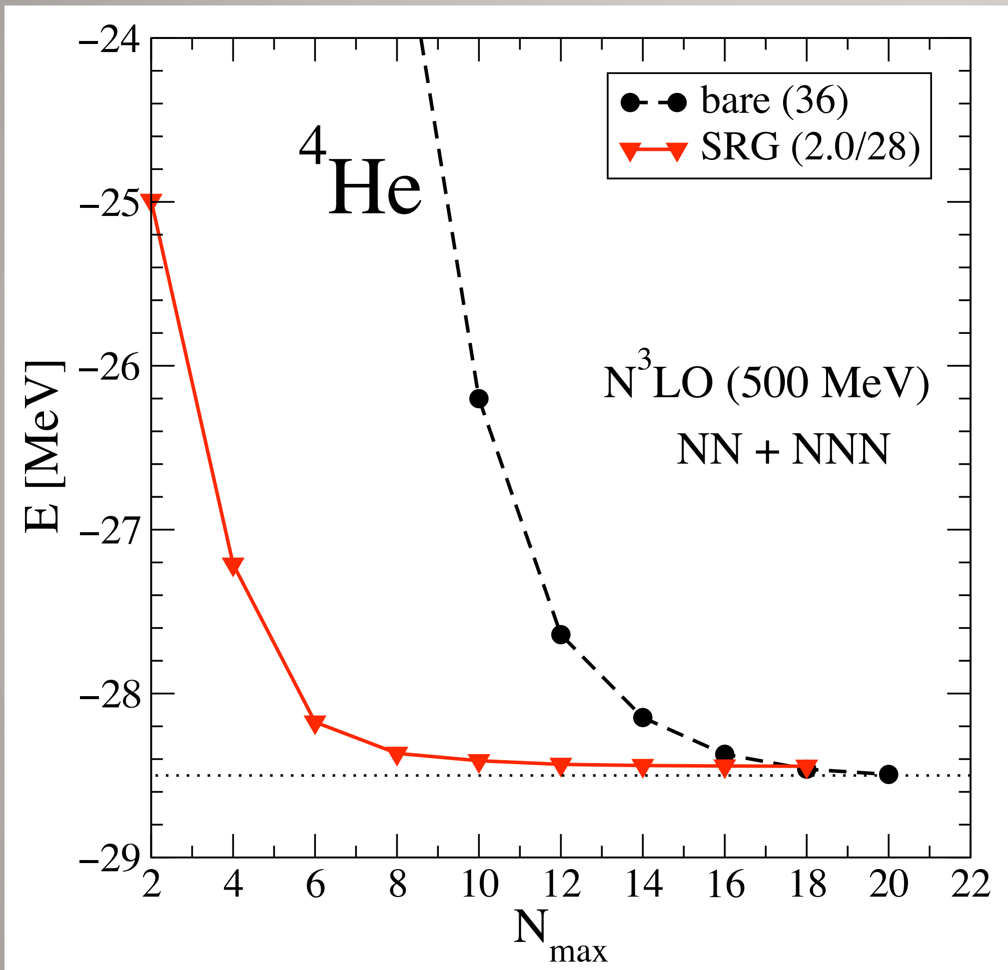
- Finite harmonic oscillator (HO) basis
  - *A*-nucleon HO basis states
  - complete $N_{max}\hbar\Omega$ model space
- ***Effective interaction tailored to model-space truncation*** for NN(+NNN) potentials
  - Okubo-Lee-Suzuki unitary transformation
- Or a **sequence of unitary transformations in momentum space**:
  - Similarity-Renormalization-Group (SRG) evolved NN(+NNN) potential



$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

Convergence to exact solution with increasing $N_{\max}$ for bound states. No coupling to continuum.

^{4}He from chiral EFT interactions: g.s. energy convergence



PRL 103, 082501 (2009) PHYSICAL REVIEW LETTERS week ending 21 AUGUST 2009

Evolution of Nuclear Many-Body Forces with the Similarity Renormalization Group

E. D. Jurgenson,[1] P. Navrátil,[2] and R. J. Furnstahl[1]

A=3 binding energy and half life constraint
c_D=-0.2, c_E=-0.205, Λ=500 MeV

Chiral N^{3}LO NN plus N^{2}LO NNN potential

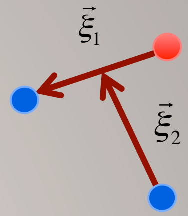
- Bare interaction (black line)
  - Strong short-range correlations
    - Large basis needed
- SRG evolved effective interaction (red line)
  - Unitary transformation

$$H_\alpha = U_\alpha H U_\alpha^+ \Rightarrow \frac{dH_\alpha}{d\alpha} = \left[\left[T, H_\alpha\right], H_\alpha\right] \quad \left(\alpha = 1/\lambda^4\right)$$

  - Two- plus *three*-body components, *four*-body omitted
  - Softens the interaction
    - Smaller basis sufficient

3*N* interaction matrix elements in HO basis

- Jacobi coordinate three-nucleon basis



$$|NiJMTM_T\rangle = \sum \langle (nlsjt, \mathcal{N}\mathcal{L}\tfrac{1}{2}\mathcal{J}\tfrac{1}{2})||NiJT\rangle \; |(nlsjt, \mathcal{N}\mathcal{L}\tfrac{1}{2}\mathcal{J}\tfrac{1}{2})JMTM_T\rangle$$

- 3*N* matrix elements in the three-nucleon Slater-determinant basis

$$\left|(nljm\tfrac{1}{2}m_t)_{(ijl)}\right\rangle = \frac{1}{\sqrt{3!}} \begin{vmatrix} \varphi_i(\vec{r}_1) & \varphi_i(\vec{r}_2) & \varphi_i(\vec{r}_3) \\ \varphi_j(\vec{r}_1) & \varphi_j(\vec{r}_2) & \varphi_j(\vec{r}_3) \\ \varphi_l(\vec{r}_1) & \varphi_l(\vec{r}_2) & \varphi_l(\vec{r}_3) \end{vmatrix} = a_l^+ a_j^+ a_i^+ |0\rangle$$

$$\begin{aligned} &\langle (nl\tfrac{1}{2}jm_j\tfrac{1}{2}m_t)_{(abc)}|V_{3\mathrm{eff},123}|(nl\tfrac{1}{2}jm_j\tfrac{1}{2}m_t)_{(def)}\rangle \\ &= \sum \langle (nl\tfrac{1}{2}jm_j\tfrac{1}{2}m_t)_{(abc)}|NiJMTM_T;N_{\mathrm{c.m.}}L_{\mathrm{c.m.}}M_{\mathrm{c.m.}}\rangle \; \langle NiJT|V_{3\mathrm{eff},123}|N'i'JT\rangle \; \langle N'i'JMTM_T;N_{\mathrm{c.m.}}L_{\mathrm{c.m.}}M_{\mathrm{c.m.}}|(nl\tfrac{1}{2}jm_j\tfrac{1}{2}m_t)_{(def)}\rangle \end{aligned}$$

3N interaction matrix elements in HO basis

- Transformation

PHYSICAL REVIEW C **68**, 034305 (2003)

$$
\begin{aligned}
&\langle (nl\tfrac{1}{2}jm_j\tfrac{1}{2}m_t)_{(abc)}|NiJMTM_T;N_{\mathrm{c.m.}}L_{\mathrm{c.m.}}M_{\mathrm{c.m.}}\rangle\\
&\quad=\delta_{2n_a+l_a+2n_b+l_b+2n_c+l_c,N+2N_{\mathrm{c.m.}}+L_{\mathrm{c.m.}}}\delta_{m_{j_a}+m_{j_b}+m_{j_c},M+M_{\mathrm{c.m.}}}\delta_{m_{t_a}+m_{t_b}+m_{t_c},M_T}\\
&\qquad\times\sqrt{6}\sum\langle (nlsjt,\mathcal{N}\mathcal{L}\tfrac{1}{2}\mathcal{J}\tfrac{1}{2})||NiJT\rangle\tfrac{1}{2}(1-(-1)^{l+s+t})(l_am_a\tfrac{1}{2}m_{s_a}|j_am_{j_a})(l_bm_b\tfrac{1}{2}m_{s_b}|j_bm_{j_b})(l_cm_c\tfrac{1}{2}m_{s_c}|j_cm_{j_c})\\
&\qquad\times(\tfrac{1}{2}m_{t_a}\tfrac{1}{2}m_{t_b}|tm_t)(tm_t\tfrac{1}{2}m_{t_c}|TM_T)(\tfrac{1}{2}m_{s_a}\tfrac{1}{2}m_{s_b}|sm_s)(l_bm_bl_am_a|\Lambda m_\Lambda)(L_{12}M_{12}lm_l|\Lambda m_\Lambda)(l_cm_cL_{12}M_{12}|\lambda m_\lambda)\\
&\qquad\times(L_{\mathrm{c.m.}}M_{\mathrm{c.m.}}\mathcal{L}\mathcal{M}_{\mathcal{L}}|\lambda m_\lambda)(\mathcal{L}\mathcal{M}_{\mathcal{L}}\tfrac{1}{2}m_{s_c}|\mathcal{J}\mathcal{M}_{\mathcal{J}})(lm_lsm_s|jm_j)(jm_j\mathcal{J}\mathcal{M}_{\mathcal{J}}|JM)\\
&\qquad\times\langle n_cl_cN_{12}L_{12}\lambda|N_{\mathrm{c.m.}}L_{\mathrm{c.m.}}\mathcal{N}\mathcal{L}\lambda\rangle_{\frac{1}{2}}\langle n_bl_bn_al_a\Lambda|N_{12}L_{12}nl\Lambda\rangle_1,
\end{aligned}
$$

- Implemented in the *p*-shell NCSM $N_{\max}$=4 ($N_{\max}$=6 for ^{6}Li) calculations
  - E3Max=max($2n_a+l_a+2n_b+l_b+2n_c+l_c$)=8

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3N interaction matrix elements in HO basis

- Transformation
  - Introduce an intermediate J-coupling

$$\{|N_{CM}L_{CM}\rangle|NiJT\rangle\}^{\mathcal{J}\mathcal{M}} \qquad \{\{|a\rangle|b\rangle\}^{J_{12}}|c\rangle\}^{\mathcal{J}\mathcal{M}}$$

PHYSICAL REVIEW C **73**, 064002 (2006)

$$\langle abc|N_{CM}L_{CM}M_{CM};NiJM\rangle = \sum (j_a m_a j_b m_b | J_{ab}M_{ab})(J_{ab}M_{ab}j_c m_c | \mathcal{J}\mathcal{M})\langle n_{12}l_{12}s_{12}j_{12};n_3 l_3 I_3|NiJ\rangle\langle((ab)J_{ab},c)\mathcal{J}|(N_{CM}L_{CM},\alpha)\mathcal{J}\rangle$$

$$|\alpha\rangle = |n_{12}n_3[(l_{12}s_{12})j_{12}(l_3 1/2)I_3]J M_J(t_{12}1/2)T M_T\rangle \qquad T \equiv \langle((ab)J_{ab},c)\mathcal{J}|(N_{CM}L_{CM},\alpha)\mathcal{J}\rangle$$

- Implemented in the p-shell NCSM N_{max}=8 calculations
  - E3Max= max($2n_a+l_a+2n_b+l_b+2n_c+l_c$)=11

- The main problem: Huge number of 3N matrix elements

$$T = \sum_{\mathcal{L}_{12}S_3L_3L_{12}\mathcal{L}\Lambda} \sqrt{\hat{j}_{12}\hat{I}_3\hat{L}_3\hat{S}_3} \begin{Bmatrix} l_{12} & l_3 & L_3 \\ s_{12} & 1/2 & S_3 \\ j_{12} & I_3 & J \end{Bmatrix}$$
$$\times(-)^{L_3+S_3+l_{c.m.}+\mathcal{J}}\sqrt{\hat{\mathcal{L}}\hat{J}} \begin{Bmatrix} l_{c.m.} & L_3 & \mathcal{L} \\ S_3 & \mathcal{J} & J \end{Bmatrix} \sqrt{\hat{L}_{12}\hat{s}_{12}\hat{j}_a\hat{j}_b}$$
$$\times \begin{Bmatrix} l_a & l_b & L_{12} \\ 1/2 & 1/2 & s_{12} \\ j_a & j_b & J_{12} \end{Bmatrix} \sqrt{\hat{J}_{12}\hat{j}_c\hat{\mathcal{L}}\hat{S}_3} \begin{Bmatrix} L_{12} & s_{12} & J_{12} \\ l_c & 1/2 & j_c \\ \mathcal{L} & S_3 & \mathcal{J} \end{Bmatrix}$$
$$\times(-)^{l_{12}+l_3-L_3}(-)^{l_{c.m.}+l_3+l_{12}+\mathcal{L}}\sqrt{\hat{\Lambda}\hat{L}_3} \begin{Bmatrix} l_{c.m.} & l_3 & \Lambda \\ l_{12} & \mathcal{L} & L_3 \end{Bmatrix}$$
$$\times(-)^{\mathcal{L}_{12}+l_c-\Lambda}(-)^{l_c+L_{12}-\mathcal{L}}(-)^{l_c+l_{12}+\mathcal{L}_{12}+\mathcal{L}}\sqrt{\hat{\Lambda}\hat{L}_{12}}$$
$$\times \begin{Bmatrix} l_c & \mathcal{L}_{12} & \Lambda \\ l_{12} & \mathcal{L} & L_{12} \end{Bmatrix} [n_{c.m.}l_{c.m.}, n_3 l_3 : \Lambda; N_{12}\mathcal{L}_{12}, n_c l_c : \Lambda]_d$$
$$\times [N_{12}\mathcal{L}_{12}, n_{12}l_{12} : L_{12}; n_a l_a, n_b l_b : L_{12}]_{d'}$$

$3N$ interaction matrix elements in HO basis

- Transformation
  - Introduce an intermediate J-coupling

$$\{|N_{CM}L_{CM}\rangle|NiJT\rangle\}^{\mathcal{J}\mathcal{M}} \qquad \{\{|a\rangle|b\rangle\}^{J_{12}}|c\rangle\}^{\mathcal{J}\mathcal{M}}$$

PHYSICAL REVIEW C **73**, 064002 (2006)

$$\langle abc|N_{CM}L_{CM}M_{CM};NiJM\rangle = \sum (j_a m_a j_b m_b | J_{ab}M_{ab})(J_{ab}M_{ab} j_c m_c | \mathcal{J}\mathcal{M})\langle n_{12}l_{12}s_{12}j_{12};n_3 l_3 I_3|NiJ\rangle\langle((ab)J_{ab},c)\mathcal{J}|(N_{CM}L_{CM},\alpha)\mathcal{J}\rangle$$

$$|\alpha\rangle = |n_{12}n_3[(l_{12}s_{12})j_{12}(l_3 1/2)I_3]J M_J (t_{12}1/2)T M_T\rangle \qquad T \equiv \langle((ab)J_{ab},c)\mathcal{J}|(N_{CM}L_{CM},\alpha)\mathcal{J}\rangle$$

- New developments (R. Roth *et al.*):
  - Store 3N matrix elements in the J-coupled basis
  - Uncouple on the fly
  - Use a smart ordering to facilitate efficient uncoupling

    PRL **107**, 072501 (2011)
- Implemented up to E3Max= $\max(2n_a+l_a+2n_b+l_b+2n_c+l_c)=16$
  - Good for p-shell NCSM N_{max}=13 calculations

$$T = \sum_{\mathcal{L}_{12}S_3L_3L_{12}\mathcal{L}\Lambda} \sqrt{\hat{j}_{12}\hat{I}_3\hat{L}_3\hat{S}_3}\begin{Bmatrix} l_{12} & l_3 & L_3 \\ s_{12} & 1/2 & S_3 \\ j_{12} & I_3 & J \end{Bmatrix}$$
$$\times(-)^{L_3+S_3+l_{\text{c.m.}}+\mathcal{J}}\sqrt{\hat{\mathcal{L}}\hat{J}}\begin{Bmatrix} l_{\text{c.m.}} & L_3 & \mathcal{L} \\ S_3 & \mathcal{J} & J \end{Bmatrix}\sqrt{\hat{L}_{12}\hat{s}_{12}\hat{j}_a\hat{j}_b}$$
$$\times\begin{Bmatrix} l_a & l_b & L_{12} \\ 1/2 & 1/2 & s_{12} \\ j_a & j_b & J_{12} \end{Bmatrix}\sqrt{\hat{J}_{12}\hat{j}_c\hat{\mathcal{L}}\hat{S}_3}\begin{Bmatrix} L_{12} & s_{12} & J_{12} \\ l_c & 1/2 & j_c \\ \mathcal{L} & S_3 & \mathcal{J} \end{Bmatrix}$$
$$\times(-)^{l_{12}+l_3-L_3}(-)^{l_{\text{c.m.}}+l_3+l_{12}+\mathcal{L}}\sqrt{\hat{\Lambda}\hat{L}_3}\begin{Bmatrix} l_{\text{c.m.}} & l_3 & \Lambda \\ l_{12} & \mathcal{L} & L_3 \end{Bmatrix}$$
$$\times(-)^{\mathcal{L}_{12}+l_c-\Lambda}(-)^{l_c+L_{12}-\mathcal{L}}(-)^{l_c+l_{12}+\mathcal{L}_{12}+\mathcal{L}}\sqrt{\hat{\Lambda}\hat{L}_{12}}$$
$$\times\begin{Bmatrix} l_c & \mathcal{L}_{12} & \Lambda \\ l_{12} & \mathcal{L} & L_{12} \end{Bmatrix}[n_{\text{c.m.}}l_{\text{c.m.}}, n_3l_3:\Lambda; N_{12}\mathcal{L}_{12}, n_cl_c:\Lambda]_d$$
$$\times[N_{12}\mathcal{L}_{12}, n_{12}l_{12}:L_{12}; n_al_a, n_bl_b:L_{12}]_{d'}$$

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3*N* interaction matrix elements in HO basis

- Transformation
  - Introduce an intermediate *J*-coupling

$$\{|N_{CM}L_{CM}\rangle|NiJT\rangle\}^{\mathcal{J}\mathcal{M}} \qquad \{\{|a\rangle|b\rangle\}^{J_{12}}|c\rangle\}^{\mathcal{J}\mathcal{M}}$$

PHYSICAL REVIEW C **73**, 064002 (2006)

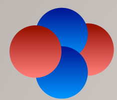
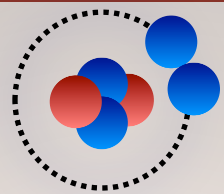
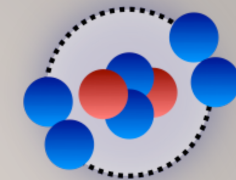
$$\langle abc|N_{CM}L_{CM}M_{CM};NiJM\rangle = \sum (j_a m_a j_b m_b | J_{ab}M_{ab})(J_{ab}M_{ab} j_c m_c | \mathcal{J}\mathcal{M})\langle n_{12}l_{12}s_{12}j_{12};n_3 l_3 I_3|NiJ\rangle\langle((ab)J_{ab},c)\mathcal{J}|(N_{CM}L_{CM},\alpha)\mathcal{J}\rangle$$

$$|\alpha\rangle = |n_{12}n_3[(l_{12}s_{12})j_{12}(l_3 1/2)I_3]JM_J(t_{12}1/2)TM_T\rangle \qquad T \equiv \langle((ab)J_{ab},c)\mathcal{J}|(N_{CM}L_{CM},\alpha)\mathcal{J}\rangle$$

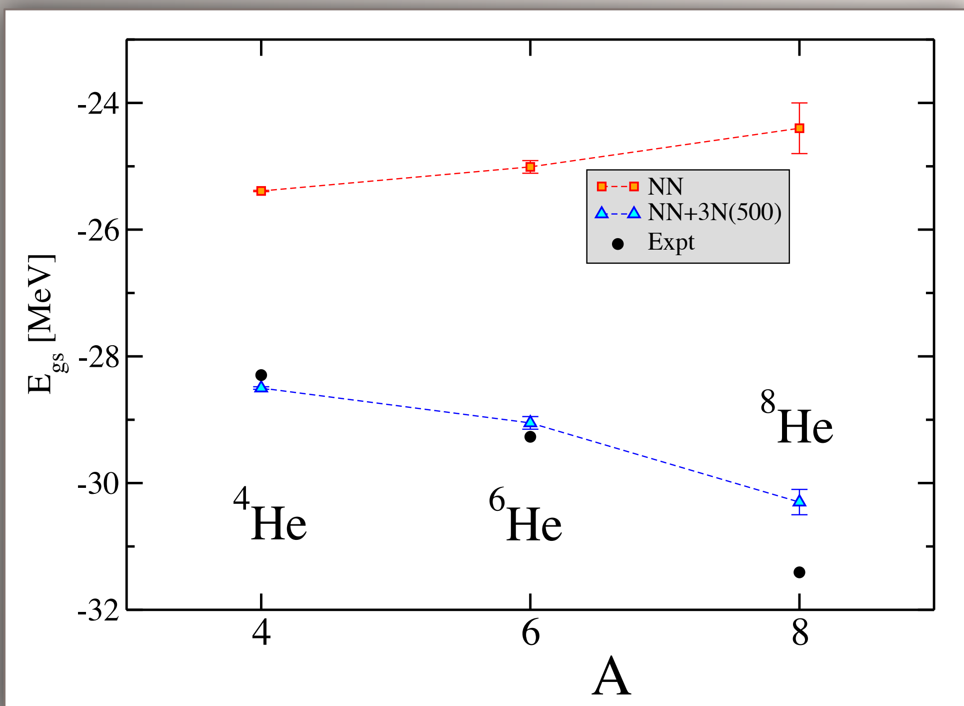
  - However, **E3Max=16 not sufficient** for medium mass nuclei and perhaps also not enough for the reactions and scattering
  - Further improvements needed, e,g.:
    - Three sums in *T* can be performed, with two 9j and three 6j coefficients replaced by a 12j and a 6j coefficient. Code speedup significant… More work needed!

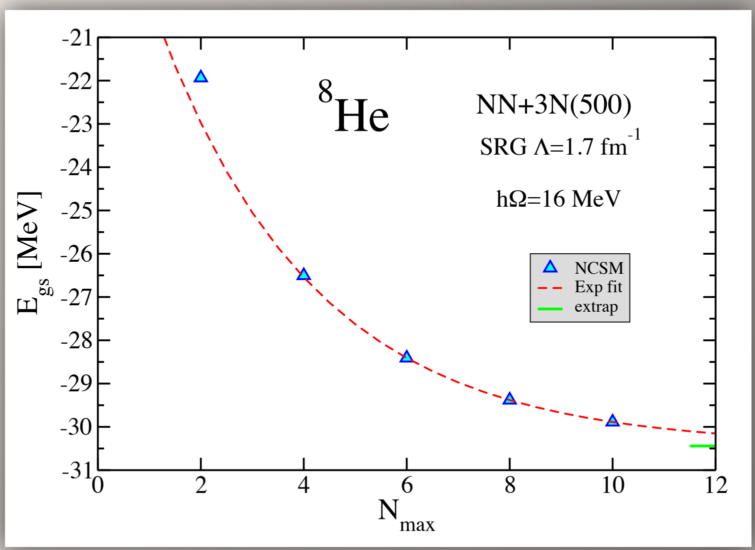
$$T = \sum_{\mathcal{L}_{12}S_3L_3L_{12}\mathcal{L}\Lambda} \sqrt{\hat{j}_{12}\hat{I}_3\hat{L}_3\hat{S}_3} \begin{Bmatrix} l_{12} & l_3 & L_3 \\ s_{12} & 1/2 & S_3 \\ j_{12} & I_3 & J \end{Bmatrix}$$
$$\times(-)^{L_3+S_3+l_{c.m.}+\mathcal{J}}\sqrt{\hat{\mathcal{L}}\hat{J}} \begin{Bmatrix} l_{c.m.} & L_3 & \mathcal{L} \\ S_3 & \mathcal{J} & J \end{Bmatrix} \sqrt{\hat{L}_{12}\hat{s}_{12}\hat{j}_a\hat{j}_b}$$
$$\times \begin{Bmatrix} l_a & l_b & L_{12} \\ 1/2 & 1/2 & s_{12} \\ j_a & j_b & J_{12} \end{Bmatrix} \sqrt{\hat{J}_{12}\hat{j}_c\hat{\mathcal{L}}\hat{S}_3} \begin{Bmatrix} L_{12} & s_{12} & J_{12} \\ l_c & 1/2 & j_c \\ \mathcal{L} & S_3 & \mathcal{J} \end{Bmatrix}$$
$$\times(-)^{l_{12}+l_3-L_3}(-)^{l_{c.m.}+l_3+l_{12}+\mathcal{L}}\sqrt{\hat{\Lambda}\hat{L}_3} \begin{Bmatrix} l_{c.m.} & l_3 & \Lambda \\ l_{12} & \mathcal{L} & L_3 \end{Bmatrix}$$
$$\times(-)^{\mathcal{L}_{12}+l_c-\Lambda}(-)^{l_c+L_{12}-\mathcal{L}}(-)^{l_c+l_{12}+\mathcal{L}_{12}+\mathcal{L}}\sqrt{\hat{\Lambda}\hat{L}_{12}}$$
$$\times \begin{Bmatrix} l_c & \mathcal{L}_{12} & \Lambda \\ l_{12} & \mathcal{L} & L_{12} \end{Bmatrix} [n_{c.m.}l_{c.m.}, n_3 l_3 : \Lambda; N_{12}\mathcal{L}_{12}, n_c l_c : \Lambda]_d$$
$$\times [N_{12}\mathcal{L}_{12}, n_{12}l_{12} : L_{12}; n_a l_a, n_b l_b : L_{12}]_{d'}$$

NNN interaction effects in neutron rich nuclei: He isotopes

^{4}He  ^{6}He  ^{8}He 

- ^{6}He and ^{8}He with SRG-evolved chiral N^{3}LO NN + N^{2}LO NNN
  - chiral N^{3}LO NN: ^{4}He underbound, ^{6}He and ^{8}He **unbound**
  - chiral N^{3}LO NN + N^{2}LO NNN: ^{4}He OK, both ^{6}He and ^{8}He **bound**





NNN interaction important to bind neutron rich nuclei

^{6}He half-life

Precision measurement of ^{6}He beta decay

PHYSICAL REVIEW C **86**, 035506 (2012)

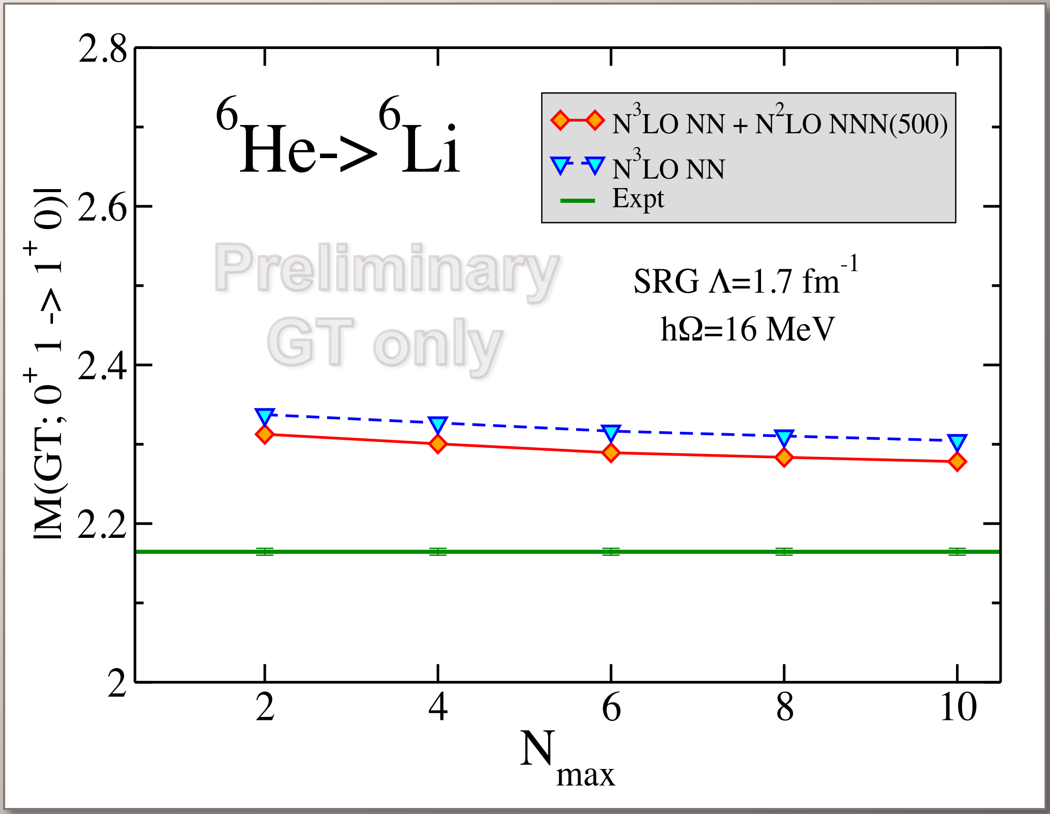
Precision measurement of the ^{6}He half-life and the weak axial current in nuclei

A. Knecht,[1,*] R. Hong,[1] D. W. Zumwalt,[1] B. G. Delbridge,[1] A. García,[1] P. Müller,[2] H. E. Swanson,[1] I. S. Towner,[3] S. Utsuno,[1] W. Williams,[2,†] and C. Wrede[1,‡]

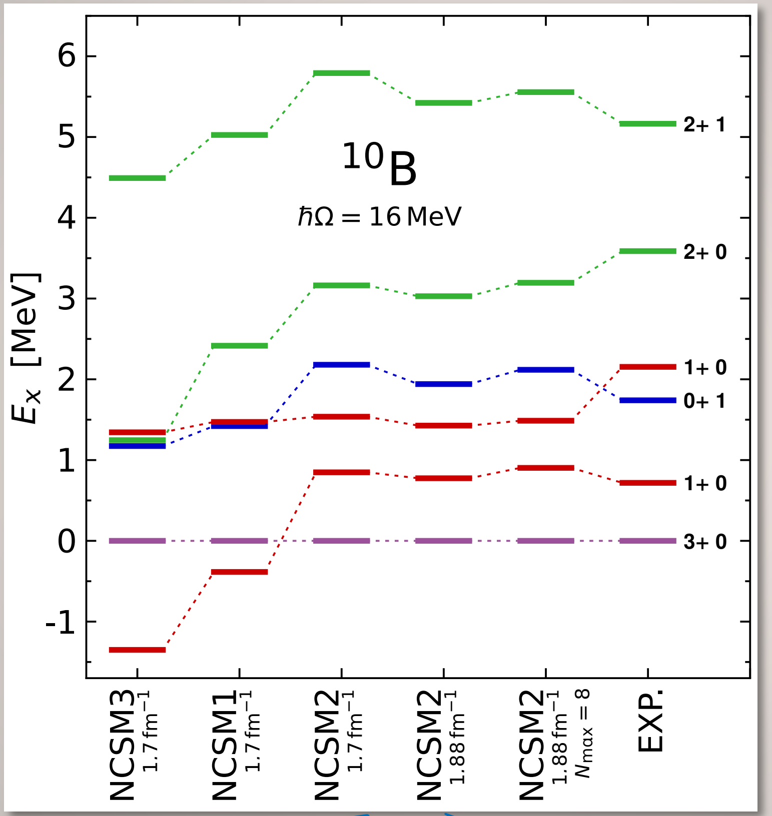
… challenge and test of *ab initio* calculations, nuclear forces and currents

Improvement with the NNN interaction

MEC must be included



^{10}B states very sensitive to 3N interaction

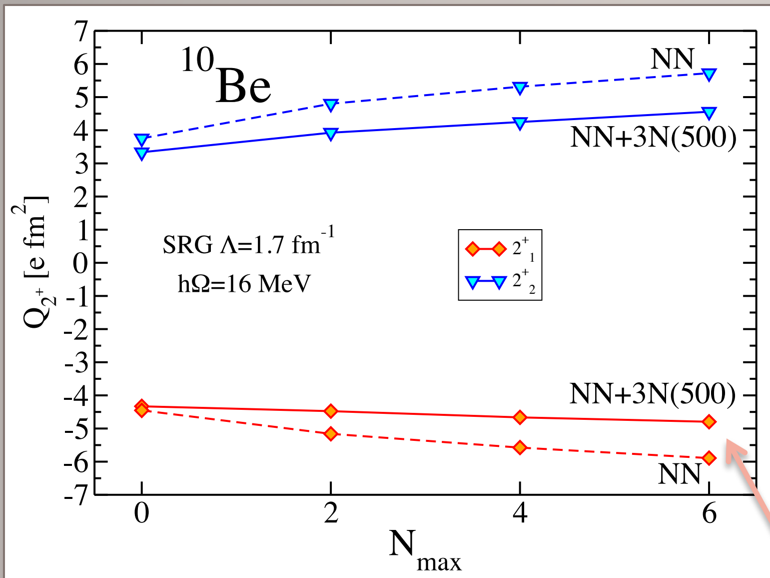


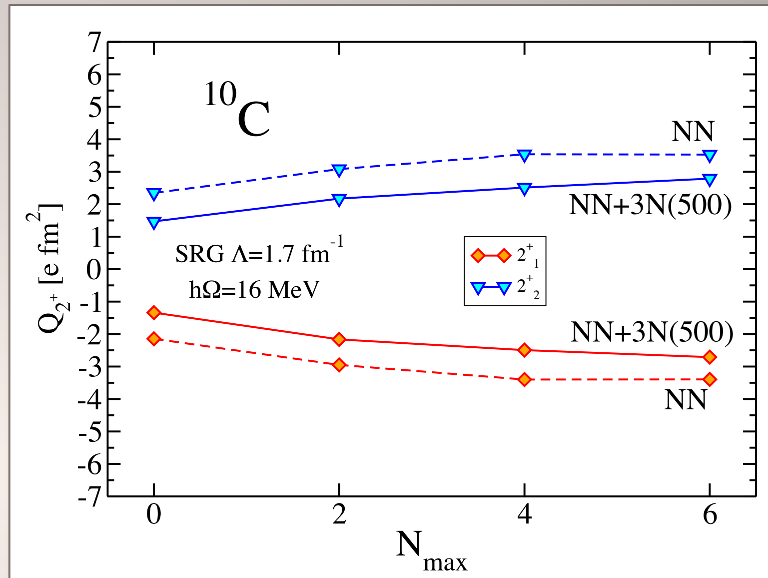
chiral NN

chiral NN+3N(400)

chiral NN+3N(500)

Properties of low lying states if ^{10}Be and ^{10}C





Q_{2+1}<0 from Coulomb excitation at TRIUMF

	NCSM: CD-Bonn 2000	GFMC: AV18+IL7	experiment
^{10}Be $B(E2;2^+_1 \rightarrow 0^+_1)$	9.8(4)	8.8(4)	9.2(3)
^{10}Be $B(E2;2^+_2 \rightarrow 0^+_1)$	0.2(2)	1.8(1)	0.11(2)
^{10}C $B(E2;2^+_1 \rightarrow 0^+_1)$	10(2)	15.3(1.4)	8.8(3)

^{10}C and ^{10}Be high-precision Q moment measurement proposed

Recent 2^+_1 state lifetime measurements at ANL and Coulomb excitations at TRIUMF

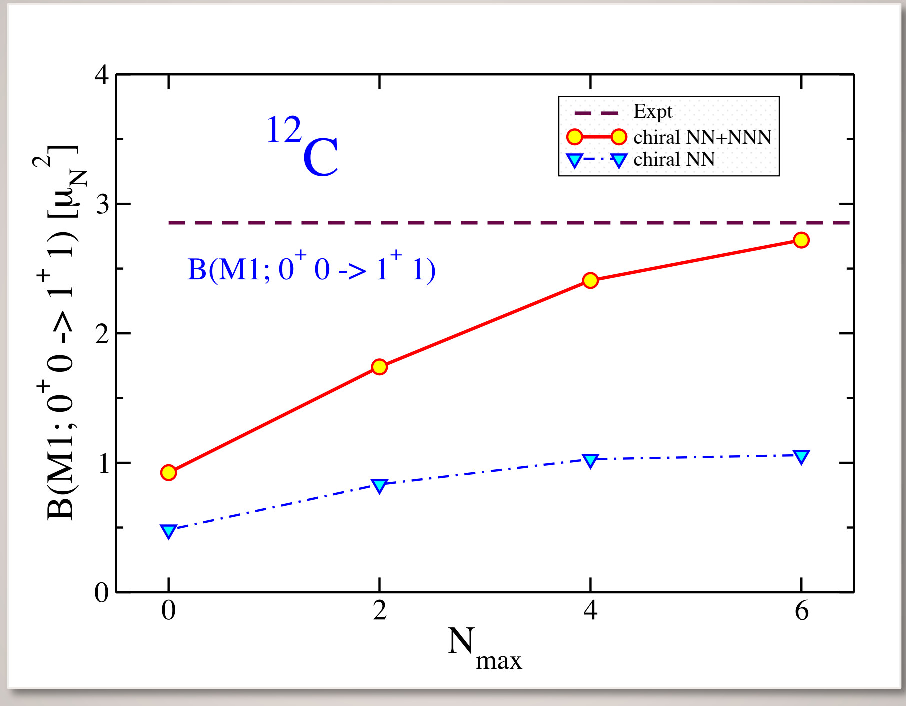
PHYSICAL REVIEW C **86**, 041303(R) (2012)

Reorientation-effect measurement of the $\langle 2^+_1 \| \hat{E}2 \| 2^+_1 \rangle$ matrix element in ^{10}Be

J. N. Orce,[1,2,*] T. E. Drake,[3] M. K. Djongolov,[1] P. Navrátil,[1,4] S. Triambak,[1,5] G. C. Ball,[1] H. Al Falou,[1,6] R. Churchman,[1] D. S. Cross,[7] P. Finlay,[8] C. Forssén,[9] A. B. Garnsworthy,[1] P. E. Garrett,[8] G. Hackman,[1] A. B. Hayes,[10] R. Kshetri,[1,7] J. Lassen,[1] K. G. Leach,[8] R. Li,[1] J. Meissner,[1] C. J. Pearson,[1] E. T. Rand,[8] F. Sarazin,[11] S. K. L. Sjue,[1] M. A. Stoyer,[4] C. S. Sumithrarachchi,[8] C. E. Svensson,[8] E. R. Tardiff,[1] A. Teigelhoefer,[1] S. J. Williams,[1,†] J. Wong,[8] and C. Y. Wu[4]

TRIUMF

M1 transitions in ^{12}C sensitive to 3N interaction



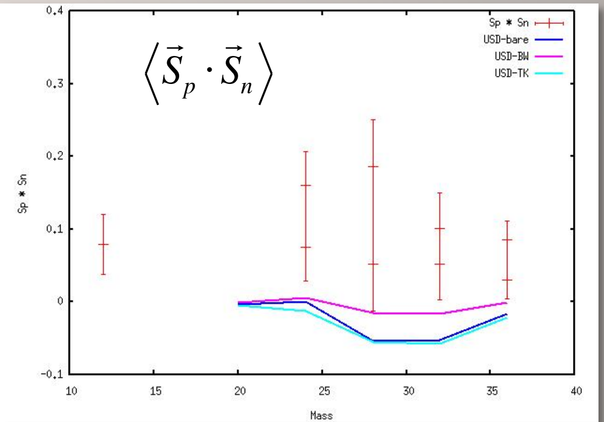
Chiral 3N interaction changes occupations of the $p_{3/2}$ and $p_{1/2}$ orbits
("increases the gap" between them)
Enhances the M1 transition from the g.s. to 1^+ 1 state

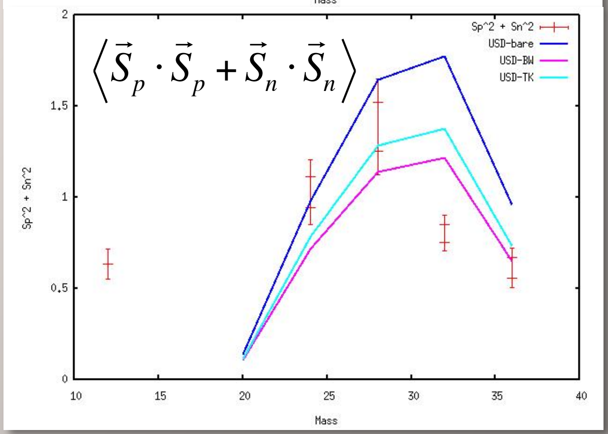
Similar increase of the Gamow-Teller transition between g.s. of $^{12}B(^{12}N)$ and ^{12}C

Tensor correlations and 3N effects in ground states of ^{4}He and ^{12}C

- Tensor correlations related to $\langle \vec{S}_p \cdot \vec{S}_n \rangle$ and $\langle \vec{S}_p \cdot \vec{S}_p + \vec{S}_n \cdot \vec{S}_n \rangle$
  - $\vec{S}_p = \frac{1}{2}\sum_{i=1}^{A}(\frac{1}{2}+t_{z,i})\,\vec{\sigma}_i \quad , \quad \vec{S}_n = \frac{1}{2}\sum_{i=1}^{A}(\frac{1}{2}-t_{z,i})\,\vec{\sigma}_i$ … spin operators
- Experiment: Atsushi Tamii *et al.*
- *Ab initio* NCSM:
  - ^{12}C N_{max}=6 only

	$\langle \vec{S}_p \cdot \vec{S}_p + \vec{S}_n \cdot \vec{S}_n \rangle$	$\langle \vec{S}_p \cdot \vec{S}_n \rangle$	$\langle \vec{S}^2 \rangle$
^{4}He Minnesota NN	0.04	-0.02	0
^{4}He chiral NN	0.19	0.04	0.27
^{4}He chiral NN+3N(500)	0.22	0.05	0.32
^{12}C chiral NN	0.50	0.065	0.63
^{12}C chiral NN+3N(400)	0.68	0.061	0.80
^{12}C chiral NN+3N(500)	1.01	0.065	1.14





^{12}C: chiral NN+3N(400)
the best agreement with experiment

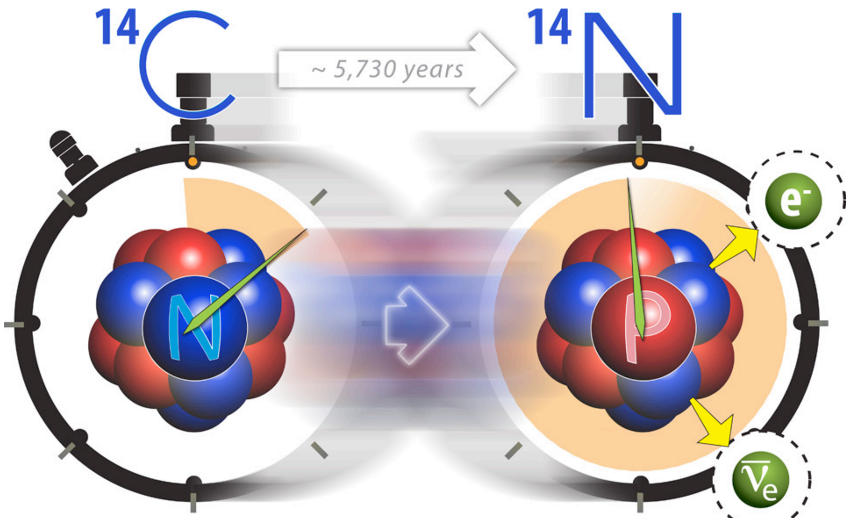
“Anomalous Long Lifetime of Carbon-14”

Objectives

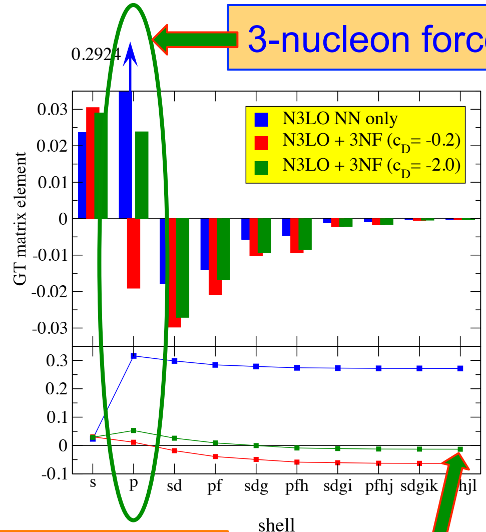
- Solve the puzzle of the long but useful lifetime of ^{14}C
- Determine the microscopic origin of the suppressed β-decay rate

Impact

- Establishes a major role for strong 3-nucleon forces in nuclei
- Verifies accuracy of *ab initio* microscopic nuclear theory



3-nucleon forces suppress critical component



net decay rate
Is very small

- Dimension of matrix solved for 8 lowest states ~ 1×10^9
- Solution takes ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL

PRL 106, 202502 (2011) PHYSICAL REVIEW LETTERS week ending 20 MAY 2011

Origin of the Anomalous Long Lifetime of ^{14}C

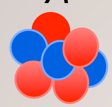
P. Maris,[1] J. P. Vary,[1] P. Navrátil,[2,3] W. E. Ormand,[3,4] H. Nam,[5] and D. J. Dean[5]

TRIUMF

Extending no-core shell model beyond bound states

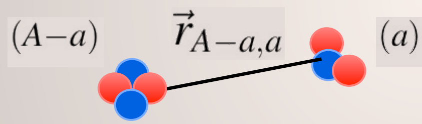
Include more many nucleon correlations…

NCSM →

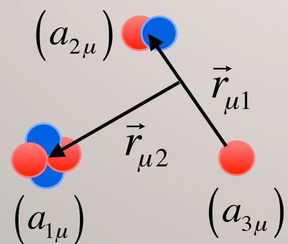


$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

+



+



$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

+

…

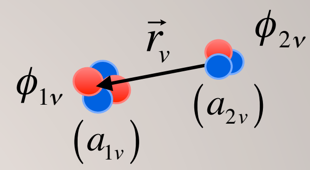
…using the Resonating Group Method (RGM) ideas

Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_{\kappa} \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$

$(a_{1\kappa} = A)$

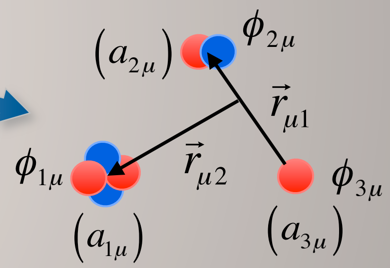
$$+ \sum_{\nu} \hat{A}_{\nu} \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right) \phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_{\nu}(\vec{r}_{\nu})$$



$$a_{1\nu} + a_{2\nu} = A$$

$$+ \sum_{\mu} \hat{A}_{\mu} \phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right) \phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right) \phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right) G_{\mu}(\vec{r}_{\mu 1}, \vec{r}_{\mu 2})$$

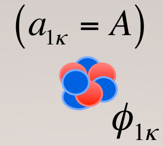
$$+ \cdots$$



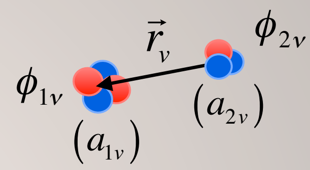
$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_{\kappa} \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$



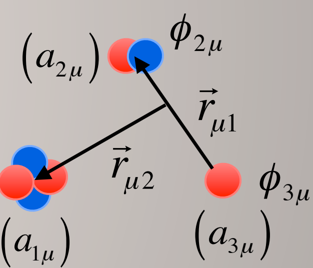
$$+ \sum_{\nu} \hat{A}_{\nu} \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right) \phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_{\nu}(\vec{r}_{\nu})$$



$$a_{1\nu} + a_{2\nu} = A$$

$$+ \sum_{\mu} \hat{A}_{\mu} \phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right) \phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right) \phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right) G_{\mu}(\vec{r}_{\mu 1}, \vec{r}_{\mu 2})$$

$$+ \cdots$$

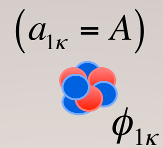


$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

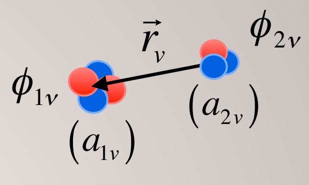
- ϕ : antisymmetric cluster wave functions
  - $\{\xi\}$: Translationally invariant internal coordinates (Jacobi relative coordinates)
  - These are known, they are an input

Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_\kappa \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$



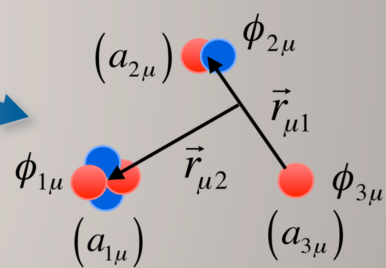
$$+ \sum_{\nu} \hat{A}_\nu \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right) \phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_\nu(\vec{r}_\nu)$$



$$a_{1\nu} + a_{2\nu} = A$$

$$+ \sum_{\mu} \hat{A}_\mu \phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right) \phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right) \phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right) G_\mu(\vec{R}_{\mu 1}, \vec{R}_{\mu 2})$$

$$+ \cdots$$



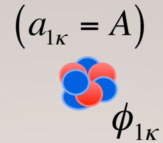
$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

- **A_ν, A_μ** : intercluster antisymmetrizers
  - Antisymmetrize the wave function for exchanges of nucleons between clusters
  - Example:

$$a_{1\nu} = A - 1,\ a_{2\nu} = 1 \quad \Rightarrow \quad \hat{A}_\nu = \frac{1}{\sqrt{A}}\left[1 - \sum_{i=1}^{A-1} \hat{P}_{iA}\right]$$

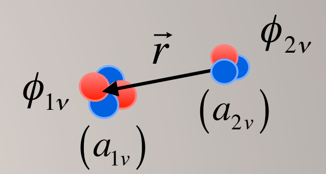
Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} \boxed{c_\kappa} \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$



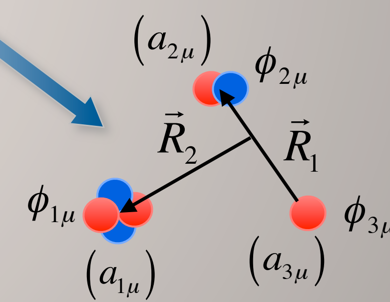
$$a_{1\nu} + a_{2\nu} = A$$

$$+ \sum_{\nu} \int \boxed{g_\nu(\vec{r}\,)}\, \hat{A}_\nu \left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r} - \vec{r}_\nu)\right] d\vec{r}$$



$$+ \sum_{\mu} \iint \boxed{G_\mu(\vec{R}_1, \vec{R}_2)}\, \hat{A}_\mu \left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)\delta(\vec{R}_1 - \vec{R}_{\mu 1})\delta(\vec{R}_2 - \vec{R}_{\mu 2})\right] d\vec{R}_1 d\vec{R}_2$$

$$+ \cdots$$



$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

- ***c***, ***g*** and ***G***: discrete and continuous linear variational amplitudes
  - Unknowns to be determined

TRIUMF

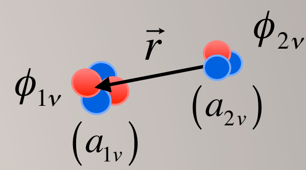
Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_{\kappa} \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$

$(a_{1\kappa} = A)$

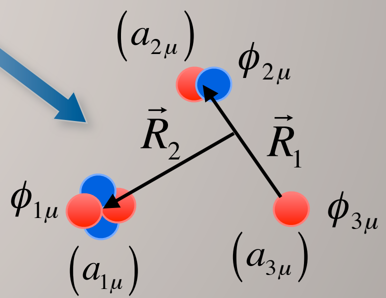
$a_{1\nu} + a_{2\nu} = A$

$$+\sum_{\nu}\int g_{\nu}(\vec{r}\,)\ \hat{A}_{\nu}\left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r}-\vec{r}_{\nu})\right]d\vec{r}$$



$$+\sum_{\mu}\iint G_{\mu}(\vec{R}_1,\vec{R}_2)\ \hat{A}_{\mu}\left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)\delta(\vec{R}_1-\vec{R}_{\mu 1})\delta(\vec{R}_2-\vec{R}_{\mu 2})\right]d\vec{R}_1 d\vec{R}_2$$

$$+\ \cdots$$



$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$

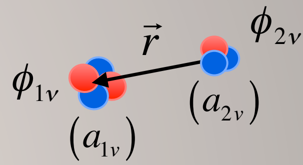
- Discrete and continuous set of basis functions
  - Non-orthogonal
  - Over-complete

Binary cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_{\kappa} \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$

$$a_{1\nu} + a_{2\nu} = A$$

$$+\sum_{\nu} \int g_{\nu}(\vec{r}\,)\; \hat{A}_{\nu}\left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r} - \vec{r}_{\nu})\right]d\vec{r}$$



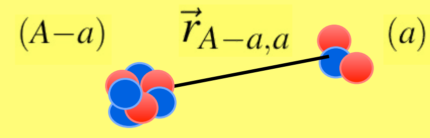
$$+\sum_{\mu} \iint G_{\mu}(\vec{R}_1,\vec{R}_2)\; \hat{A}_{\mu}\left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)\delta(\vec{R}_1 - \vec{R}_{\mu 1})\delta(\vec{R}_2 - \vec{R}_{\mu 2})\right]d\vec{R}_1 d\vec{R}_2$$

$$+ \cdots$$

- In practice: function space limited by using relatively simple forms of Ψ chosen according to physical intuition and energetical arguments
  - Most common: expansion over binary-cluster basis

The *ab initio* NCSM/RGM in a snapshot

- Ansatz: $\Psi^{(A)} = \sum_\nu \int d\vec{r}\, \varphi_\nu(\vec{r})\, \hat{\mathcal{A}}\, \Phi^{(A-a,a)}_{\nu\vec{r}}$



$$\psi^{(A-a)}_{1\nu}\, \psi^{(a)}_{2\nu}\, \delta(\vec{r} - \vec{r}_{A-a,a})$$

eigenstates of $H_{(A\text{-}a)}$ and $H_{(a)}$ in the *ab initio* NCSM basis

- Many-body Schrödinger equation:

$$H\Psi^{(A)} = E\Psi^{(A)}$$

$$T_{\rm rel}(r) + \mathcal{V}_{\rm rel} + \bar{V}_{\rm Coul}(r) + H_{(A-a)} + H_{(a)}$$

realistic nuclear Hamiltonian

$$\sum_\nu \int d\vec{r} \left[\mathcal{H}^{(A-a,a)}_{\mu\nu}(\vec{r}\,', \vec{r}) - E\,\mathcal{N}^{(A-a,a)}_{\mu\nu}(\vec{r}\,', \vec{r}) \right] \varphi_\nu(\vec{r}) = 0$$

$$\langle \Phi^{(A-a,a)}_{\mu\vec{r}\,'} | \hat{\mathcal{A}} H \hat{\mathcal{A}} | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$$

Hamiltonian kernel

$$\langle \Phi^{(A-a,a)}_{\mu\vec{r}\,'} | \hat{\mathcal{A}}^2 | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$$

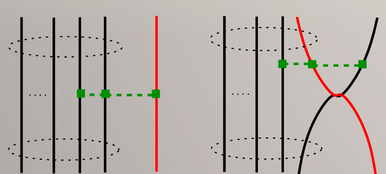
Norm kernel

Including 3N interaction in the NCSM/RGM Single-nucleon projectile:

$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \right| \hat{A}_{\nu'} V^{NNN} \hat{A}_{\nu} \left| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left\langle (A-1) \; r' \; (a'=1) \right| V^{NNN} \left(1 - \sum_{i=1}^{A-1} \hat{P}_{iA} \right) \left| (a=1) \; r \; (A-1) \right\rangle$$

$$\mathcal{V}^{NNN}_{\nu'\nu}(r,r') = \sum R_{n'l'}(r') R_{nl}(r) \left[\frac{(A-1)(A-2)}{2} \langle \Phi^{J^\pi T}_{\nu' n'} | V_{A-2A-1A}(1 - 2P_{A-1A}) | \Phi^{J^\pi T}_{\nu n} \rangle - \frac{(A-1)(A-2)(A-3)}{2} \langle \Phi^{J^\pi T}_{\nu' n'} | P_{A-1A} V_{A-3A-2A-1} | \Phi^{J^\pi T}_{\nu n} \rangle \right] .$$

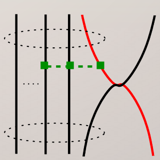
Direct potential: in the model space (interaction is localized!)



(a) (b)

$$\propto {}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \right| a^+_i a^+_j a_l a_k \left| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

Exchange potential: in the model space (interaction is localized!)

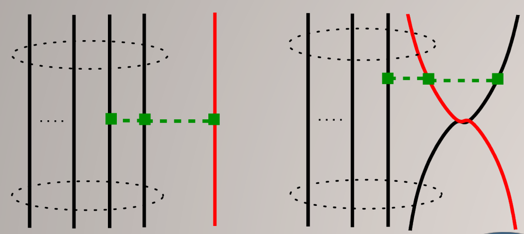


(c)

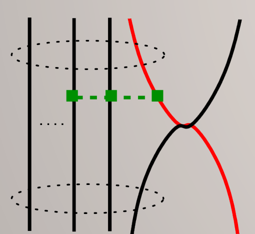
$$\propto {}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \right| a^+_h a^+_i a^+_j a_m a_l a_k \left| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

Including 3N interaction challenging: more than *2 body density required*

Including 3N interaction in the NCSM/RGM: Direct and exchange terms



(a) (b)



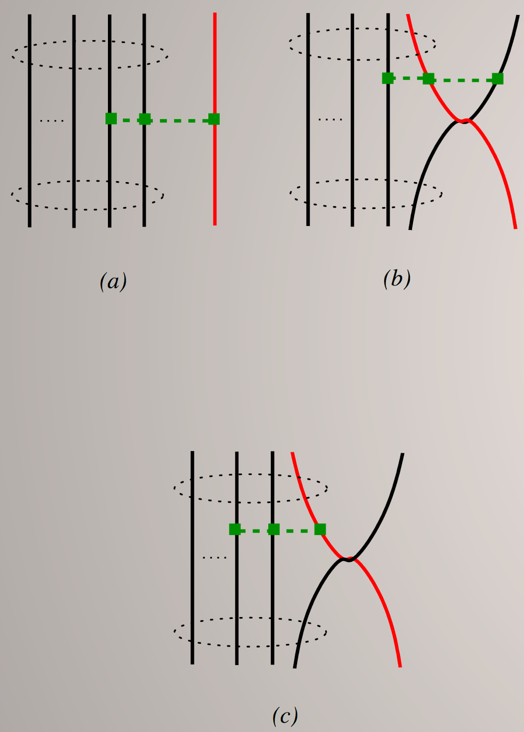
(c)

$$\sum \hat{s}\hat{s}'\hat{j}\hat{j}'\hat{\tau}\hat{K}\,(-1)^{J_1'+j'+J}(-1)^{j_0+J_0-j+2j'}(-1)^{T_1+1/2+T}(-1)^{1/2+T_0+t_0+1}$$
$$\left\{\begin{array}{ccc} J_1 & 1/2 & s \\ l & J & j \end{array}\right\}\left\{\begin{array}{ccc} J_1' & 1/2 & s' \\ l' & J & j' \end{array}\right\}$$
$$\left\{\begin{array}{ccc} J_1 & K & J_1' \\ j' & J & j \end{array}\right\}\left\{\begin{array}{ccc} j_0' & j_0 & K \\ j & j' & J_0 \end{array}\right\}$$
$$\left\{\begin{array}{ccc} T_1 & \tau & T_1' \\ 1/2 & T & 1/2 \end{array}\right\}\left\{\begin{array}{ccc} t_0' & t_0 & \tau \\ 1/2 & 1/2 & T_0 \end{array}\right\}$$
$$\left\langle \left[(n_a'l_a'j_a' : n_b'l_b'j_b')\, j_0't_0' :\; n'l'j'\right] J_0T_0 \right| V_{A-2A-1A}(1-2P_{A-1A}) \left| \left[\left(n_al_aj_a :\; n_bl_bj_b\right) j_0t_0 : nlj\right] J_0T_0 \right\rangle$$
$$\left\langle \alpha_{A-1}'J_1'T_1' \left|\left|\left| \left[\left[a^\dagger_{n_a'l_a'j_a'}a^\dagger_{n_b'l_b'j_b'}\right]^{j_0't_0'}\left[\tilde{a}_{n_al_aj_a}\tilde{a}_{n_bl_bj_b}\right]^{j_0t_0}\right]^{K\tau} \right|\right|\right| \alpha_{A-1}J_1T_1 \right\rangle$$

$$\sum \hat{s}\hat{s}'\hat{j}\hat{j}'\hat{\tau}\hat{K}\hat{J}_0\hat{T}_0\hat{g}'\hat{t}_g'\hat{j}_0'\hat{t}_0'\hat{k}'\hat{t}_k'\,(-1)^{J_1'+j'+J}(-1)^{j+j_a'+j_b'+j_0'+J_0+k'}(-1)^{T_1+1/2+T}(-1)^{1-T_0-\tau+t_0'+t_k'}$$
$$\left\{\begin{array}{ccc} J_1 & 1/2 & s \\ l & J & j \end{array}\right\}\left\{\begin{array}{ccc} J_1' & 1/2 & s' \\ l' & J & j' \end{array}\right\}$$
$$\left\{\begin{array}{ccc} J_1 & K & J_1' \\ j' & J & j \end{array}\right\}\left\{\begin{array}{ccc} g' & J_0 & K \\ j_0' & k' & j_b' \end{array}\right\}\left\{\begin{array}{ccc} k' & j_0' & K \\ j' & j & j_a' \end{array}\right\}$$
$$\left\{\begin{array}{ccc} T_1 & \tau & T_1' \\ 1/2 & T & 1/2 \end{array}\right\}\left\{\begin{array}{ccc} t_g' & T_0 & \tau \\ t_0' & t_k' & 1/2 \end{array}\right\}\left\{\begin{array}{ccc} t_k' & t_0' & \tau \\ 1/2 & 1/2 & 1/2 \end{array}\right\}$$
$$\left\langle \left[\left(n'l'j' :\; n_a'l_a'j_a'\right) j_0't_0' : n_b'l_b'j_b'\right] J_0T_0 \right| V_{A-3\,A-2\,A-1} \left| \left[(n_\alpha l_\alpha j_\alpha : n_al_aj_a)\, j_0t_0 :\; n_bl_bj_b\right] J_0T_0 \right\rangle$$
$$\left\langle \alpha_{A-1}'J_1'T_1' \left|\left|\left| \left[\left\{\left[a^\dagger_{nlj}a^\dagger_{n_a'l_a'j_a'}\right]^{k't_k'} a^\dagger_{n_b'l_b'j_b'}\right\}^{g't_g'}\left\{\left[\tilde{a}_{n_\alpha l_\alpha j_\alpha}\tilde{a}_{n_al_aj_a}\right]^{j_0t_0}\tilde{a}_{n_bl_bj_b}\right\}^{J_0T_0}\right]^{K\tau} \right|\right|\right| \alpha_{A-1}J_1T_1 \right\rangle$$

G. Hupin: Kernel derivations with many-body densities.
Use of existing codes:
Applicable to A=3,4 targets

Including 3N interaction in the NCSM/RGM: Direct and exchange terms

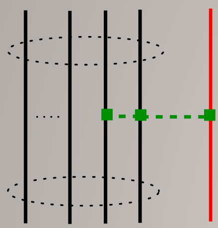


J. Langhammer:

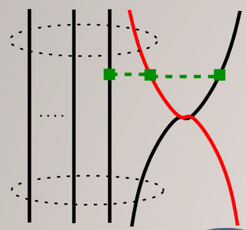
Kernel derivations without the angular momentum re-coupling and the many-body density factorization.

Kernel calculations directly from the target eigenvectors:
Applicable to *p*-shell nuclei targets
The same strategy possible for multi-nucleon projectiles and *A*>4 targets

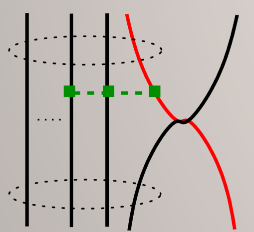
Including 3N interaction in the NCSM/RGM: Direct and exchange terms



(a)



(b)



(c)

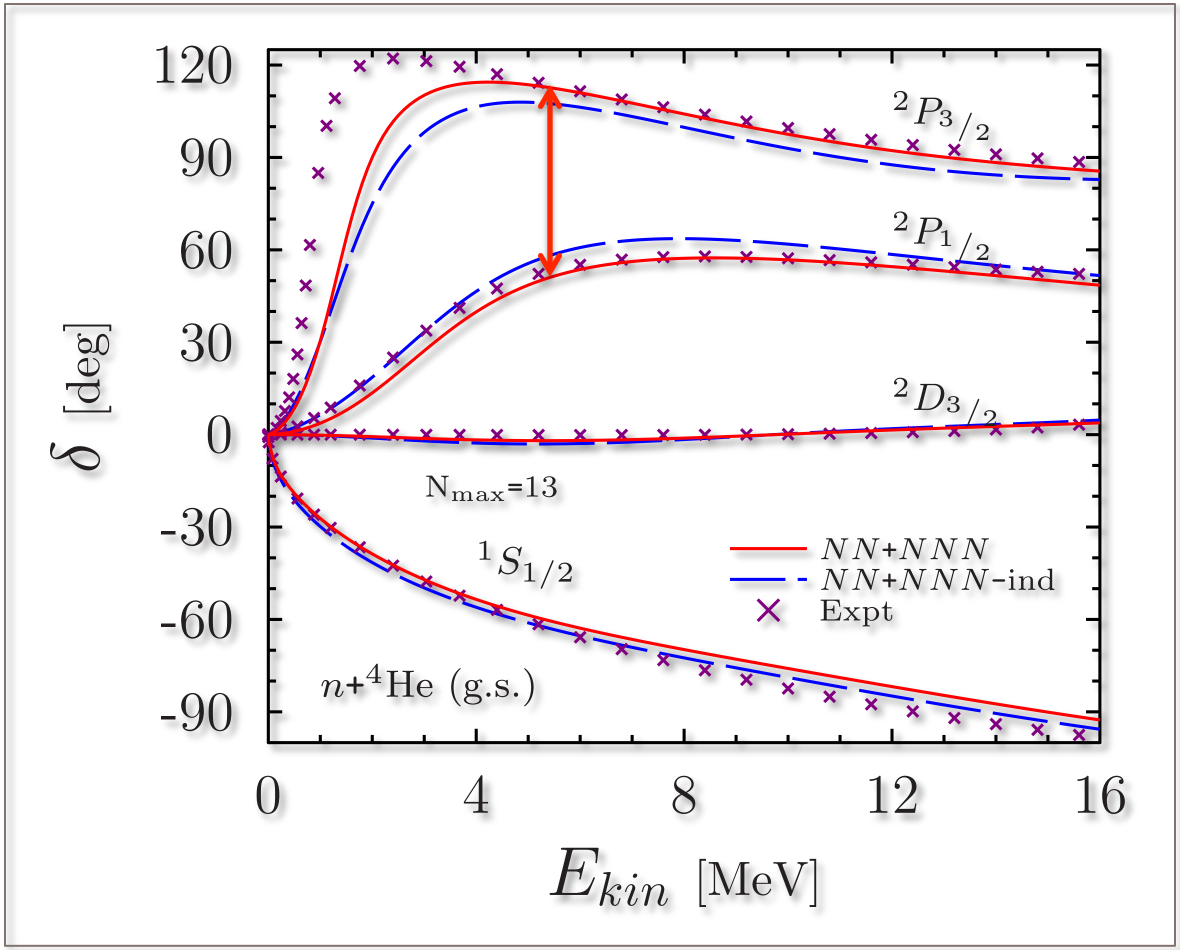
$$
\begin{aligned}
&\langle \epsilon^{J\pi T}_{\nu' n'} | \hat{V}_{A-2\,A-1\,A}(1-\hat{T}_{A-1,A}-\hat{T}_{A-2,A}) | \epsilon^{J\pi T}_{\nu n} \rangle \\
&= \sum_{M_1 m_j} \sum_{M_{T_1} m_t} \left(\begin{array}{cc|c} I_1 & j & J \\ M_1 & m_j & M_J \end{array} \right) \left(\begin{array}{cc|c} T_1 & \frac{1}{2} & T \\ M_{T_1} & m_t & M_T \end{array} \right) \\
&\sum_{M'_1 m'_j} \sum_{M'_{T_1} m'_t} \left(\begin{array}{cc|c} I'_1 & j' & J \\ M'_1 & m'_j & M'_J \end{array} \right) \left(\begin{array}{cc|c} T'_1 & \frac{1}{2} & T \\ M'_{T_1} & m'_t & M'_T \end{array} \right) \\
&\frac{1}{2(A-1)(A-2)} \sum_{\beta_{A-2}} \sum_{\beta_{A-1}} \sum_{\beta'_{A-2}} \sum_{\beta'_{A-1}} \\
&\langle \Psi' I'_1 M'_1 T'_1 M'_{T_1} | \hat{a}^\dagger_{\beta_{A-1}} \hat{a}^\dagger_{\beta_{A-2}} \hat{a}_{\beta'_{A-2}} \hat{a}_{\beta'_{A-1}} | \Psi I_1 M_1 T_1 M_{T_1} \rangle \\
&{}_a\langle \beta_{A-2} \beta_{A-1} n' l' j' m'_j m'_t | \hat{V} | \beta'_{A-2} \beta'_{A-1} n l j m_j m_t \rangle_a
\end{aligned}
$$

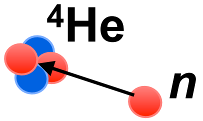
$$
\begin{aligned}
&\langle \epsilon^{J\pi T}_{\nu' n'} | \hat{V}_{A-3\,A-2\,A} \hat{T}_{A-1,A} | \epsilon^{J\pi T}_{\nu n} \rangle \\
&= \sum_{M_1 m_j} \sum_{M_{T_1} m_t} \left(\begin{array}{cc|c} I_1 & j & J \\ M_1 & m_j & M_J \end{array} \right) \left(\begin{array}{cc|c} T_1 & \frac{1}{2} & T \\ M_{T_1} & m_t & M_T \end{array} \right) \\
&\sum_{M'_1 m'_j} \sum_{M'_{T_1} m'_t} \left(\begin{array}{cc|c} I'_1 & j' & J \\ M'_1 & m'_j & M'_J \end{array} \right) \left(\begin{array}{cc|c} T'_1 & \frac{1}{2} & T \\ M'_{T_1} & m'_t & M'_T \end{array} \right) \\
&\frac{1}{6} \frac{1}{(A-1)(A-2)(A-3)} \sum_{\beta_{A-3}} \sum_{\beta_{A-2}} \sum_{\beta'_{A-3}} \sum_{\beta'_{A-2}} \sum_{\beta'_{A-1}} \\
&\langle \Psi' I'_1 M'_1 T'_1 M'_{T_1} | \hat{a}^\dagger_{nljm_j\frac{1}{2}m_t} \hat{a}^\dagger_{\beta_{A-2}} \hat{a}^\dagger_{\beta_{A-3}} \hat{a}_{\beta'_{A-3}} \hat{a}_{\beta'_{A-2}} \hat{a}_{\beta'_{A-1}} | \Psi I_1 M_1 T_1 M_{T_1} \rangle \\
&{}_a\langle \beta_{A-3} \beta_{A-2} n' l' j' m'_j \tfrac{1}{2} m'_t | \hat{V}_{A-3\,A-2\,A} | \beta'_{A-3} \beta'_{A-2} \beta'_{A-1} \rangle_a
\end{aligned}
$$

Computational challenge: Large scale parallelization, target eigenvectors for multiple M values

n-^{4}He scattering: NN vs. NN+NNN interactions, first results

G. Hupin, J. Langhammer, S. Quaglioni, P. Navrátil, R. Roth, work in progress





chiral NN+NNN(500)
chiral NN+NNN-induced
SRG λ=2 fm^{-1}
HO N_{max}=13, ħΩ=20 MeV

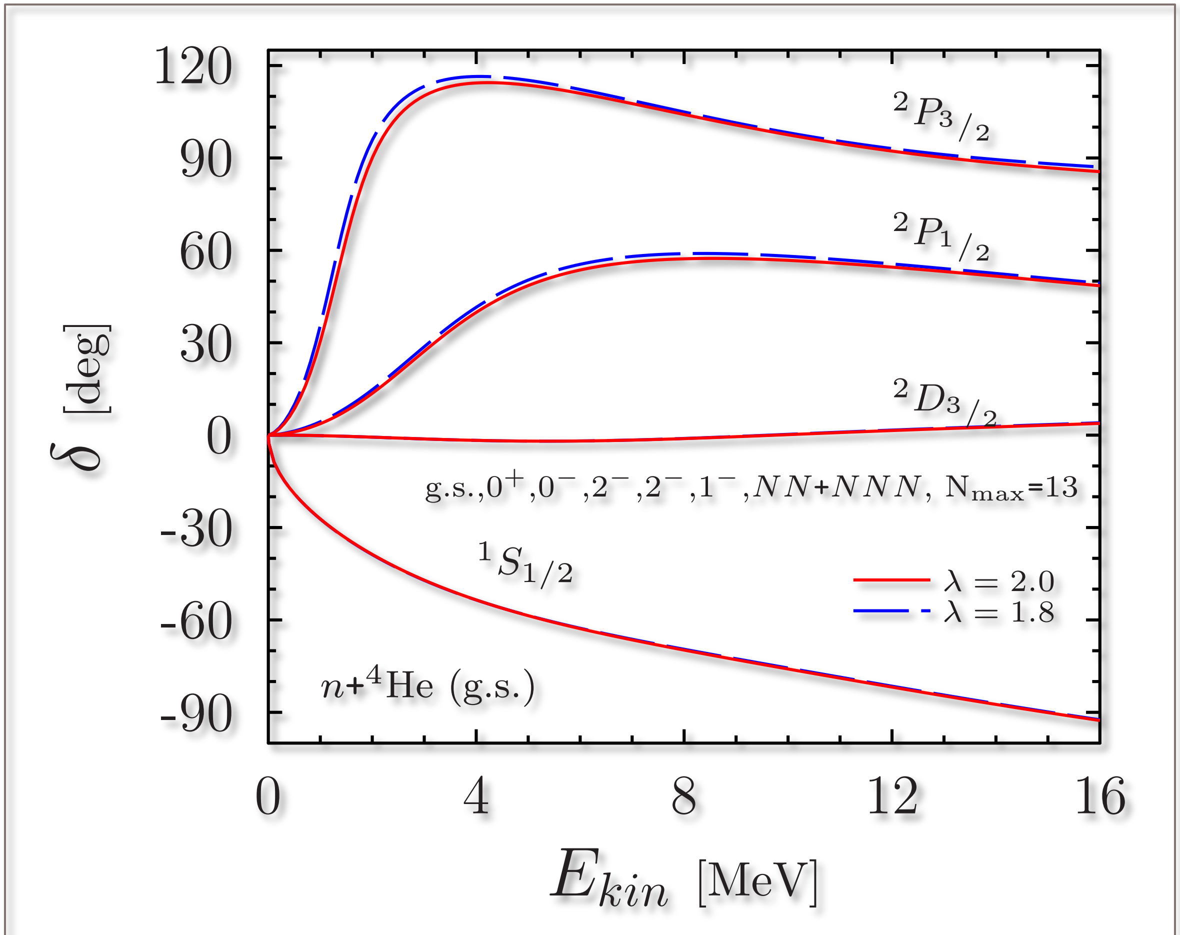
^{4}He g.s. and 5 excited states

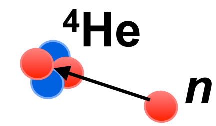
The largest splitting between the P-waves obtained with the chiral NN+NNN interaction

TRIUMF

n-^{4}He scattering: NN vs. NN+NNN interactions, first results

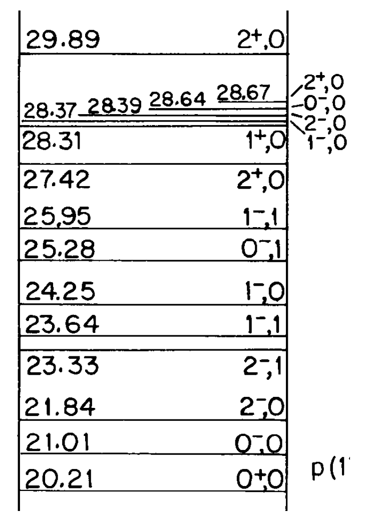
G. Hupin, J. Langhammer, S. Quaglioni, P. Navrátil, R. Roth, work in progress





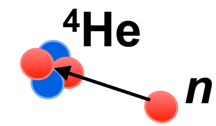
chiral NN+NNN(500)
SRG λ=2 fm^{-1} & 1.88 fm^{-1}
HO N_{max}=13, hΩ=20 MeV

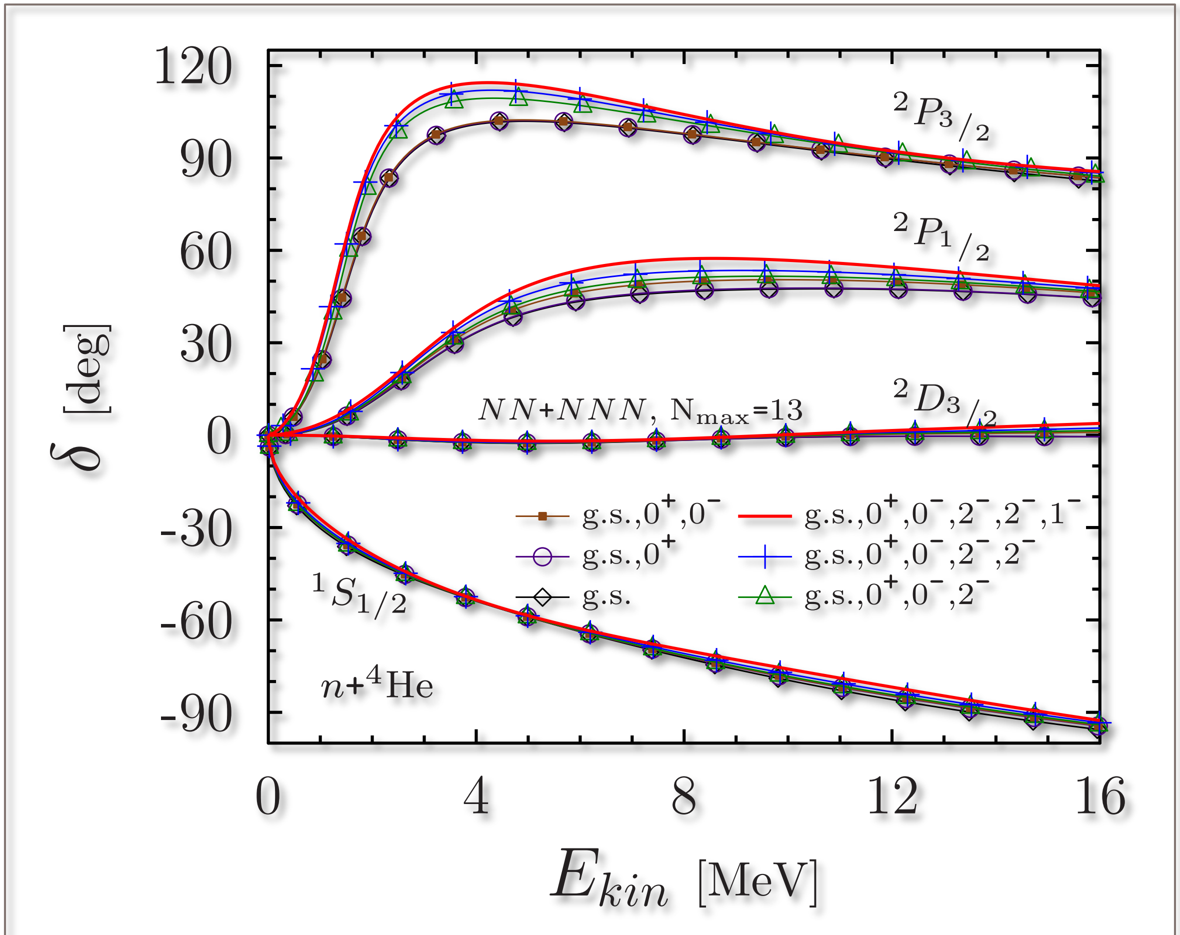
^{4}He g.s. and 5 excited states



n-^{4}He scattering: NN vs. NN+NNN interactions, first results

G. Hupin, J. Langhammer, S. Quaglioni, P. Navrátil, R. Roth, work in progress



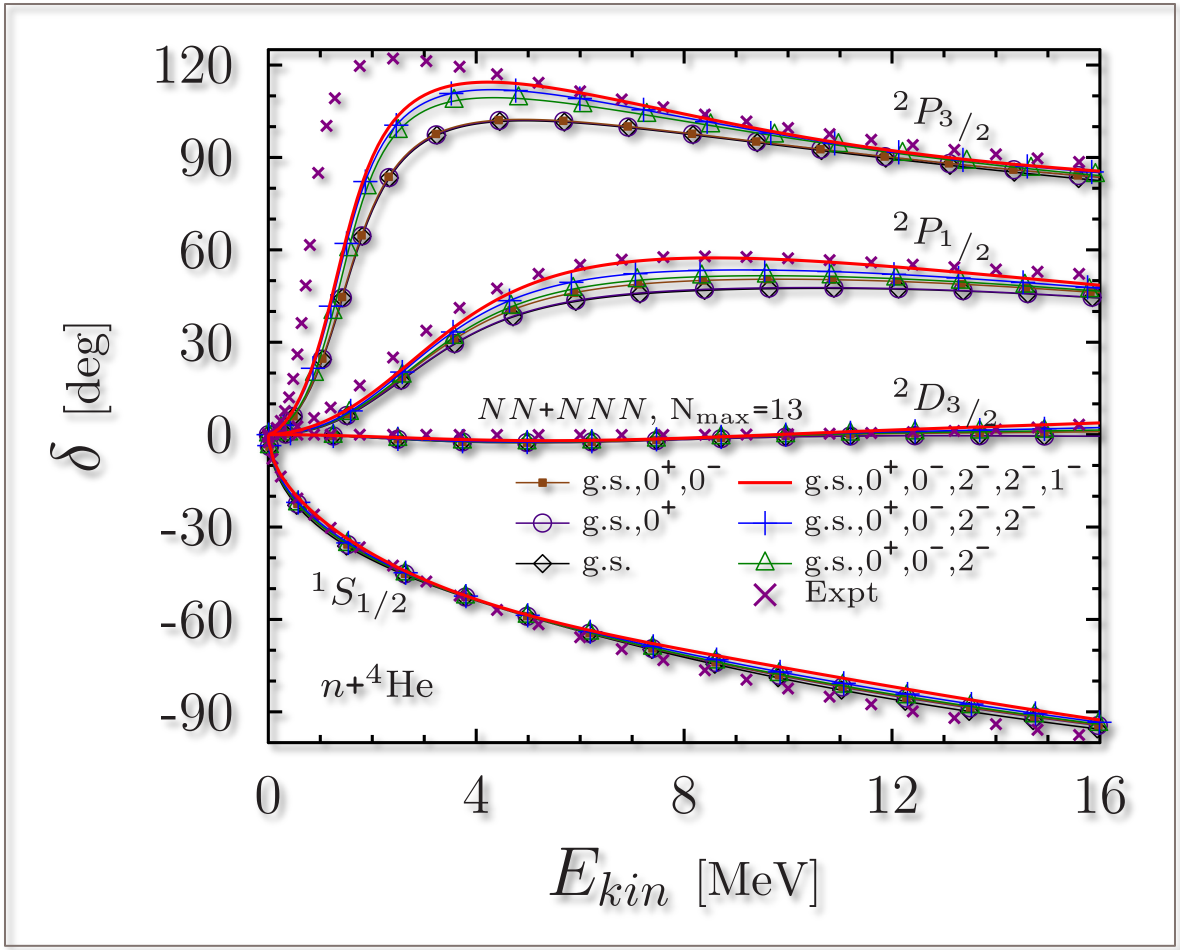


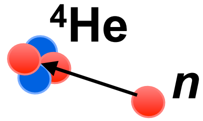
chiral NN+NNN(500)
SRG λ=2 fm^{-1}
HO N_{max}=13, hΩ=20 MeV

Different ^{4}He excited states impact different partial waves

n-^{4}He scattering: NN vs. NN+NNN interactions, first results

G. Hupin, J. Langhammer, S. Quaglioni, P. Navrátil, R. Roth, work in progress





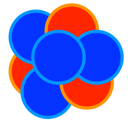
chiral NN+NNN(500)
SRG λ=2 fm^{-1}
HO N_{max}=13, hΩ=20 MeV

Different ^{4}He excited states impact different partial waves

Better reproduction of data with the increase of number of ^{4}He excited states
… still **not enough**

New developments: NCSM with continuum

NCSM

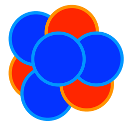


$$\left|\Psi_A^{J^\pi T}\right\rangle = \sum_{Ni} c_{Ni} \left|ANiJ^\pi T\right\rangle$$

TRIUMF

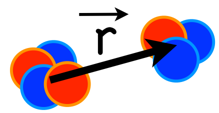
New developments: NCSM with continuum

NCSM



$$\left|\Psi_A^{J^\pi T}\right\rangle = \sum_{Ni} c_{Ni} \left|ANiJ^\pi T\right\rangle$$

NCSM/RGM



$$|\Psi_A^{J^\pi T}\rangle = \sum_\nu \int d\vec{r} \chi_\nu(\vec{r}) \hat{A} \Phi_{\nu\vec{r}}^{J^\pi T(A-a,a)}$$

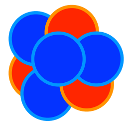
$$\mathcal{H}\chi = E\mathcal{N}\chi$$

$$\bar{\chi} = \mathcal{N}^{+\frac{1}{2}}\chi$$

$$\boxed{(\mathcal{N}^{-\frac{1}{2}}\mathcal{H}\mathcal{N}^{-\frac{1}{2}})\bar{\chi} = E\bar{\chi}}$$

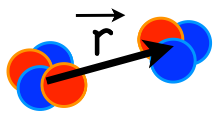
New developments: NCSM with continuum

NCSM



$$\left|\Psi_A^{J^\pi T}\right\rangle = \sum_{Ni} c_{Ni} \left|ANiJ^\pi T\right\rangle$$

NCSM/RGM



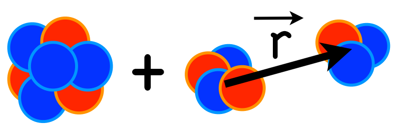
$$|\Psi_A^{J^\pi T}\rangle = \sum_{\nu} \int d\vec{r} \chi_\nu(\vec{r}) \hat{A} \Phi_{\nu \vec{r}}^{J^\pi T (A-a,a)}$$

$$\mathcal{H}\chi = E\mathcal{N}\chi$$

$$\bar{\chi} = \mathcal{N}^{+\frac{1}{2}}\chi$$

$$(\mathcal{N}^{-\frac{1}{2}}\mathcal{H}\mathcal{N}^{-\frac{1}{2}})\bar{\chi} = E\bar{\chi}$$

NCSMC



S. Baroni, P. N., and S. Quaglioni,
PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

$$|\Psi_A^{J^\pi T}\rangle = \sum_{\lambda} c_\lambda |A\lambda J^\pi T\rangle + \sum_{\nu} \int d\vec{r} \left(\sum_{\nu'} \int d\vec{r}\,' \mathcal{N}_{\nu\nu'}^{-\frac{1}{2}}(\vec{r}, \vec{r}\,') \bar{\chi}_{\nu'}(\vec{r}\,') \right) \hat{A} \Phi_{\nu \vec{r}}^{J^\pi T (A-a,a)}$$

$$\begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \mathcal{N}^{-\frac{1}{2}}\mathcal{H}\mathcal{N}^{-\frac{1}{2}} \end{pmatrix} \begin{pmatrix} c \\ \bar{\chi} \end{pmatrix} = E \begin{pmatrix} 1 & \bar{g} \\ \bar{g} & 1 \end{pmatrix} \begin{pmatrix} c \\ \bar{\chi} \end{pmatrix}$$

NCSMC formalism

Start from

$$\begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \overline{\mathcal{H}} \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix} = E \begin{pmatrix} 1 & \bar{g} \\ \bar{g} & 1 \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix}$$

NCSM sector:

$$(H_{NCSM})_{\lambda\lambda'} = \langle A\lambda J^\pi T|\hat{H}|A\lambda' J^\pi T\rangle = \varepsilon_\lambda^{J^\pi T}\delta_{\lambda\lambda'}$$

NCSM/RGM sector:

$$\overline{\mathcal{H}}_{\nu\nu'}(r,r') = \sum_{\mu\mu'} \int\int dy dy' y^2 y'^2 \mathcal{N}_{\nu\mu}^{-\frac{1}{2}}(r,y)\mathcal{H}_{\mu\mu'}(y,y')\mathcal{N}_{\mu'\nu'}^{-\frac{1}{2}}(y',r')$$

NCSMC formalism

Start from

$$\begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \overline{\mathcal{H}} \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix} = E \begin{pmatrix} 1 & \bar{g} \\ \bar{g} & 1 \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix}$$

Coupling:

$$\bar{g}_{\lambda\nu}(r) = \sum_{\nu'} \int dr' r'^2 \langle A\lambda J^\pi T | \hat{\mathcal{A}}_{\nu'} \Phi^{J^\pi T}_{\nu' r'} \rangle \, \mathcal{N}^{-\frac{1}{2}}_{\nu'\nu}(r', r)$$

$$\bar{h}_{\lambda\nu}(r) = \sum_{\nu'} \int dr' r'^2 \langle A\lambda J^\pi T | \hat{H} \hat{\mathcal{A}}_{\nu'} | \Phi^{J^\pi T}_{\nu' r'} \rangle \, \mathcal{N}^{-\frac{1}{2}}_{\nu'\nu}(r', r)$$

Calculation of *g* from SD wave functions:

$$\begin{aligned} g_{\lambda\nu n} &= \langle A\lambda J^\pi T | \hat{\mathcal{A}}_\nu \Phi^{J^\pi T}_{\nu n} \rangle \\ &= \frac{1}{\langle n\ell 00, \ell | 00 n\ell, \ell \rangle_{\frac{1}{(A-1)}}} \, {}_{SD}\langle A\lambda J^\pi T | \hat{\mathcal{A}}_\nu \Phi^{J^\pi T}_{\nu n} \rangle_{SD} \\ &= \frac{1}{\langle n\ell 00, \ell | 00 n\ell, \ell \rangle_{\frac{1}{(A-1)}}} \frac{1}{\hat{J}\hat{T}} \sum_j (-1)^{I_1+J+j} \hat{s}\hat{j} \begin{Bmatrix} I_1 & \frac{1}{2} & s \\ \ell & J & j \end{Bmatrix} {}_{SD}\langle A\lambda J^\pi T ||| a^\dagger_{n\ell j\frac{1}{2}} ||| A-1 \alpha_1 I_1^{\pi_1} T_1 \rangle_{SD} \end{aligned}$$

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NCSMC coupling due to the 3N interaction

$$\langle A\lambda J^\pi T|V_{3N}\mathcal{A}\left[|A-1\alpha_1 I_1 T_1\rangle\varphi_{nlj}(A)\right]^{(J^\pi T)} =$$

$$\frac{1}{12}\sum(I_1 M_1 jm|JM)(T_1 M_{T_1}\tfrac{1}{2}m_t|TM_T)$$

$$\langle\beta_1\beta_2\beta_3|V_{3N}|\beta_{1'}\beta_{2'}(nljmm_t)\rangle$$

$$\langle A\lambda JMTM_T|a^\dagger_{\beta_3}a^\dagger_{\beta_2}a^\dagger_{\beta_1}a_{\beta_{1'}}a_{\beta_{2'}}|A-1\alpha_1 I_1 M_1 T_1 M_{T_1}\rangle$$

Straightforward to calculate

NCSMC formalism

Start from

$$\begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \overline{\mathcal{H}} \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix} = E \begin{pmatrix} 1 & \bar{g} \\ \bar{g} & 1 \end{pmatrix} \begin{pmatrix} c \\ \chi \end{pmatrix}$$

$$N^{\lambda\lambda'}_{\nu r \nu' r'} = \begin{pmatrix} \delta_{\lambda\lambda'} & \bar{g}_{\lambda\nu'}(r') \\ \bar{g}_{\lambda'\nu}(r) & \delta_{\nu\nu'} \frac{\delta(r-r')}{rr'} \end{pmatrix}$$

Orthogonalization:

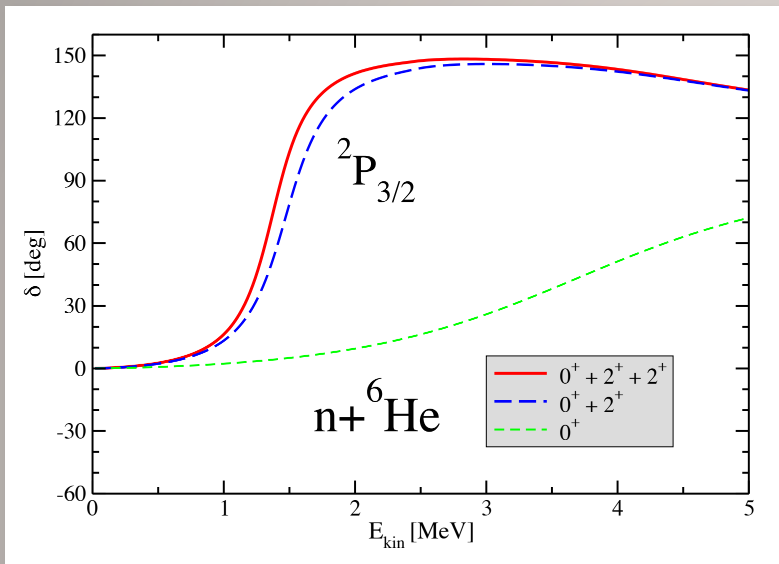
$$\overline{H} = N^{-\frac{1}{2}} \begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \overline{\mathcal{H}} \end{pmatrix} N^{-\frac{1}{2}} \qquad \begin{pmatrix} \bar{c} \\ \bar{\chi} \end{pmatrix} = N^{+\frac{1}{2}} \begin{pmatrix} c \\ \chi \end{pmatrix}$$

Solve with generalized microscopic R-matrix

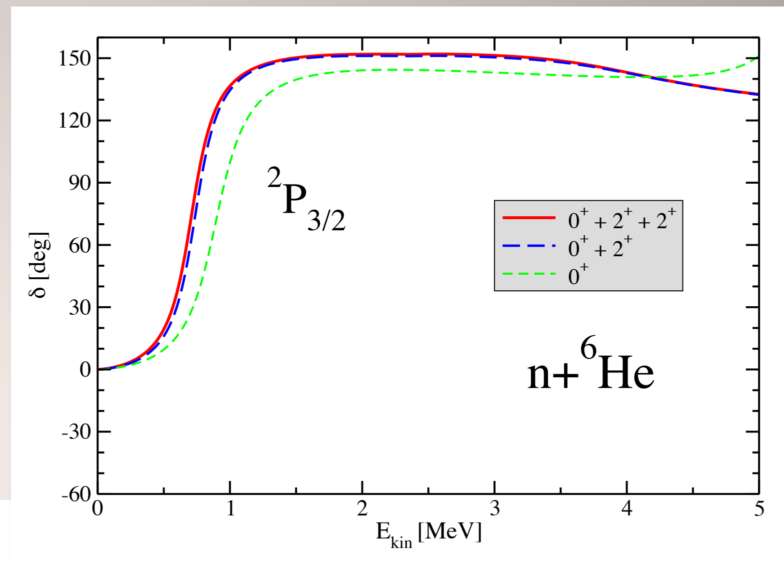
$$(\hat{\overline{H}} + \hat{L} - E) \begin{pmatrix} \bar{c} \\ \bar{\chi} \end{pmatrix} = \hat{L} \begin{pmatrix} \bar{c} \\ \bar{\chi} \end{pmatrix}$$

Bloch operator → $\hat{L}_\nu = \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{2}\delta(r-a)(\frac{d}{dr} - \frac{B_\nu}{r}) \end{pmatrix}$

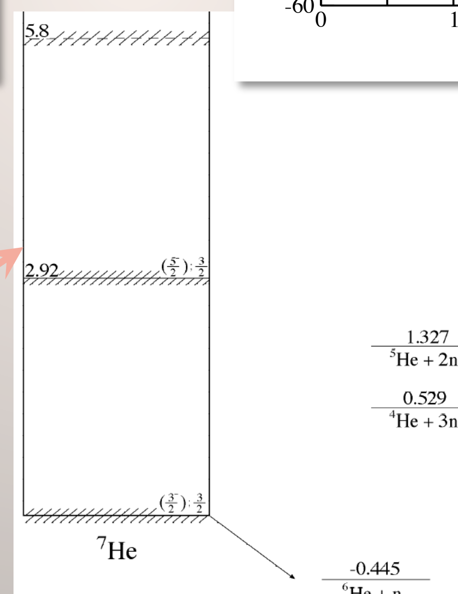
NCSM with continuum: ^{7}He ↔ ^{6}He+n

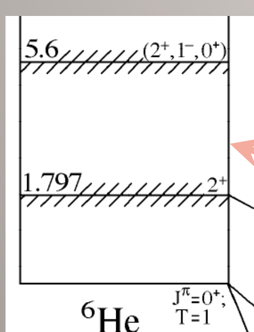


NCSM/RGM
with up to three ^{6}He states



NCSMC
with up to three ^{6}He states
and four ^{7}He eigenstates
More **7-nucleon correlations**
Fewer target states needed





Expt.

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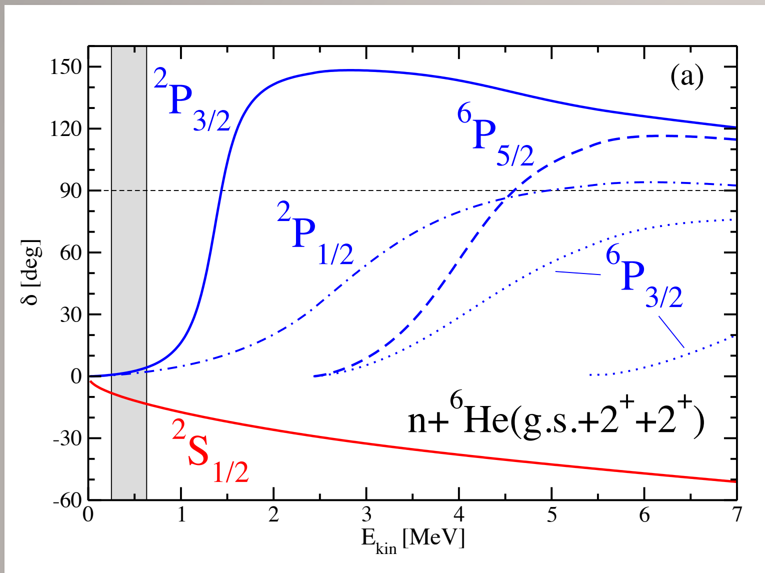
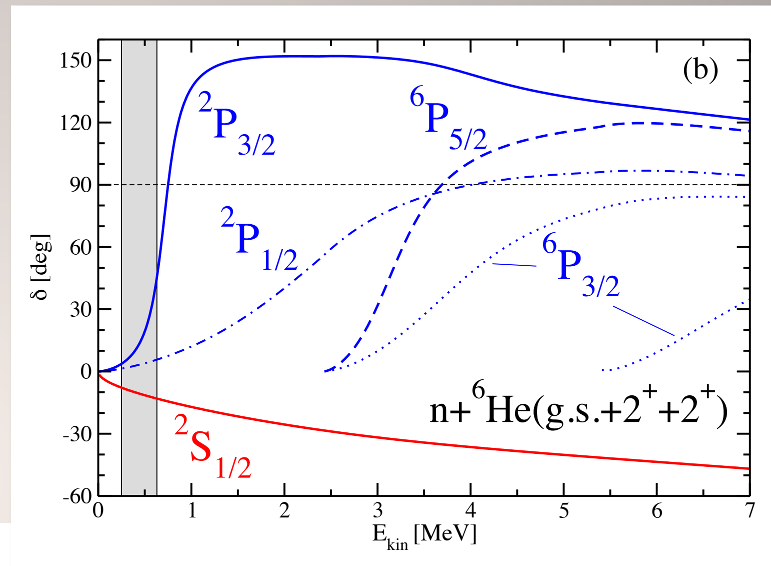
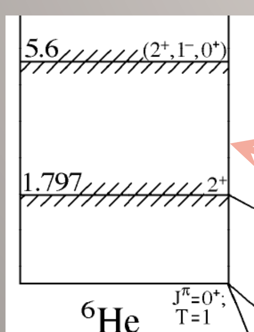
NCSM with continuum: ^{7}He ↔ ^{6}He+*n*



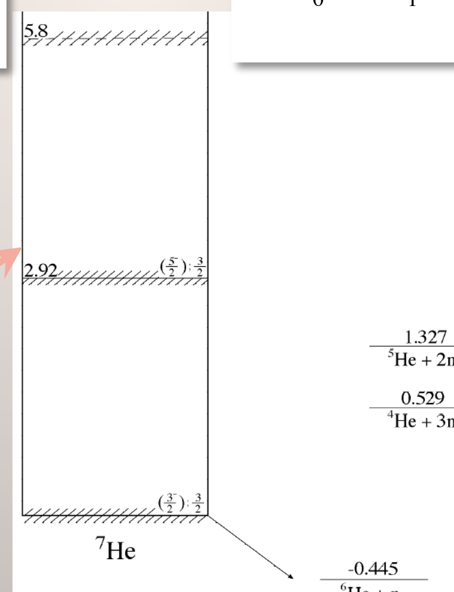
NCSM/RGM
with three ^{6}He states



NCSMC
with three ^{6}He states
and ten ^{7}He eigenstates
More **7-nucleon correlations**
Fewer target states needed



Expt.



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^{7}He: NCSMC vs. NCSM/RGM vs. NCSM

J^π	experiment			NCSMC		NCSM/RGM		NCSM
	E_R	Γ	Ref.	E_R	Γ	E_R	Γ	E_R
$3/2^-$	0.430(3)	0.182(5)	[2]	0.71	0.30	1.39	0.46	1.30
$5/2^-$	3.35(10)	1.99(17)	[40]	3.13	1.07	4.00	1.75	4.56
$1/2^-$	3.03(10)	2	[11]	2.39	2.89	2.66	3.02	3.26
	3.53	10	[15]					
	1.0(1)	0.75(8)	[5]					

[11] A. H. Wuosmaa *et al.*, Phys. Rev. C **72**, 061301 (2005).

- NCSMC and NSCM/RGM energies where phase shift derivative maximal
- NCSMC and NSCM/RGM widths from the derivatives of phase shifts

$$\Gamma = \left.\frac{2}{\partial\delta(E_{kin})/\partial E_{kin}}\right|_{E_{kin}=E_R}$$

Experimental controversy: Existence of low-lying 1/2$^-$ state … not seen in these calculations

Best agreement with the neutron pick-up and proton-removal reactions experiments [11]

TRIUMF

Conclusions and Outlook

- 3N interaction applications in many-body calculations
  - Technically solved for NCSM
  - Medium mass nuclei: The HO cut for 3N matrix elements needs to be increased beyond E3max=16 – further algorithmic development required
  - Promising results for scattering within the NCSM/RGM

- We developed a new unified approach to nuclear bound and unbound states
  - Merging of the NCSM and the NCSM/RGM

PRL **110**, 022505 (2013)

- We demonstrated its capabilities in calculations of ^{7}He resonances
- 3N interaction inclusion straightforward - under way

- Outlook:
  - Problems with the 3N interaction input for medium mass nuclei solvable
  - Extension of the NCSMC formalism to composite projectiles (deuteron, ^{3}H, ^{3}He, ^{4}He)
  - Extension of the formalism to coupling of three-body clusters (^{6}He ~ ^{4}He+n+n)

Collaborators

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