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

Ab Initio Nuclear Structure & Reaction Theory: No-Core Shell Model with Continuum Approach

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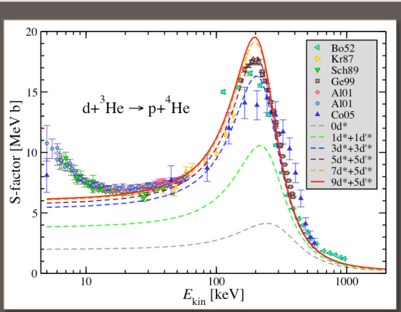
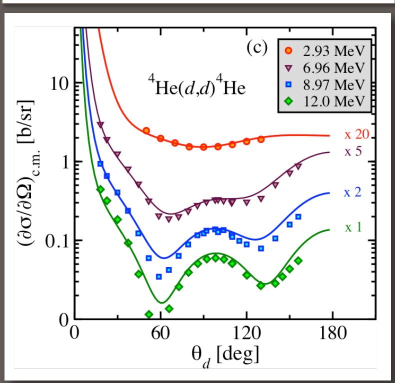
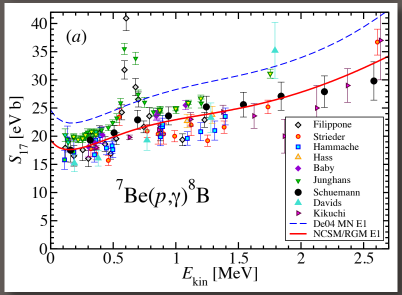
Petr Navratil | TRIUMF







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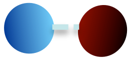
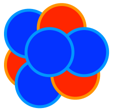
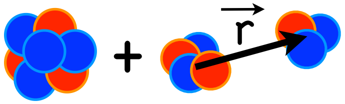
Un accélérateur de la démarche scientifique canadienne

Outline

- Lecture 1
  - Introduction to nuclear reaction theory
- Lecture 2
  - Nuclear forces
    - chiral EFT, two-nucleon, three-nucleon
  - Nuclear many-body calculations for bound states
    - No-core shell model (NCSM)
  - Similarity Renormalization Group
- Lecture 3
  - Nuclear many-body calculations including continuum
    - NCSM with the Resonating Group Method (NCSM/RGM)
    - NCSM with continuum (NCSMC)
- Lecture 4
  - Applications to exotic nuclei and astrophysics
    - ^{7}He, ^{11}Be, ^{10}C(p,p), ^{11}C(p,γ)^{12}N
    - ^{7}Be(p,γ)^{8}B, ^{3}He(α,γ)^{7}Be, ^{3}H(α,γ)^{7}Li, ^{3}He(d,p)^{4}He, ^{3}H(d,n)^{4}He
    - Progress towards ^{2}H(α,γ)^{6}Li, ^{4}He(nn,γ)^{6}He,

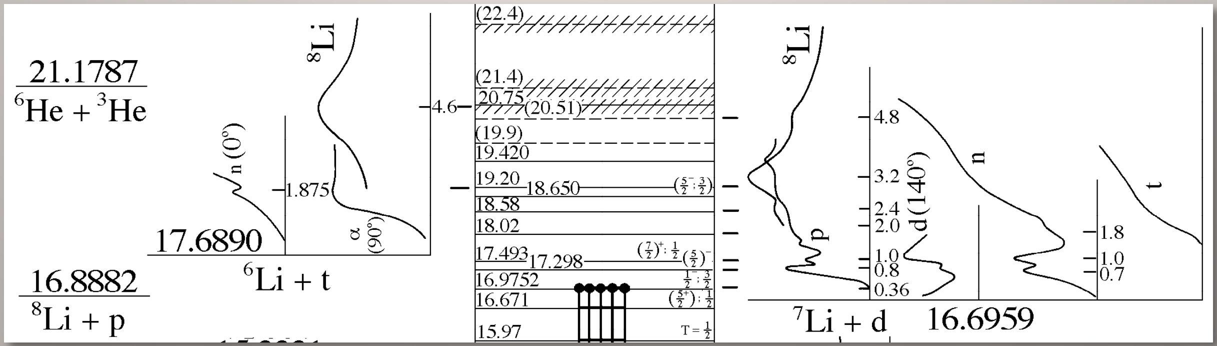






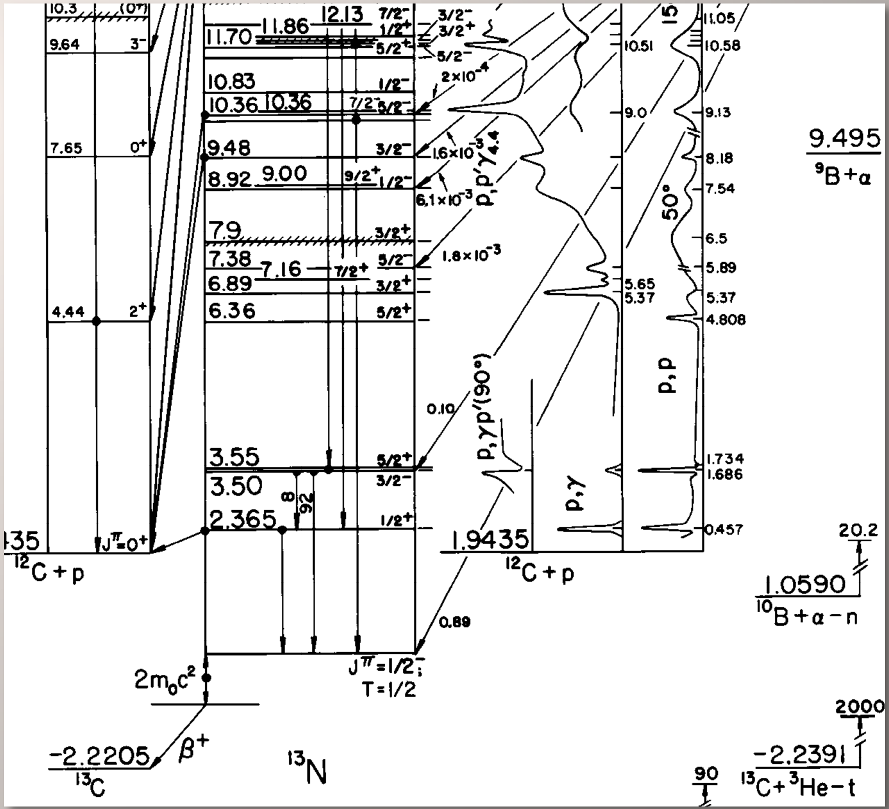
Nuclear reactions

- A+B➔C+D ; A(B,C)D
  - conserve
    - number of nucleons
    - charge
    - energy
    - momentum
    - angular momentum
    - parity (strong, electromagnetic)
  - Q-value: $Q = M_A c^2 + M_B c^2 – M_C c^2 – M_D c^2$
    - Exothermic: Q>0 – increase of kinetic energy in the final state
    - Endothermic: Q<0 – decrease of kinetic energy in the final state



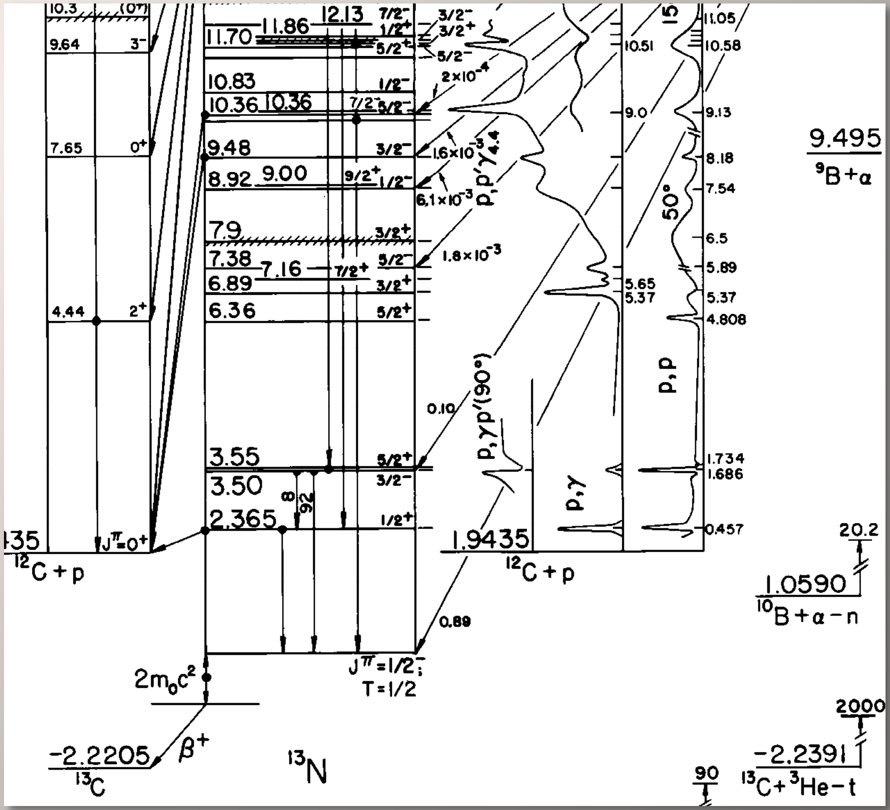
Nuclear reactions - kinds

- Elastic scattering
  - $p+{}^4He \rightarrow p+{}^4He$; ${}^4He(p,p){}^4He$; ${}^1H(\alpha,p){}^4He$
  - $n+{}^4He \rightarrow n+{}^4He$; ${}^4He(n,n){}^4He$
  - $\boxed{{}^{12}C(p,p){}^{12}C}$
  - ${}^3He(\alpha,\alpha){}^3He$
- Inelastic scattering
  - $\boxed{{}^{12}C(p,p'){}^{12}C^*(2^+)}$
  - ${}^{196}Pt({}^{11}Be,{}^{11}Be^*){}^{196}Pt$
    - inverse kinematics, Coulomb excitation
- Transfer reactions
  - ${}^7Li(d,p){}^8Li$
  - ${}^3H(d,n){}^4He$ (fusion)
  - ${}^{11}B(p,\alpha){}^8Be^*$
  - $\boxed{{}^{12}C(p,\alpha){}^9B}$
- Charge exchange reactions
  - ${}^7Li(p,n){}^7Be$
- Breakup reactions
  - $d+{}^{10}B \rightarrow p+n+{}^{10}B$
- Capture reactions (electromagnetic)
  - ${}^7Be(p,\gamma){}^8B$
  - ${}^3He(\alpha,\gamma){}^7Be$
  - $\boxed{{}^{12}C(p,\gamma){}^{13}N}$
- Photo-disintegration (electromagnetic)
  - $\gamma+{}^{11}Be \rightarrow {}^{10}Be+n$
- Fission
  - $n+{}^{235}U \rightarrow C^*+D^*$



Nuclear reactions – times and energy scales

- Direct reactions
  - fast
  - **involve few nucleons**
  - high incident energies
  - typical examples: transfer and breakup
  - DWBA theory
    - neglects antisymmetrization
- Resonance reactions
  - peaks in the cross sections
  - resonances: long-lived configurations of nucleons
  - various lifetimes
  - typically at low energies
    - elastic, inelastic scattering
    - capture
  - at high energies collective giant resonances
  - nuclear many-body theory
- Compound nucleus reactions
  - low energy reactions
  - slow
  - compound nucleus formation, equilibrium
  - **decay independent on the details of the initial channel**
  - typical examples
    - neutron-induced reactions on heavy nuclei
  - Hauser-Feshbach theory



Kinematics of binary reactions

- Center of mass

$$\vec{R}_{cm} = \left(M_A \vec{r}_A + M_B \vec{r}_B\right) / \left(M_A + M_B\right)$$

$$\vec{P}_{cm} = \vec{p}_A + \vec{p}_B$$

- Relative motion

$$\vec{r}_{AB} = \vec{r}_A - \vec{r}_B$$

$$\vec{p}_{AB} = \left(M_B \vec{p}_A - M_A \vec{p}_B\right) / \left(M_A + M_B\right)$$

- Total kinetic energy

$$E_{totkin} = \frac{\vec{p}_A^{\,2}}{2M_A} + \frac{\vec{p}_B^{\,2}}{2M_B} = \frac{\vec{P}_{cm}^{\,2}}{2(M_A + M_B)} + \frac{\vec{p}_{AB}^{\,2}}{2\mu_{AB}} \quad ; \quad \mu_{AB} = \frac{M_A M_B}{M_A + M_B} \quad ; \quad E_{kin} = \frac{\vec{p}_{AB}^{\,2}}{2\mu_{AB}}$$

  - center of mass energy and momentum conserved in reaction

Laboratory and CM scattering angles

- Laboratory – target (B) at rest: $v_B=0$
  - Relative kinetic energy

$$E_{kin} = \frac{M_B}{M_A + M_B} E_A = \tfrac{1}{2}\mu_{AB} v_A^2$$

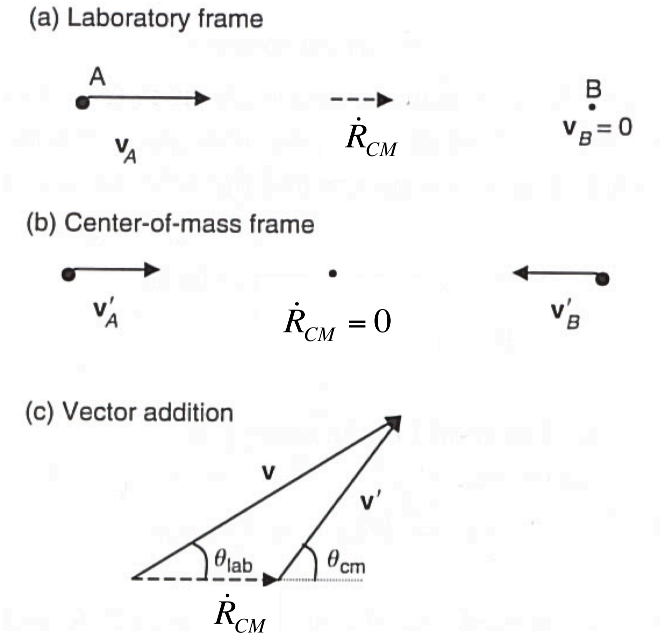
  - velocity relations

$$\vec{v} = \vec{v}' + \dot{\vec{R}}_{CM}$$

  - measured angle of nucleus C

$$v_C \sin\theta_{lab} = v_C' \sin\theta_{CM}$$

$$v_C \cos\theta_{lab} = v_C' \cos\theta_{CM} + \dot{R}_{CM}$$



$$\tan\theta_{lab} = \frac{v_C' \sin\theta_{CM}}{v_C' \cos\theta_{CM} + \dot{R}_{CM}} = \frac{\sin\theta_{CM}}{\cos\theta_{CM} + \rho} \quad ; \quad \rho = \sqrt{\frac{M_A M_C}{M_B M_D} \frac{E_{kin}}{Q + E_{kin}}}$$

Using the energy conservation: $\frac{\vec{p}_{AB}^{\,2}}{2\mu_{AB}} + Q = \frac{\vec{p}_{CD}^{\,2}}{2\mu_{CD}}$

Cross section

- Asymptotic wave function for a short range potential

$$H_{tot} = \frac{\vec{P}_{CM}^2}{2M} + H \quad ; \quad H = \frac{\vec{p}^2}{2\mu} + V(r)$$

$$\Psi(\vec{r}_1, \vec{r}_2) = e^{i\vec{K}_{CM}\cdot\vec{R}_{CM}}\psi(\vec{r}) \quad ; \quad \vec{P}_{CM} = \hbar\vec{K}_{CM}$$

$$H\psi(\vec{r}) = E\psi(\vec{r})$$

  - if $\quad rV(r) \to 0 \quad \text{for } r \to \infty$
  - then $\boxed{\psi(\vec{r}) \to e^{i\vec{k}\cdot\vec{r}} + f(\theta,\varphi)\frac{e^{ikr}}{r}}$; $\vec{p} = \hbar\vec{k}$

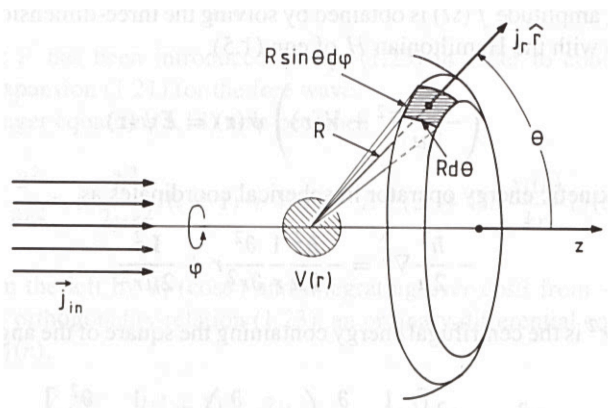
- Differential cross section

$$d\sigma(\Omega) = \frac{\text{probability current into } d\Omega \text{ in the direction } \Omega}{\text{probability current density of the incident wave}}$$

$$\vec{j} = \frac{\hbar}{2\mu i}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)$$

$$\vec{j}_{in} = \frac{\hbar\vec{k}_i}{\mu_i} = \vec{v}_i$$

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{j_r R^2}{|\,\vec{j}_{in}\,|} = |f(\theta,\varphi)|^2}$$



$$\frac{d\sigma}{d\Omega_{CM}}d\Omega_{CM} = \frac{d\sigma}{d\Omega_{lab}}d\Omega_{lab} \Rightarrow \boxed{\frac{d\sigma}{d\Omega_{lab}} = \frac{\left(1+\rho^2+2\rho\cos\theta\right)^{3/2}}{|1+\rho\cos\theta|}\frac{d\sigma}{d\Omega_{CM}}}$$

Calculation of scattering amplitude

- Simplest case: Central short-range potential, no Coulomb

$$H\psi(\vec{r}) = E\psi(\vec{r})$$

$$\left(-\frac{\hbar^2}{2\mu}\vec{\nabla}^2 + V(r)\right)\psi(\vec{r}) = E\psi(\vec{r}) \quad ; \quad -\frac{\hbar^2}{2\mu}\vec{\nabla}^2 = -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\vec{L}^2}{2\mu r^2}$$

  - The (initial) expansion plane wave expansion

$$e^{i\vec{k}\cdot\vec{r}} = 4\pi\sum_{l,m} i^l j_l(kr) Y^*_{lm}(\hat{k})\, Y_{lm}(\hat{r}) = \sum_l (2l+1) i^l j_l(kr) P_l(\cos\theta) \quad ; \quad \vec{k}\cdot\vec{r} = kr\cos\theta$$

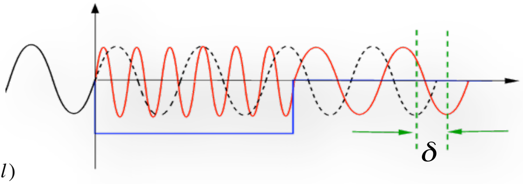
  - No dependence on azimuthal angle φ

$$\psi(\vec{r}) = \frac{1}{kr}\sum_l (2l+1) i^l u_l(r) P_l(\cos\theta) \quad ; \quad \vec{L}^2 P_l(\cos\theta) = \hbar^2 l(l+1) P_l(\cos\theta)$$

$$\boxed{\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \frac{2\mu}{\hbar^2}V(r) + k^2\right)u_l(r) = 0} \quad ; \quad k^2 = 2\mu E/\hbar^2$$

Equation to solve

  - Assume V(r)~0 for *r* ≥ *a* (valid for a nuclear potential)



$$u_l(r) \to b_l\, kr\left(\cos\delta_l\, j_l(kr) + \sin\delta_l\, n_l(kr)\right) \quad \text{for} \quad r \geq a$$

$$\to b_l\left(\cos\delta_l \sin(kr - \tfrac{\pi}{2}l) + \sin\delta_l \cos(kr - \tfrac{\pi}{2}l)\right) = b_l\, e^{-i\delta_l}\,\frac{e^{2i\delta_l}e^{i(kr-\frac{\pi}{2}l)} - e^{-i(kr-\frac{\pi}{2}l)}}{2i} \quad \text{for} \quad r \to \infty$$

  - We introduced phase shift δ_l . For V=0 the phase shift is zero: δ_l=0

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Calculation of scattering amplitude

- To find the amplitude *f(θ)* we use

$$f(\theta) = \sum_l (2l+1) f_l P_l(\cos\theta)$$

- Then we match

$$\psi(\vec{r}) \to e^{i\vec{k}\cdot\vec{r}} + f(\theta,\varphi)\frac{e^{ikr}}{r} = \sum_l (2l+1)(i^l j_l(kr) + f_l \frac{e^{ikr}}{r}) P_l(\cos\theta) \to \frac{1}{2ik}\sum_l (2l+1)(i^l \frac{e^{i(kr-\frac{\pi}{2}l)} - e^{-i(kr-\frac{\pi}{2}l)}}{r} + 2ik f_l \frac{e^{ikr}}{r}) P_l(\cos\theta)$$

$$= \boxed{\frac{1}{2ikr}\sum_l (2l+1)((-1)^{l+1} e^{-ikr} + (1+2ik f_l)e^{ikr}) P_l(\cos\theta)}$$

- with

$$\psi(\vec{r}) = \frac{1}{kr}\sum_l (2l+1) i^l u_l(r) P_l(\cos\theta) \to \frac{1}{kr}\sum_l (2l+1) i^l b_l e^{-i\delta_l} \frac{e^{2i\delta_l} e^{i(kr-\frac{\pi}{2}l)} - e^{-i(kr-\frac{\pi}{2}l)}}{2i} P_l(\cos\theta)$$

$$= \boxed{\frac{1}{2ikr}\sum_l (2l+1) b_l e^{-i\delta_l}\left((-1)^{l+1} e^{-ikr} + e^{2i\delta_l} e^{ikr}\right) P_l(\cos\theta)} \quad \text{for} \quad r \to \infty$$

- and set $b_l = e^{i\delta_l}$ and $1 + 2ik f_l = e^{2i\delta_l} \Rightarrow f_l = (S_l - 1)/2ik$
- S-matrix (element) S or collision matrix U: $S_l = e^{2i\delta_l}$

- Cross section: $\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{1}{4k^2}\sum_{l,l'} (2l+1)(2l'+1)(S_l - 1)(S^*_{l'} - 1) P_l(\cos\theta) P_{l'}(\cos\theta)$

Charge particle scattering

- Rutherford scattering

$$V_C(r) = \frac{Z_1 Z_2 e^2}{r} \quad ; \quad \left(-\frac{\hbar^2}{2\mu}\vec{\nabla}^2 + V_C(r)\right)\psi_C(\vec{r}) = E\psi_C(\vec{r})$$

$$\psi_C(k\hat{z},\vec{r}) = \sum_l (2l+1) i^l P_l(\cos\theta)\frac{1}{kr}F_l(\eta,kr)e^{i\sigma_l(\eta)} \quad ; \quad \eta = \frac{Z_1 Z_2 e^2}{\hbar v} \quad \ldots \quad \text{Sommerfeld parameter}$$

$$\sigma_l(\eta) = \arg\Gamma(l+1+i\eta) \quad \ldots \quad \text{Coulomb phase shift}$$

  - Regular and irregular Coulomb functions

$$F_l(0,kr) = kr\, j_l(kr) \quad ; \quad G_l(0,kr) = kr\, n_l(kr)$$

$$F_l(\eta,kr) \to \sin(kr - \eta\ln 2kr - l\tfrac{\pi}{2} + \sigma_l) \quad ; \quad G_l(\eta,kr) \to \cos(kr - \eta\ln 2kr - l\tfrac{\pi}{2} + \sigma_l) \quad \text{for} \quad r \to \infty$$

$$H_l^{(\pm)}(\eta,kr) = G_l(\eta,kr) \pm i F_l(\eta,kr)$$

  - Coulomb scattering amplitude

$$\psi_C(k\hat{z},\vec{r}) \to e^{i(kz+\eta\ln[k(r-z)])} + f_C(\theta)\frac{e^{i(kr-\eta\ln 2kr)}}{r} \quad \text{for} \quad \mathrm{r} \to \infty$$

$$f_C(\theta) = \frac{1}{2ik}\sum_l (2l+1)\left(e^{2i\sigma_l} - 1\right)P_l(\cos\theta) = -\frac{\eta}{2k\sin^2\frac{\theta}{2}}\; e^{-i\eta\ln(\sin^2\frac{\theta}{2})+2i\sigma_0}$$

  - Rutherford cross section

$$\frac{d\sigma_R}{d\Omega} = \left|f_C(\theta)\right|^2 = \frac{\eta^2}{4k^2\sin^4\frac{\theta}{2}}$$

Gamow factor

$$\psi_C(0) = \Gamma(1+i\eta)e^{-\eta\pi/2}$$

$$\left|\psi_C(0)\right|^2 \approx 2\pi\eta\, e^{-2\eta\pi} \quad \text{for} \quad \eta >> 1$$

…relevant for low-energy charged nuclear reactions - astrophysics

Charge particle scattering

- Nuclear plus Coulomb scattering

$$\left(-\frac{\hbar^2}{2\mu}\vec{\nabla}^2+V_C(r)+V(r)\right)\psi(\vec{r})=E\psi(\vec{r})$$

$$\psi(\vec{r})=\frac{1}{kr}\sum_l(2l+1)i^l\,e^{i\sigma_l}u_l(r)P_l(\cos\theta)$$

$$\psi(\vec{r})=\psi_C(\vec{r})+\psi_N(\vec{r})$$

$$\psi_N(\vec{r})\rightarrow f_N(\theta)\frac{e^{i[kr-\eta\ln(2kr)]}}{r}\quad\text{for}\quad r\rightarrow\infty$$

  - only outgoing Coulomb function in the nuclear part of the wave function

$$\psi(\vec{r})=\psi_C(\vec{r})+\frac{1}{kr}\sum_l(2l+1)i^l\,e^{i\sigma_l}f_l^N\,H_l^{(+)}(\eta,kr)P_l(\cos\theta)$$

$$f_l^N=\frac{1}{2i}(S_l^N-1)\quad;\quad S_l^N=e^{2i\delta_l^N}$$

    - nuclear phase shift

  - scattering amplitude – Coulomb plus nuclear

$$f(\theta)=f_C(\theta)+f_N(\theta)$$

$$f_N(\theta)=\frac{1}{2ik}\sum_l(2l+1)e^{2i\sigma_l}(e^{2i\delta_l^N}-1)P_l(\cos\theta)$$

  - Cross section $\frac{d\sigma}{d\Omega}=\left|f(\theta)\right|^2=\frac{d\sigma_R}{d\Omega}+2\,\mathrm{Re}\left[f_C^*(\theta)f_N(\theta)\right]+\left|f_N(\theta)\right|^2$

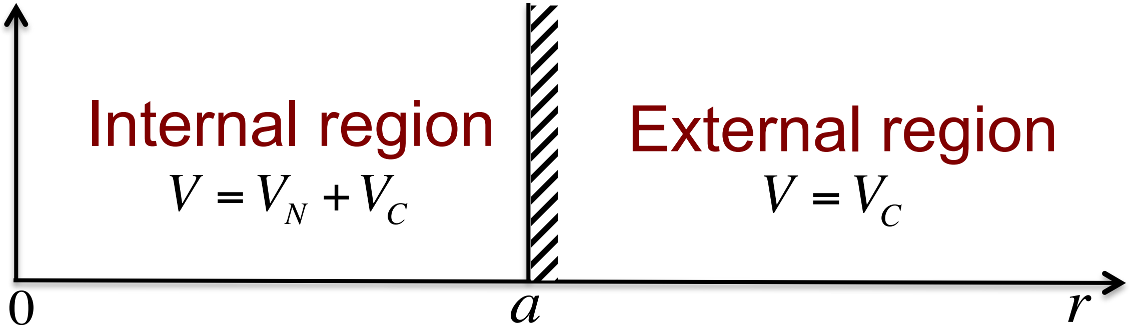
How to solve scattering equations?

$$\psi(\vec{r})=\frac{1}{kr}\sum_{l}(2l+1)i^{l}e^{i\sigma_{l}}u_{l}(r)P_{l}(\cos\theta) \quad ; \quad \vec{L}^{2}P_{l}(\cos\theta)=\hbar^{2}l(l+1)P_{l}(\cos\theta)$$

$$\left(\frac{d^{2}}{dr^{2}}-\frac{l(l+1)}{r^{2}}-\frac{2\mu}{\hbar^{2}}V(r)+k^{2}\right)u_{l}(r)=0 \quad ; \quad k^{2}=2\mu E/\hbar^{2}$$

$$\left(T_{l}(r)+V(r)-E\right)u_{l}(r)=0 \quad ; \quad T_{l}(r)=-\frac{\hbar^{2}}{2\mu}\left(\frac{d^{2}}{dr^{2}}-\frac{l(l+1)}{r^{2}}\right)$$

- Many methods… let’s apply Microscopic R-matrix on a Lagrange mesh
  - Very efficient also for the case of non-local potentials
  - Powerful for coupled channel problem



Internal region

$V=V_N+V_C$

External region

$V=V_C$

  - Solution in the external region

$$u_{l}(r)=\frac{i}{2}\left(H_{l}^{(-)}(\eta,kr)-S_{l}H_{l}^{(+)}(\eta,kr)\right)\equiv I_{l}(kr)-S_{l}O_{l}(kr)$$

Microscopic R-matrix on a Lagrange mesh

- Internal region

$$u_l(r) = \sum_{n=1}^{N} A_{ln}\, f_n(r) \quad ; \quad N \text{ Lagrange basis functions } f_n(r)$$

associated with a Lagrange mesh of N points $ax_n \in [0,a]$

x_n ... zero of shifted Legendre polynomials: $P_N(2x_n - 1) = 0$

$$f_n(r) = (-1)^{N-n} a^{-1/2} \sqrt{\frac{1-x_n}{x_n}}\, \frac{r}{r - ax_n} P_N(\tfrac{2r}{a} - 1)$$

$$f_{n'}(ax_n) = \frac{1}{\sqrt{a\lambda_n}} \delta_{n,n'} \quad \ldots \quad \text{zero at all mesh points except one}$$

- λ_n … weights of the Gauss-Legendre quadrature approximation of the integral

$$\int_0^1 g(x)dx \approx \sum_{n=1}^{N} \lambda_n g(x_n)$$

- Lagrange basis functions orthonormal within the quadrature approximation

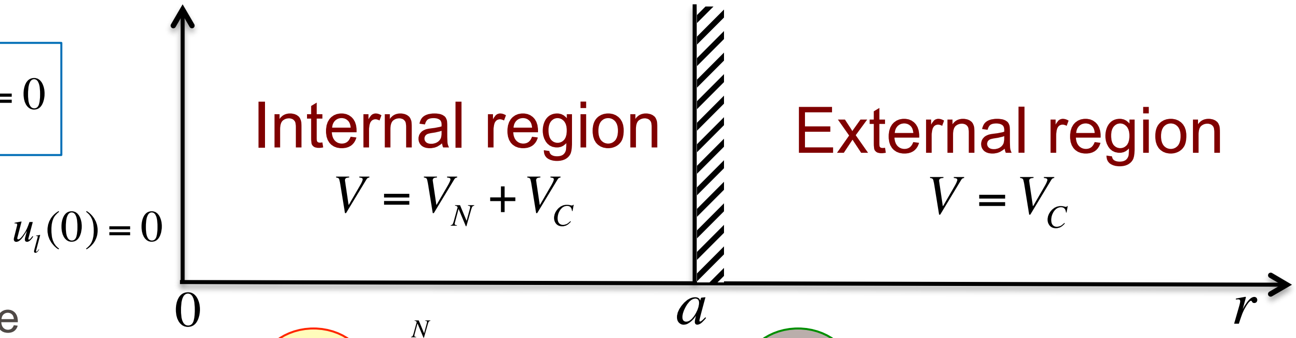
$$\int_0^a f_n(r) f_{n'}(r) dr \approx \delta_{n,n'}$$

- Matrix element calculation trivial $\langle f_n | V | f_{n'} \rangle = \int_0^a f_n(r) V(r) f_{n'}(r) dr \approx V(ax_n)\delta_{n,n'}$

Microscopic R-matrix on a Lagrange mesh

- Back to solving the Schrödinger equation

$$\boxed{\left(T_l(r)+V(r)-E\right)u_l(r)=0}$$



$u_l(0)=0$

Internal region

$V=V_N+V_C$

External region

$V=V_C$

$$u_l(r)=\sum_{n=1}^{N}A_{ln}\,f_n(r) \qquad u_l(r)=I_l(kr)-S_l O_l(kr)$$

- Logarithmic-derivative matching at *r*=*a* facilitated by the Bloch operator

$$\mathcal{L}=\frac{\hbar^2}{2\mu}\delta(r-a)\left(\frac{d}{dr}-B\right)\quad\ldots\quad B\text{ boundary condition, for scattering }B=0$$

$$\left(T_l(r)+V(r)+\mathcal{L}-E\right)u_l(r)=\mathcal{L}\,u_l(r)$$

$$\boxed{T_l+\mathcal{L}\quad\ldots\quad\text{Hermitian on }r\in[0,a]}$$

$$\sum_{n=1}^{N}\left(C_{n'n}-E\delta_{n,n'}\right)A_{ln}=f_{n'}(a)\frac{\hbar^2k}{2\mu}\left[I_l'(ka)-S_lO_l'(ka)\right]$$

$$C_{n'n}=\left\langle f_{n'}\middle|T_l+V+\mathcal{L}\middle|f_n\right\rangle=\int_0^a dr\,f_{n'}(r)\left[T_l(r)+V(r)+\mathcal{L}\right]f_n(r)$$

1) Invert *C-E* to get A_{ln} & u_l in the internal region

2) Match u_l to the external solution at *r*=*a*

3) Obtain R-matrix R_l & S-matrix S_l

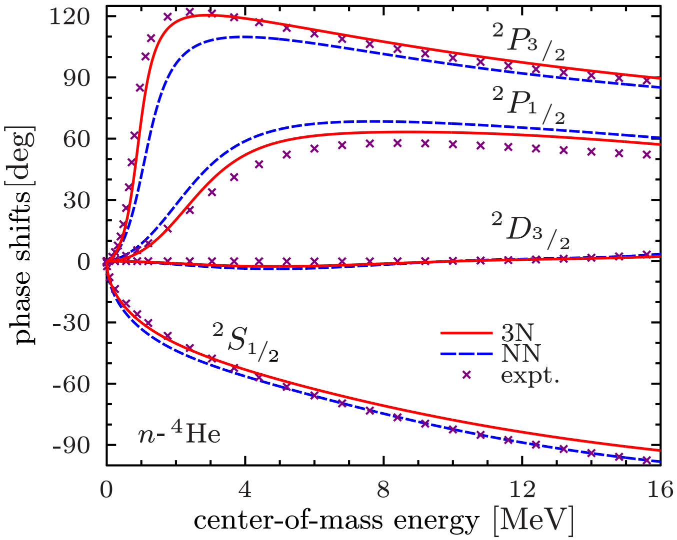
$$R_l=\frac{\hbar^2}{2\mu a}\sum_{n,n'=1}^{N}f_n(a)\left[C-E1\right]^{-1}_{nn'}f_{n'}(a)\quad;\quad\boxed{S_l=e^{2i\delta_l}=\frac{I_l(ka)-kaR_lI_l'(ka)}{O_l(ka)-kaR_lO_l'(ka)}}$$

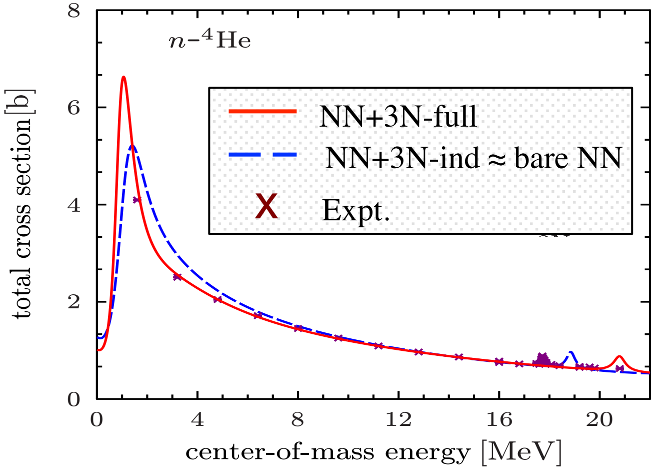
Phase shift properties

- Example: n-^{4}He elastic scattering

$$\frac{d\sigma_{el}}{d\Omega} = \frac{1}{4k^2}\sum_{l,l'}(2l+1)(2l'+1)(S_l-1)(S^*_{l'}-1)P_l(\cos\theta)P_{l'}(\cos\theta) \quad ; \quad S_l = e^{2i\delta_l}$$

$$\sigma_{el} = \frac{\pi}{k^2}\sum_l (2l+1)\left|S_l-1\right| = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\delta_l \quad ; \quad \delta_l = \delta_{l,res} + \delta_{l,bg}$$





- Phase shift increasing – attractive interaction :
  - A sharp resonance in l=1 $^{2s+1}l_J$=$^2P_{3/2}$
  - A broad resonance in l=1 $^2P_{1/2}$
- Phase shift ~ 0 – interaction ~0
  - l=2 $^2D_{3/2}$
- Phase shift decreasing – no resonance
  - l=0 $^2S_{1/2}$ – Pauli-forbidden bound state

- An isolated resonance can be phenomenologically described by a Breit-Wigner shape

$$\sigma_l^{res}(E) \approx \frac{4\pi}{k^2}(2l+1)\frac{\Gamma^2/4}{(E-E_r)+\Gamma^2/4} = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_{l,res}(E)$$

$$\delta_{l,res}(E) = \arctan\left(\frac{\Gamma/2}{E_r-E}\right)(+n(E)\pi) \quad ; \quad \delta_{l,bg} \approx 0$$

$$\Gamma \approx 2\Big/\left(\frac{d\delta}{dE}\right)_{E=E_r} \ldots \text{ resonance width, } E_r \text{ resonance energy, } \tau \approx \hbar/\Gamma \text{ time delay}$$

Phase shift properties

- S-matrix near an isolated resonance

$$S(E) = e^{2i\delta_{bg}} \frac{E - E_r - i\Gamma/2}{E - E_r + i\Gamma/2}$$

$S(E)$ continued to complex energy E: Pole at $E_p = E_r - i\Gamma/2$

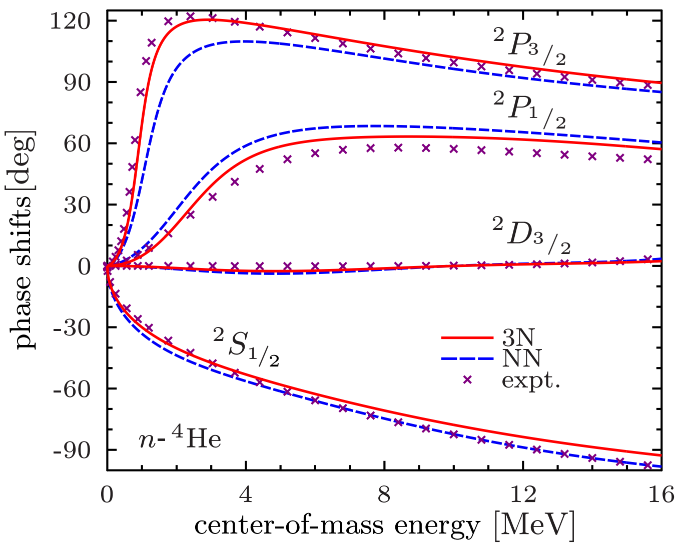
  - used to define the resonance E_r and Γ
  - n-^{4}He $3/2^-$: E~ 0.96 – i 0.92/2 MeV
  - n-^{4}He $1/2^-$: E~ 1.9 – i 6.1/2 MeV

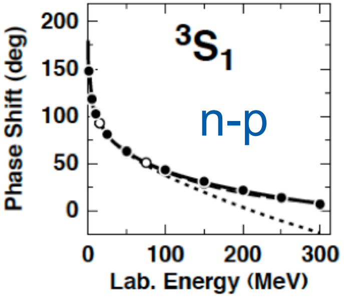
- l=0 neutral scattering (neutron S-wave scattering)
  - special case: neutral unbound poles called virtual states

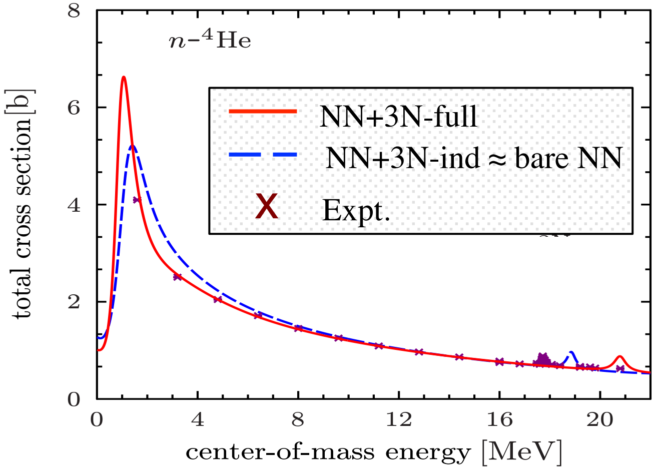
$$S(k) = -\frac{k + i/a_0}{k - i/a_0} \quad \ldots \quad \text{pole at } k_p = i/a_0$$

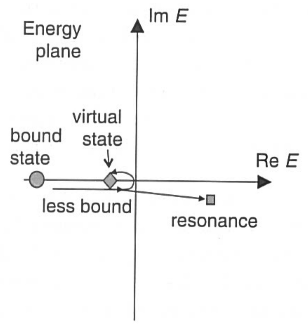
$$\delta(k) = -\arctan(a_0 k) \quad \ldots \quad k\cot\delta(k) = -1/a_0$$

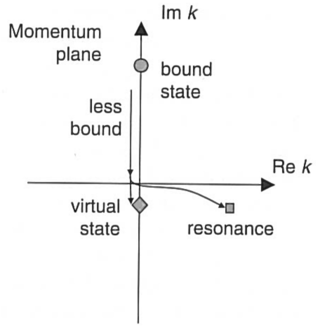
$$a_0 \quad \ldots \quad l = 0 \text{ scattering length}$$

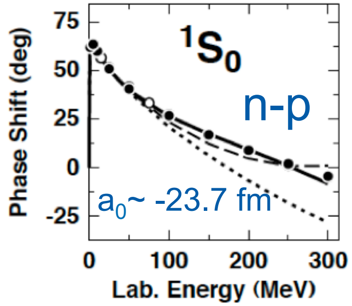












Multi-channel scattering & reactions

- Binary collisions – $A_1+A_2 \rightarrow A_1+A_2$; $A_1+A_2 \rightarrow A^*_1+A^*_2$; $A_1+A_2 \rightarrow A_3+A_4$ …

$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \hat{A}_\nu \left[\left(\left|A-a\;\alpha_1 I_1^{\pi_1}\right\rangle \left|a\;\alpha_2 I_2^{\pi_2}\right\rangle \right)^{(s)} Y_\ell(\hat{r}_{A-a,a}) \right]^{(J^\pi)} \frac{u_\nu^{J^\pi}(r_{A-a,a})}{r_{A-a,a}}$$

$$\nu \equiv \left\{ A-a\;\alpha_1 I_1^{\pi_1}; a\;\alpha_2 I_2^{\pi_2}; s\ell \right\} \quad \text{channel q.n.} \quad ; \quad \hat{A}_\nu \ldots \text{antisymmetrizer}$$

$$\vec{r}_{A-a,a} = \frac{1}{A-a}\sum_{i=1}^{A-a}\vec{r}_i - \frac{1}{a}\sum_{j=A-a+1}^{A}\vec{r}_j \qquad \vec{s} = \vec{I}_1 + \vec{I}_2 \quad ; \quad \vec{J} = \vec{s} + \vec{\ell}$$

  - *(A-a,a)* … defines a mass partition
  - *s* … channel spin, *l* ... relative orbital momentum, *J* ... total momentum
  - Hamiltonian

$$H = H_{(A-a)} + H_{(a)} + T_{rel} + V_{rel} \quad ; \quad T_{rel} = \frac{\hbar^2}{2\mu_{A-a,a}}\nabla^2_{A-a,a} \quad ; \quad V_{rel} \to V_{C,rel} = \frac{Z_{A-a}Z_a e^2}{r_{A-a,a\alpha}} \quad \text{for} \quad r_{A-a,a} \to \infty$$

$$H_{(A-a)}\left|A-a\;\alpha_1 I_1^{\pi_1}\right\rangle = E_{\alpha_1}^{I_1^{\pi 1}}\left|A-a\;\alpha_1 I_1^{\pi_1}\right\rangle$$

$$H_{(a)}\left|a\;\alpha_2 I_2^{\pi_2}\right\rangle = E_{\alpha_2}^{I_2^{\pi 2}}\left|a\;\alpha_2 I_2^{\pi_2}\right\rangle$$

  - Coupled channel equations $\quad H\left|\psi^{J^\pi T}\right\rangle = E\left|\psi^{J^\pi T}\right\rangle$

Multi-channel scattering & reactions

- Wave function expansion considering the beam in the ***k**$_i$* direction

$$\left|\psi^{J^\pi T}\right\rangle = \frac{4\pi}{k_i}\sqrt{v_i}\sum_{\alpha s \ell s_i \ell_i J} i^{\ell_i} Y^*_{\ell_i m_i}(\hat{k}_i)(s_i m_{si}\, \ell_i m_i \mid JM) e^{i\sigma_{\ell_i}} \hat{A}_\alpha \left[\left(\left|A-a\,\alpha_1 I_1^{\pi_1}\right\rangle \left|a\,\alpha_2 I_2^{\pi_2}\right\rangle\right)^{(s)} Y_\ell(\hat{r}_{A-a,a})\right]_M^{(J^\pi)} \frac{u^{J^\pi}_{\alpha s\ell,\,\alpha_i s_i \ell_i}(r_{A-a,a})}{r_{A-a,a}}$$

$$\alpha \equiv \left\{A-a\,\alpha_1 I_1^{\pi_1}; a\,\alpha_2 I_2^{\pi_2}\right\}$$

Beam in the $\hat{z}$ direction ($\vec{k}_i = k_i\hat{z}$): $Y^*_{\ell_i m_i}(\hat{z}) = \delta_{m_i,0}\sqrt{\dfrac{2\ell_i+1}{4\pi}}$

$$u^{J^\pi}_{\alpha s\ell,\,\alpha_i s_i \ell_i}(r_{A-a,a}) \rightarrow \frac{i}{2}\frac{1}{\sqrt{v_\alpha}}\left[H^{(-)}_{\ell_i}(\eta_\alpha, k_\alpha r_{A-a,a})\delta_{\alpha,\alpha_i}\delta_{\ell,\ell_i}\delta_{s,s_i} - S^{J^\pi}_{\alpha s\ell,\alpha_i s_i \ell_i} H^{(+)}_{\ell}(\eta_\alpha, k_\alpha r_{A-a,a})\right] \quad \text{for} \quad r_{A-a,a} \rightarrow \infty$$

$S^{J^\pi}_{\alpha s\ell,\alpha_i s_i \ell_i}$ … symmetric and unitary S-matrix

$\hat{A}_\alpha \rightarrow 1$ for $r_{A-a,a} \rightarrow \infty$ … no antisymetrization for separated nuclei

- Scattering amplitude follows from the asymptotic expansion

$$f_{\alpha s m_s,\alpha_i s_i m_{si}}(\theta_\alpha) = \delta_{\alpha,\alpha_i}\delta_{s,s_i}\delta_{m_s,m_{si}} f_{C\alpha_i}(\theta_{\alpha_i}) + \frac{2\pi i}{k_i}\sum_{J\ell\ell_i M m m_i} i^{\ell_i-\ell}(s_i m_{si}\, \ell_i m_i \mid JM)(s m_s \ell m \mid JM) e^{i(\sigma_\ell+\sigma_{\ell_i})}\left[\delta_{\alpha,\alpha_i}\delta_{s,s_i}\delta_{\ell,\ell_i} - S^{J^\pi}_{\alpha s\ell,\alpha_i s_i \ell_i}\right] Y_\ell(\hat{r}_{A-a,a}) Y^*_{\ell_i m_i}(\hat{k}_i)$$

with $\vec{k}_i \cdot \vec{r}_{A-a,a} = k_i\, r_{A-a,a}\cos(\theta_\alpha)$

Multi-channel scattering & reactions

- Cross section

$$\frac{d\sigma_{\alpha,\alpha_i}}{d\Omega} = \frac{1}{(2I_{1i}+1)(2I_{2i}+1)} \sum_{sm_s s_i m_{si}} \left| f_{\alpha s m_s, \alpha_i s_i m_{si}}(\theta_\alpha) \right|^2$$

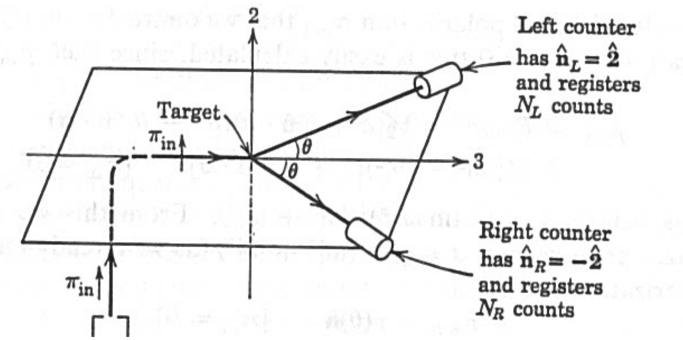
- Polarized beams
  - non-uniform distribution of the *M*-states, e.g., of the projectile

$$\frac{d\sigma^{pol}_{\alpha,\alpha_i}}{d\Omega} = \frac{d\sigma_{\alpha,\alpha_i}}{d\Omega} \sum_{Qq} t^*_{Qq} T^{\alpha,\alpha_i}_{Qq}$$

… t^*_{Qq} chracterizes spin-projection distribution

$$\left| I_2 M_2 \right\rangle \sum_{Qq} t^*_{Qq} \sqrt{2Q+1} (I_2 M_2' Q q \,|\, I_2 M_2) \left\langle I_2 M_2' \right|$$

… T^{α,α_i}_{Qq} tenzor analyzing powers



$$\tfrac{1}{2} p_y A_y = \frac{N_L - N_R}{N_L + N_R}$$

$$\frac{d\sigma^{A_y}_{\alpha,\alpha_i}}{d\Omega} = \frac{d\sigma_{\alpha,\alpha_i}}{d\Omega} \left(1 + \tfrac{1}{2} p_y A_y\right) \quad ; \quad A_y = \sqrt{2}\, i T^{\alpha,\alpha_i}_{11}$$

  - A_y analyzing power: projectile polarized in y(2)-direction, beam in z(3)-direction, reaction plane x-z

$$\frac{d\sigma^{A_y}_{\alpha,\alpha_i}}{d\Omega} = \frac{\sqrt{2}}{(2I_{1i}+1)(2I_{2i}+1)} \sum_{sm_s s_i m_{si} s_i' m_{si}'} (-1)^{I_{1i}+I_{2i}+1+s_i} \begin{Bmatrix} I_{1i} & I_{2i} & s_i' \\ 1 & s_i & I_{2i} \end{Bmatrix} \sqrt{3(2I_{2i}+1)(2s_i'+1)}\, (s_i' m_{si}' 1 1 \,|\, s_i m_{si})\, f^*_{\alpha s m_s, \alpha_i s_i' m_{si}'}(\theta_\alpha)\, f_{\alpha s m_s, \alpha_i s_i m_{si}}(\theta_\alpha)$$

Literature

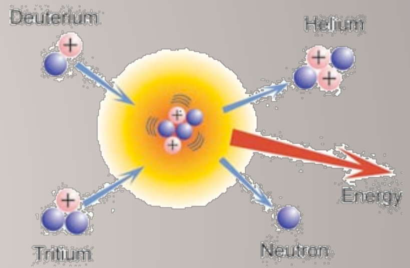
- **Nuclear Reactions for Astrophysics,**

  Ian J. Thompson and Filomena M. Nunes (Cambridge)
- **Theory of Nuclear Reactions,** P. Fröbrich and R. Lipperheide (Oxford)
- **Scattering Theory,** John R. Taylor (Dover)
- **Introduction to Nuclear Reactions (Graduate Student Series in Physics),**

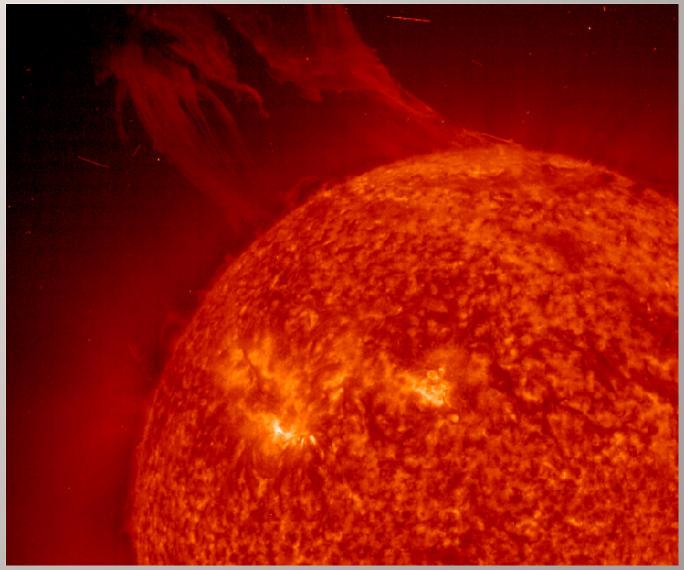
  C. A. Bertulani and P. Danielewicz (CRC Press)
- **Nuclear Reactions: An Introduction,** Hans Paetz gen. Schieck (Springer)
- **Collision Theory,** M. L. Goldhaber and K. M. Watson (Dover)
- **Direct Nuclear Reactions,** Norman K. Glendenning (World Scientific)
- **Scattering Theory of Waves and Particles,** Roger G. Newton (Springer)

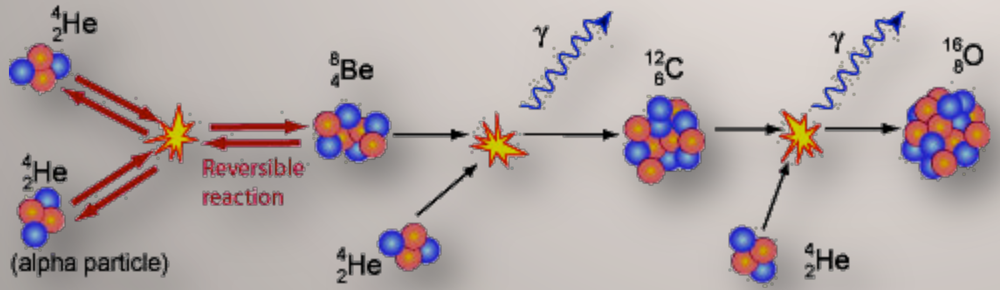
Why nuclei from first principles?

- **Goal**: Predictive theory of structure and reactions of nuclei
- Needed for
  - Physics of **exotic nuclei**, tests of fundamental symmetries
  - Understanding of nuclear reactions important for **astrophysics**
  - Understanding of reactions important for **energy generation**
  - **Double beta decay** nuclear matrix elements
  - **Neutrino-nucleus** cross sections
  - …



Understanding our Sun





What is meant by *ab initio* in nuclear physics?

- **First principles for Nuclear Physics:**

  QCD
  - Non-perturbative at low energies
  - Lattice QCD in the future

- Degrees of freedom: NUCLEONS
  - Nuclei made of nucleons
  - Interacting by nucleon-nucleon and three-nucleon potentials

- *Ab initio*

✧ All nucleons are active

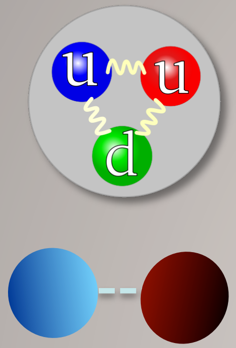
✧ Exact Pauli principle

✧ Realistic inter-nucleon interactions

  ✧ Accurate description of NN (and 3N) data

✧ Controllable approximations

From QCD to nuclei

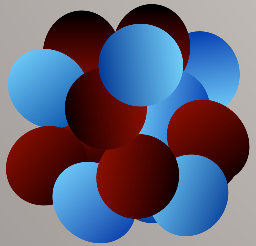


Low-energy QCD

↓

NN+3N interactions
from chiral EFT

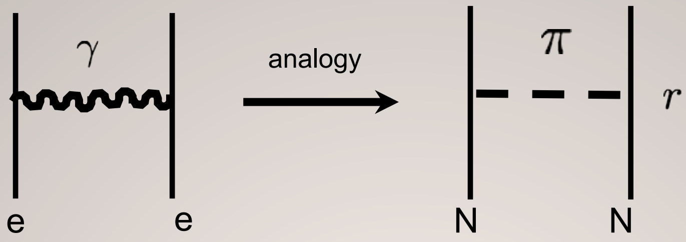
…or accurate
meson-exchange
potentials



Nuclear structure and reactions

Nuclear forces

Nucleon-Nucleon force



$r \sim \frac{1}{m}$

one-pion exchange potential (OPE)

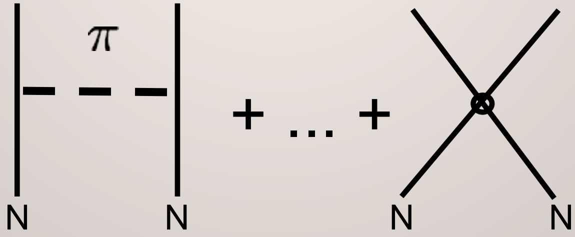
electromagnetic force:
infinite range →
exchange of massless particle

NN force:
finite range →
exchange of massive particle

Yukawa
Nobel price in 1949

Nowadays:
New vision of Effective Field Theory Links low energy physics to QCD in a systematic way

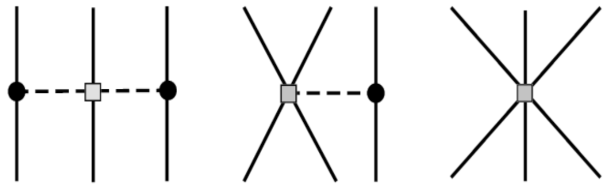
Nucleon-Nucleon force



Details of short distance physics not resolved, but captured in short range couplings →
should come from QCD
but are now fit to experiment

Many-Nucleon forces

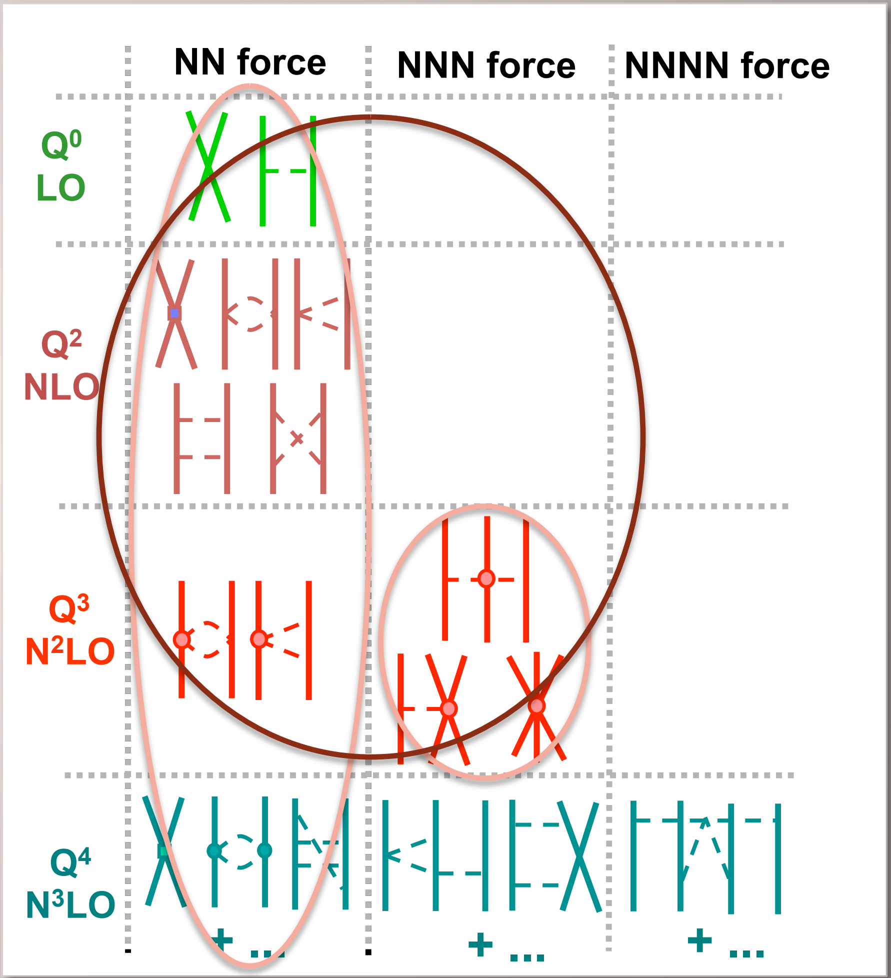
Arise due to the effective nature of nuclear forces



TRIUMF

Chiral Effective Field Theory

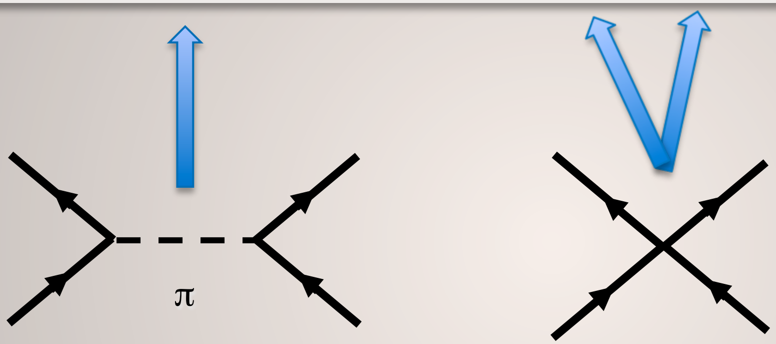
- Inter-nucleon forces from chiral effective field theory
  - Based on the symmetries of QCD
    - Chiral symmetry of QCD ($m_u \approx m_d \approx 0$), spontaneously broken with pion as the Goldstone boson
    - Degrees of freedom: nucleons + pions
  - Systematic low-momentum expansion to a given order (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

Chiral EFT NN interaction in the leading order (LO)

$$V^{\mathrm{LO}} = -\frac{g_A^2}{4F_\pi^2}\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \frac{\vec{\sigma}_1 \cdot \vec{q}\, \vec{\sigma}_2 \cdot \vec{q}}{\vec{q}^{\,2} + M_\pi^2} + C_S + C_T \vec{\sigma}_1 \cdot \vec{\sigma}_2$$



one-pion exchange

contact

C_S , C_T:
Low-energy constants (LECs) fitted to NN data

$\vec{q} = \vec{k}' - \vec{k}$ …momentum transfer

g_A=1.29 …axial-vector coupling constant

F_π=92.4 MeV …pion decay constant

Regularized, e.g., by:

$$\exp\left(-(k'/\Lambda)^{2n} - (k/\Lambda)^{2n}\right)$$

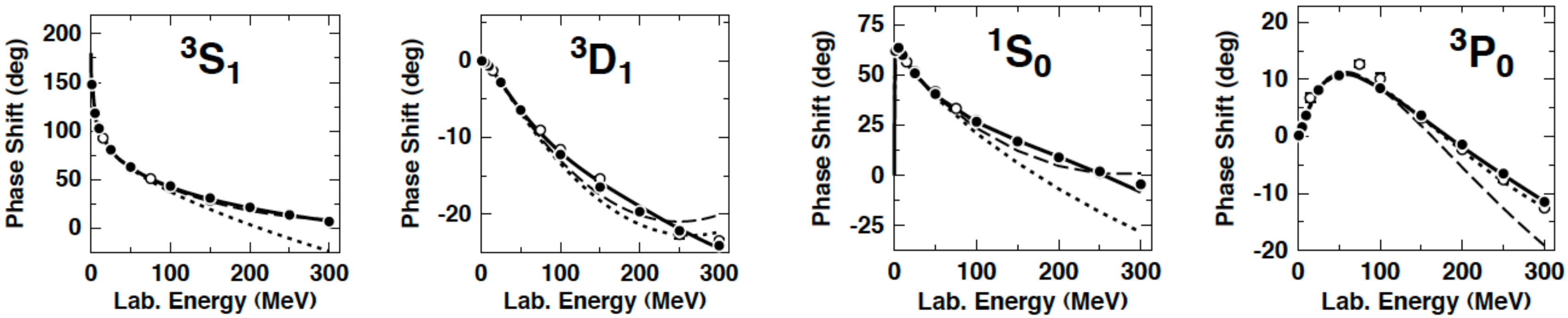
Λ ~ 500 MeV << Λ_χ~ 1 GeV

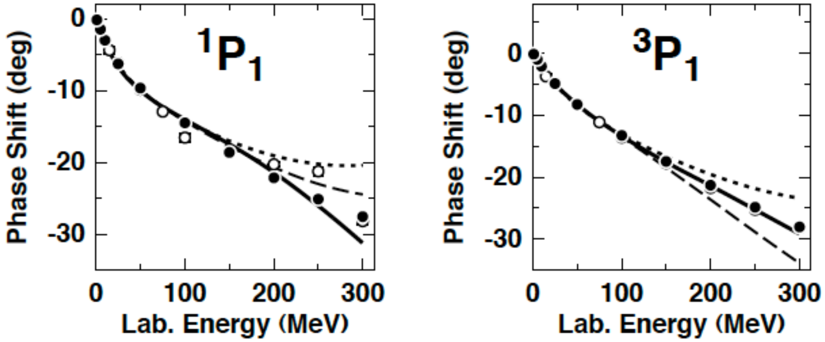
The NN interaction from chiral EFT

PHYSICAL REVIEW C **68**, 041001(R) (2003)

Accurate charge-dependent nucleon-nucleon potential at fourth order of chiral perturbation theory

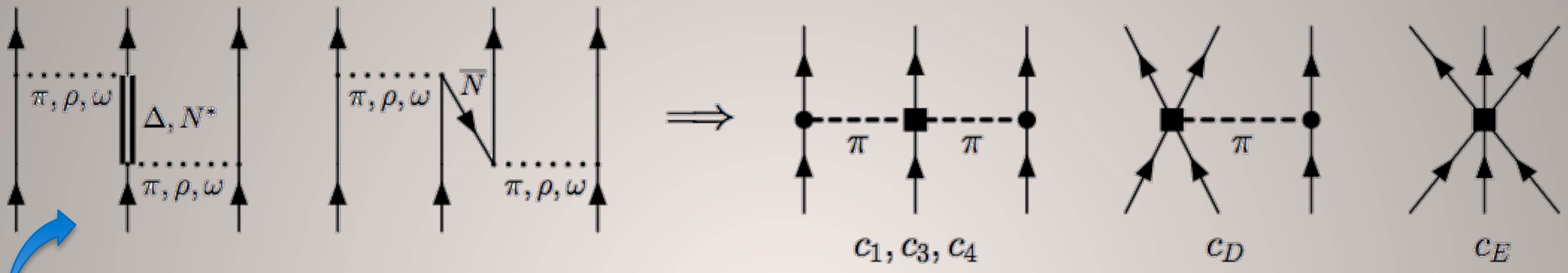
D. R. Entem[1,2,*] and R. Machleidt[1,†]





- 24 LECs fitted to the *np* scattering data and the deuteron properties
  - Including c_i LECs (i=1-4) from pion-nucleon Lagrangian

Three-nucleon forces why?



Eliminating degrees of freedom leads to three-body forces.

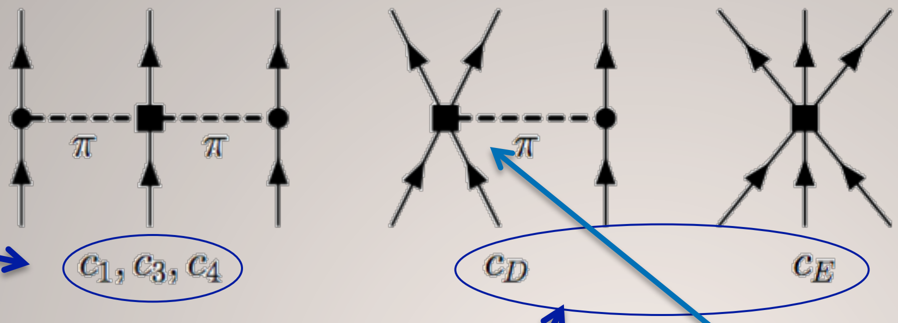
Two-pion exchange with **virtual Δ excitation** – Fujita & Miyazawa (1957)

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

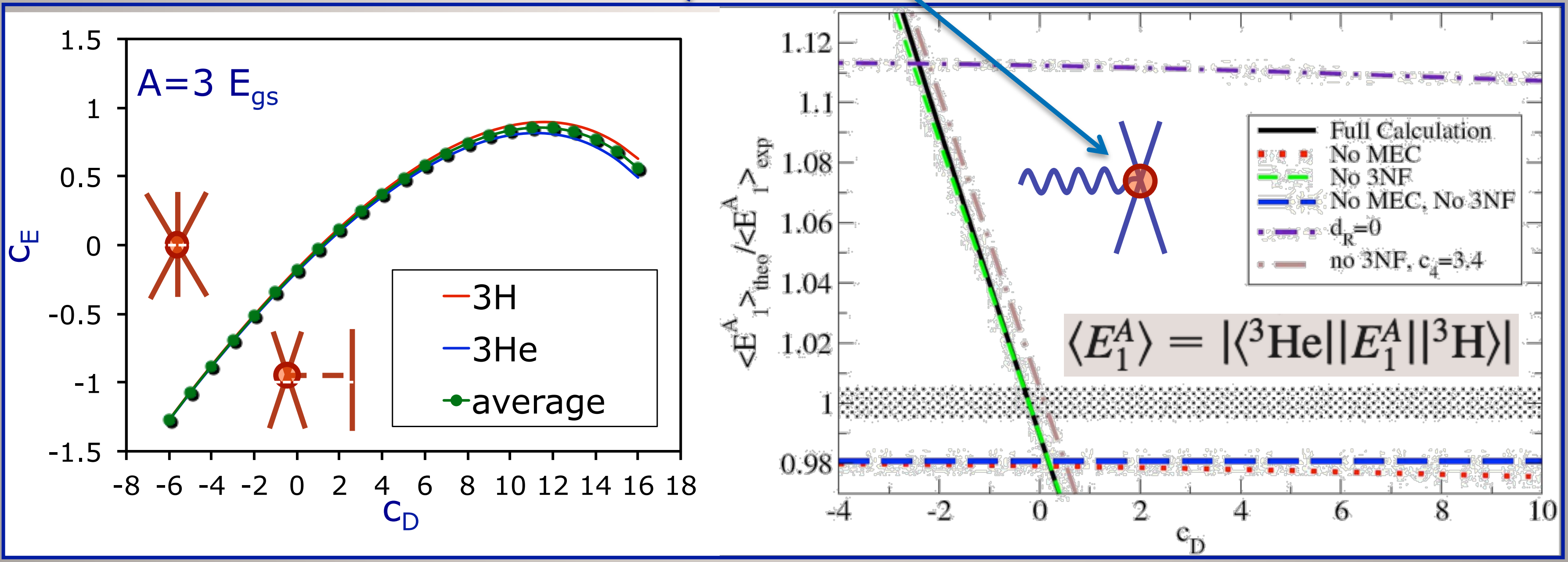
The question is not: Do three-body forces enter the description?
The only question is: How large are three-body forces?

Leading terms of the chiral NNN force

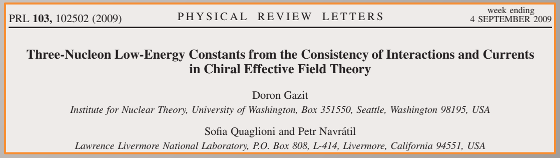
From NN & pion-nucleon scattering



Chiral EFT provides a link between the medium-range (c_D term) NNN force and the meson-exchange current appearing in nuclear beta decay



NNN parameters determined from the ^{3}H binding energy and half life



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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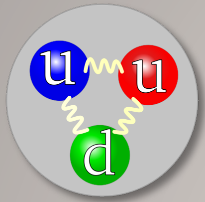
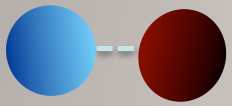
From QCD to nuclei



Low-energy QCD



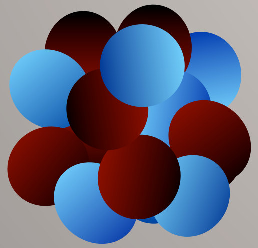
NN+3N interactions from chiral EFT

…or accurate meson-exchange potentials

$$H|\Psi\rangle = E|\Psi\rangle$$

Many-Body methods

NCSM, NCSM/RGM, NCSMC, CCM, SCGF, GFMC, HH, Nuclear Lattice EFT…



Nuclear structure and reactions

TRIUMF

The nuclear many-body problem

- Start with the microscopic *A*-nucleon Hamiltonian

$$H^{(A)}=\sum_{i=1}^{A}\frac{p_i^2}{2m}+\sum_{i<j=1}^{A}V^{2b}(\vec{r}_i-\vec{r}_j)+\left(\sum_{i<j<k=1}^{A}V_{ijk}^{3b}\right)$$

  – Nucleons interact with two- and three-nucleon forces: this yields complicated quantum correlations

- Solve the many-body Schrödinger equation

$$H^{(A)}\Psi^{(A)}(\vec{r}_1,\ \vec{r}_2,\ \dots\ \vec{r}_A)=E\Psi^{(A)}(\vec{r}_1,\ \vec{r}_2,\ \dots\ \vec{r}_A)$$

  – Negative energies (relative to a breakup threshold)– bound-state boundary conditions

    - Find eigenfunctions and eigenenergies

  – Continuum of positive energies – scattering boundary conditions

    - Find elements of the Scattering matrix

The nuclear many-body wave function

- *A* active nucleons – spatial, spin, and isospin degrees of freedom

$$\vec{r}_i \equiv \{\vec{r}_i,\ \vec{\sigma}_i,\ \vec{\tau}_i\},\ i=1,2,\cdots,A$$

- Nucleons are fermions – wave function antisymmetric

$$\Psi^{(A)}(\vec{r}_1,\ \vec{r}_2,\ \ldots\ \vec{r}_k,\ \ldots\ \vec{r}_j,\ \ldots\ \vec{r}_A) = -\Psi^{(A)}(\vec{r}_1,\ \vec{r}_2,\ \ldots\ \vec{r}_j,\ \ldots\ \vec{r}_k,\ \ldots\ \vec{r}_A)$$

- Conserved total angular momentum *J* and parity π
  - approximately conserved total isospin *T*

- We are not interested in the motion of the center of mass, but only in the intrinsic motion
  - Look for translationally invariant wave function. Two options:
    - Work with *A* - 1 translational invariant coordinates known as Jacobi coordinates
    - Work with *A* single particle coordinates and aim at exact separation between intrinsic and center of mass motion

$$\Psi^{(A)}(\vec{r}_1,\ \vec{r}_2,\ \ldots\ \vec{r}_A) = \psi^{(A)}(\vec{\xi}_1,\ \vec{\xi}_2,\ \ldots\ \vec{\xi}_{A-1})\Psi_{CM}(\vec{R}_{CM})$$

How to solve the many-body Schrödinger equation?

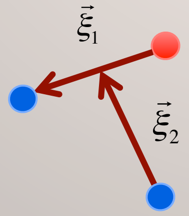
- The nuclear wave function must factorize, e.g., for free c.m. motion

$$\Psi^{(A)} = \psi^{(A)} \exp\left(-i\frac{\vec{P}_{CM}\vec{R}_{CM}}{\hbar}\right) \qquad E = \varepsilon + \frac{P^2_{CM}}{2Am}$$

- First option: solve eigenvalue problem for the intrinsic Hamiltonian
  - ☺ The c.m. motion is not present from the beginning
  - ☺ Work with 3(*A*-1) spatial degrees of freedom (Jacobi relative coordinates)
  - ☹ Jacobi coordinates do not treat the nucleons in a symmetric manner

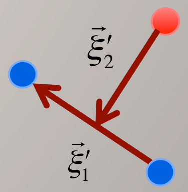
$$\hat{P}_{ij}\phi^{(A)}_{s,n}(\vec{\xi}_1,\ldots\vec{\xi}_{A-1}) = \phi^{(A)}_{s,n}(\hat{P}_{ij}\vec{\xi}_1,\ldots\ \hat{P}_{ij}\vec{\xi}_{A-1}) = \sum_{m=1}^{N} R_{nm}\phi^{(A)}_{s,m}(\vec{\xi}_1,\ldots\vec{\xi}_{A-1})$$

$$\begin{cases} \vec{\xi}_1 = \frac{1}{\sqrt{2}}(\vec{r}_1 - \vec{r}_2) \\ \vec{\xi}_2 = \sqrt{\frac{2}{3}}\left[\frac{1}{2}(\vec{r}_1 + \vec{r}_2) - \vec{r}_3\right] \end{cases}$$



$2 \leftrightarrow 3$

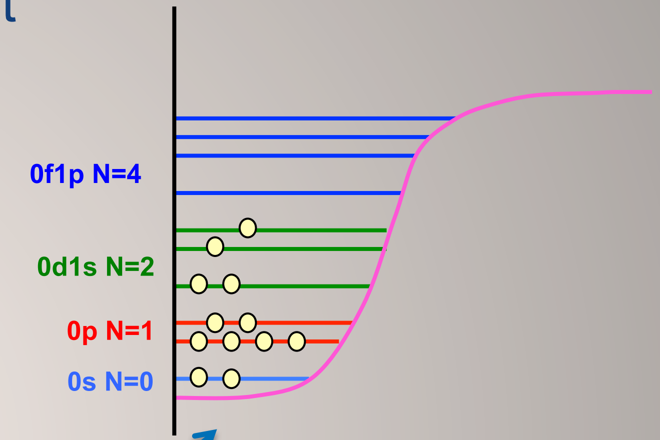
$$\begin{cases} \vec{\xi}'_1 = \frac{1}{\sqrt{2}}(\vec{r}_1 - \vec{r}_3) \\ \vec{\xi}'_2 = \sqrt{\frac{2}{3}}\left[\frac{1}{2}(\vec{r}_1 + \vec{r}_3) - \vec{r}_2\right] \end{cases}$$



How to solve the many-body Schrödinger equation (for bound states)?

- Second option: tie the system to a fixed point

$$H_{SM}^{(A)}=\sum_{i=1}^{A}\left(\frac{p_i^2}{2m}+\underset{\text{mean field}}{U_i(r_i)}\right)+\underbrace{\sum_{i<j=1}^{A}V^{2b}(\vec{r}_i-\vec{r}_j)-\sum_{i=1}^{A}U_i(r_i)}_{\text{residual interaction}}$$



  - Sum of single particle Hamiltonians

$$\left(\frac{p^2}{2m}+U\ (r\ )\right)\varphi_k(\vec{r})=\varepsilon_k\varphi_k(\vec{r})$$

The mean field determines the shell structure

  - Antisymmetrized product of single-particle wfs: use these as *A*-body basis states

$$\phi_n^{(A)}=\frac{1}{\sqrt{A!}}\begin{vmatrix}\varphi_i(\vec{r}_1) & \varphi_i(\vec{r}_2) & \dots & \varphi_i(\vec{r}_A)\\ \varphi_j(\vec{r}_1) & \varphi_j(\vec{r}_2) & & \varphi_j(\vec{r}_A)\\ & \vdots & \ddots & \vdots\\ \varphi_l(\vec{r}_1) & \varphi_l(\vec{r}_2) & \dots & \varphi_l(\vec{r}_A)\end{vmatrix}$$

Slater Determinant (SD):

- Great to implement Pauli exclusion principle
- Very convenient, especially in second quantization formalism

How to solve the many-body Schrödinger equation for bound states?

- Single-particle shell-model states are very convenient basis states for expanding the many-body wave function
- However, the introduction of the mean-field potential U destroys the invariance of the system with respect to translations
- The c.m. motion is no longer separable and remains mixed to intrinsic motion, giving rise in general to spurious effects

$$\Psi_{SM}^{(A)} = \sum_n \psi_n^{(A)}\left(\left\{\vec{\xi}_i\right\}\right) g_n(\vec{R}_{CM})$$

  - Factorization for H_{int} only when **complete convergence** reached (exact solution)

- Exception: harmonic oscillator (HO) potential is exactly separable

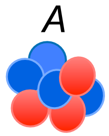
$$\sum_{i=1}^{A} \frac{1}{2} m\Omega^2 r_i^2 = \sum_{i<j=1}^{A} \frac{m\Omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2 + \frac{1}{2} Am\Omega^2 R_{CM}^2$$

$$= \sum_{i=1}^{A-1} \frac{1}{2} m\Omega^2 \xi_i^2 + \frac{1}{2} Am\Omega^2 R_{CM}^2$$

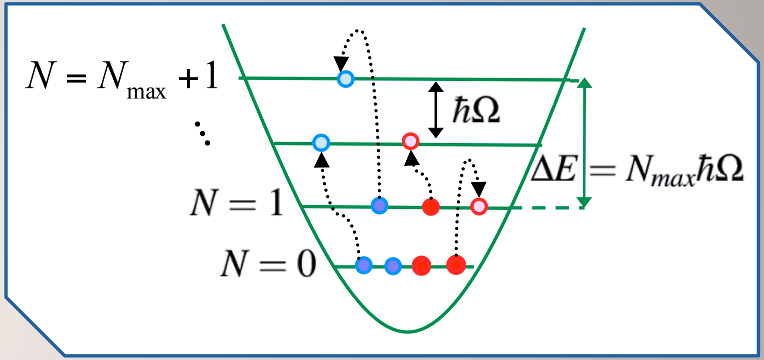
Ab initio no-core shell model (NCSM)

- An *ab initio* approach to solve the many-body Schrödinger equation for bound states (narrow resonances) starting from
  - High-precision NN+NNN interactions

    (coordinate/momentum space)
- Uses large (but finite!) expansions in HO many-body basis states



$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^{HO}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A)$$

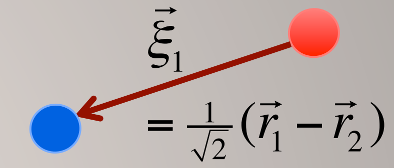


- Choice of either Jacobi relative or Cartesian single-particle coordinates according to the efficiency for the problem at hand
  - Translational invariance of the internal wave function is preserved also when single-particle Slater Determinant (SD) basis is used with $N_{\max}$ truncation
- Convergence to exact result using effective interactions (obtained from unitary transformations of the bare interaction)

$N_{\max}$ … maximal allowed HO excitation above the lowest possible *A*-nucleon configuration
Full $N_{\max}$ space: All basis states with $N \leq N_{\max}$ kept

HO multi-particle states in Jacobi coordinates

- Build many-body basis by adding one particle at the time
- Antisymmetrized two-particle states
  - Start with two-body basis states (LS coupled)



$$\left\langle \vec{\xi}_1 \vec{\sigma}_1 \vec{\sigma}_2 \vec{\tau}_1 \vec{\tau}_2 \middle| n_2 \ell_2 s_2 j_2 t_2 \right\rangle$$

$$= R_{n_2\ell_2}(\xi_1)\left[Y_{\ell_2}(\hat{\xi}_1)\otimes\left[\chi^S_{\frac{1}{2}}(\vec{\sigma}_1)\otimes\chi^S_{\frac{1}{2}}(\vec{\sigma}_2)\right]^{s_2}\right]^{j_2}\left[\chi^T_{\frac{1}{2}}(\vec{\tau}_1)\otimes\chi^T_{\frac{1}{2}}(\vec{\tau}_2)\right]^{t_2}$$

  - Now keep only antisymmetric ones, that is only those for which

$$\hat{P}_{12}\left|n_2\ell_2 s_2 j_2 t_2\right\rangle = -\left|n_2\ell_2 s_2 j_2 t_2\right\rangle \;\Rightarrow\; (-1)^{\ell_2+s_2+t_2} = -1$$

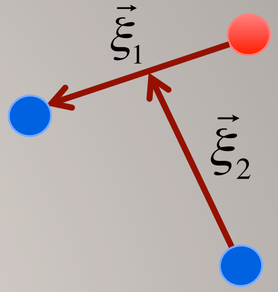
  - Total energy

$$\varepsilon_N = (N+\tfrac{3}{2})\hbar\Omega \qquad\qquad N = 2n_2+\ell_2$$

TRIUMF

HO three-particle states in Jacobi coordinates

- Add one more body



$$\left\langle \vec{\xi}_2\vec{\sigma}_3\vec{\tau}_3 \middle| N_3L_3J_3 \right\rangle = R_{N_3L_3}(\xi_2)\left[Y_{L_3}(\hat{\vec{\xi}}_2)\otimes\chi^S_{\frac{1}{2}}(\vec{\sigma}_3)\right]^{J_3}\chi^T_{\frac{1}{2}}(\vec{\tau}_3)$$

- Three-body basis (JJ coupled)

$$\left\langle \vec{\xi}_1\vec{\xi}_2\vec{\sigma}_1\vec{\sigma}_2\vec{\sigma}_3\vec{\tau}_1\vec{\tau}_2\vec{\tau}_3 \middle| \left[n_2\ell_2s_2j_2t_2;N_3L_3J_3\right]JT \right\rangle$$

Note: antisymmetric for exchange of particle 1 and 2, but not for exchange of partcles 1 and 3 or 2 and 3

$$\left|\left[n_2\ell_2s_2j_2t_2;N_3L_3J_3\right]JT\right\rangle$$

$$= \sum_{m_2,M_3} C^{JM}_{j_2m_2,J_3M_3} \sum_{m^t_2,M^t_3} C^{TM_T}_{t_2m^t_2,T_3M^t_3} \left|n_2\ell_2s_2j_2t_2\right\rangle\left|N_3L_3J_3\right\rangle$$

- Total energy: $\varepsilon_N = (N+3)\hbar\Omega$ with $N = 2n_2+\ell_2+2N_3+L_3$
- To find totally antisymmetric states, diagonalize: $\hat{A} = \frac{1}{3}(1-\hat{P}_{13}-\hat{P}_{23})$
  - Keep only antisymmetric eigenstates, that is those with eigenvalue 1

HO single-particle wave functions

- Start with single-particle HO spatial wave function, defined by radial quantum number n, orbital angular momentum l, and z-projection μ

$$\varphi_{nl\mu}(\vec{r}) = R_{nl}(r) Y_{l\mu}(\hat{r}) \qquad \varepsilon_{nl} = \left(2n + l + \tfrac{3}{2}\right)\hbar\Omega$$

- Now include the spin and isospin wave functions: $\chi^{S}_{\frac{1}{2}m_s}(\vec{\sigma}),\ \chi^{T}_{\frac{1}{2}m_t}(\vec{\tau})$
  - Uncoupled scheme

$$\varphi_{nl\mu\frac{1}{2}m_s\frac{1}{2}m_t}(\vec{r},\vec{\sigma},\vec{\tau}) = R_{nl}(r) Y_{l\mu}(\hat{r}) \chi^{S}_{\frac{1}{2}m_s}(\vec{\sigma}) \chi^{T}_{\frac{1}{2}m_t}(\vec{\tau})$$

  - j-coupled scheme

$$\varphi_{nljm_j\frac{1}{2}m_t}(\vec{r},\vec{\sigma},\vec{\tau}) = R_{nl}(r)\left[Y_l(\hat{r}) \otimes \chi^{S}_{\frac{1}{2}}(\vec{\sigma})\right]^{j}_{m_j} \chi^{T}_{\frac{1}{2}m_t}(\vec{\tau})$$

$$\left[Y_l(\hat{r}) \otimes \chi^{S}_{\frac{1}{2}}(\vec{\sigma})\right]^{j}_{m_j} = \sum_{\mu m_s} C^{j\,m_j}_{l\mu,\frac{1}{2}m_s} Y_{l\mu}(\hat{r})\ \chi^{S}_{\frac{1}{2}m_s}(\vec{\sigma})$$

Multi-particle states in the Slater Determinant basis

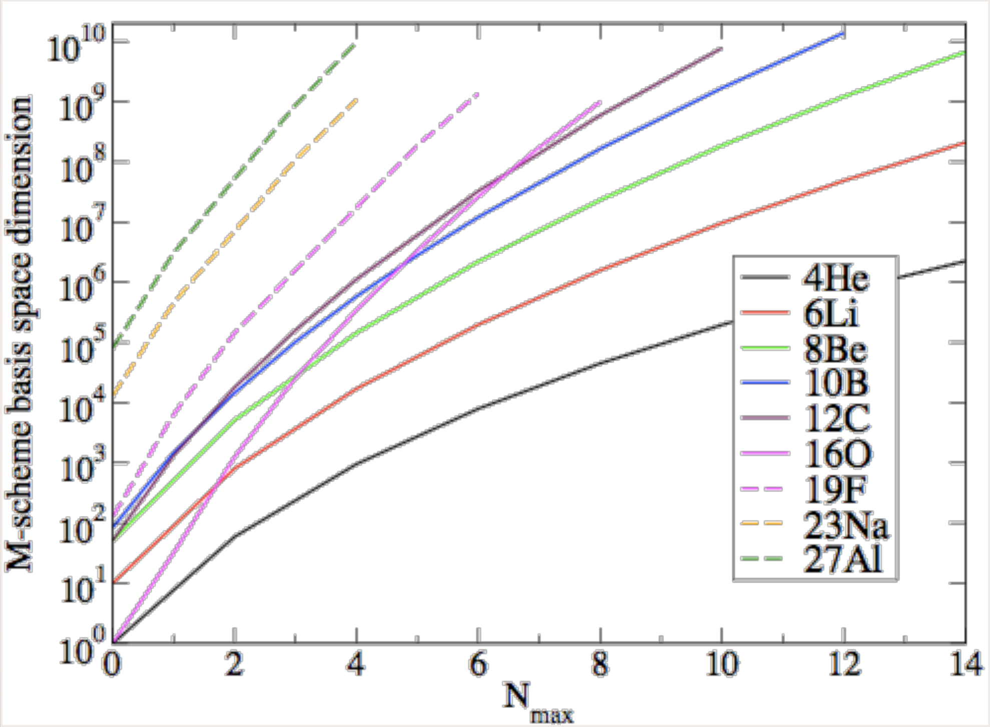
- Many-body HO Slater determinants

$$\left\langle \vec{r}_1\vec{\sigma}_1\vec{\tau}_1, \vec{r}_2\vec{\sigma}_2\vec{\tau}_2, \cdots, \vec{r}_A\vec{\sigma}_A\vec{\tau}_A \middle| a_l^+ \cdots a_j^+ a_i^+ \middle| 0 \right\rangle$$

$$= \frac{1}{\sqrt{A!}} \begin{vmatrix} \varphi_i(\vec{r}_1) & \varphi_i(\vec{r}_2) & \cdots & \varphi_i(\vec{r}_A) \\ \varphi_j(\vec{r}_1) & \varphi_j(\vec{r}_2) & & \varphi_j(\vec{r}_A) \\ & \vdots & \ddots & \vdots \\ \varphi_l(\vec{r}_1) & \varphi_l(\vec{r}_2) & \cdots & \varphi_l(\vec{r}_A) \end{vmatrix}$$

$$\varphi_{nljm_j\frac{1}{2}m_t}(\vec{r},\vec{\sigma},\vec{\tau})$$

$$= R_{nl}(r)\left[Y_l(\hat{r}) \otimes \chi^S_{\frac{1}{2}}(\vec{\sigma})\right]^j_{m_j} \chi^T_{\frac{1}{2}m_t}(\vec{\tau})$$



  - Antisymmetrization is trivial
  - Good M, M_T and parity quantum numbers, but not J and T
    - Huge number of basis states

TRIUMF

Second Quantization

- One of the most useful representations in many-body theory
  - $|0\rangle$: the state with no particles (the vacuum)
  - a_i^+ : creation operator, creates a fermion in the state i $\qquad a_i^+|0\rangle = |i\rangle, \quad a_i^+|i\rangle = 0$
  - a_i : annihilation operator, annihilates a fermion in the state i $\qquad a_i|i\rangle = |0\rangle, \quad a_i|0\rangle = 0$
  - Anticommutation relations:

$$\{a_i^+,\ a_j^+\} = \{a_i\,,\ a_j\} = 0, \qquad \{a_i^+,\ a_j\} = \{a_i\,,\ a_j^+\} = \delta_{ij}$$

Pauli principle in second quantization $\qquad a_i^+ a_j^+ = -a_j^+ a_i^+$

  - So that the Slater determinant can be written as:

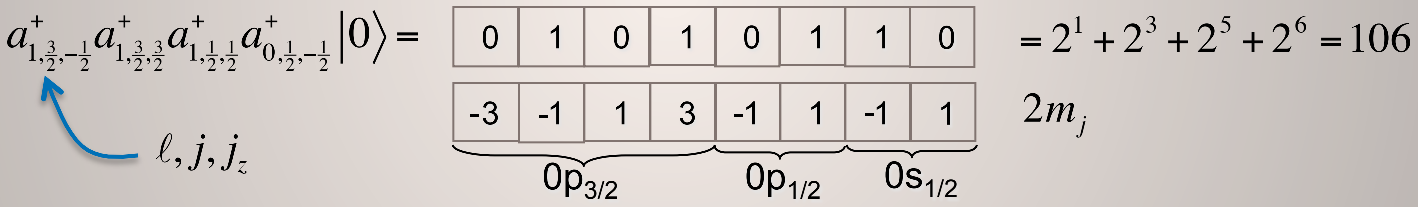
$$\phi_n^{(A)} = \frac{1}{\sqrt{A!}} \begin{vmatrix} \varphi_i(\vec{r}_1) & \varphi_i(\vec{r}_2) & \dots & \varphi_i(\vec{r}_A) \\ \varphi_j(\vec{r}_1) & \varphi_j(\vec{r}_2) & & \varphi_j(\vec{r}_A) \\ & \vdots & \ddots & \vdots \\ \varphi_l(\vec{r}_1) & \varphi_l(\vec{r}_2) & \dots & \varphi_l(\vec{r}_A) \end{vmatrix} = a_l^+ \dots a_j^+ a_i^+ |0\rangle,$$

$$l > \cdots > j > i$$

implicitly **assumes** we have **already** chosen the form of the **single-particle states**, (i = 1,2,3, ... A) as dictated by some mean-field potential

Basis states: occupation representation

- How are Slater determinants actually represented in a computer program?
  - We are dealing with fermions, so a single-particle state is either occupied or empty, which in computer language translates to either 1's or 0's
  - A very useful approach is a bit representation known as M-scheme
    - If the mean-field is spherically symmetric, the single-particle states will have good j, m_j



$$a^{+}_{1,\frac{3}{2},-\frac{1}{2}}a^{+}_{1,\frac{3}{2},\frac{3}{2}}a^{+}_{1,\frac{1}{2},\frac{1}{2}}a^{+}_{0,\frac{1}{2},-\frac{1}{2}}|0\rangle =$$

ℓ, j, j_z

0	1	0	1	0	1	1	0	$= 2^1 + 2^3 + 2^5 + 2^6 = 106$
-3	-1	1	3	-1	1	-1	1	$2m_j$
$0p_{3/2}$				$0p_{1/2}$		$0s_{1/2}$		

    - A single integer represents a complicated slater determinant
  - While the many-body states will have good M, they do not have good J. States of good J must be projected and will be a combination of Slater determinants. Same for T and M_T.

TRIUMF

Getting the eigenvalues and wave functions

- Setup Hamiltonian matrix $\langle \Phi_i | H | \Phi_j \rangle$ and diagonalize
- Lanczos algorithm
  - Bring matrix to tri-diagonal form ($\mathbf{v}_1$, $\mathbf{v}_2$ … orthonormal, H Hermitian)

$$\boxed{\begin{aligned} H\mathbf{v}_1 &= \alpha_1\mathbf{v}_1 + \beta_1\mathbf{v}_2 \\ H\mathbf{v}_2 &= \beta_1\mathbf{v}_1 + \alpha_2\mathbf{v}_2 + \beta_2\mathbf{v}_3 \\ H\mathbf{v}_3 &= \qquad\qquad \beta_2\mathbf{v}_2 + \alpha_3\mathbf{v}_3 + \beta_3\mathbf{v}_4 \\ H\mathbf{v}_4 &= \qquad\qquad\qquad\qquad \beta_3\mathbf{v}_3 + \alpha_4\mathbf{v}_4 + \beta_4\mathbf{v}_5 \end{aligned}}$$

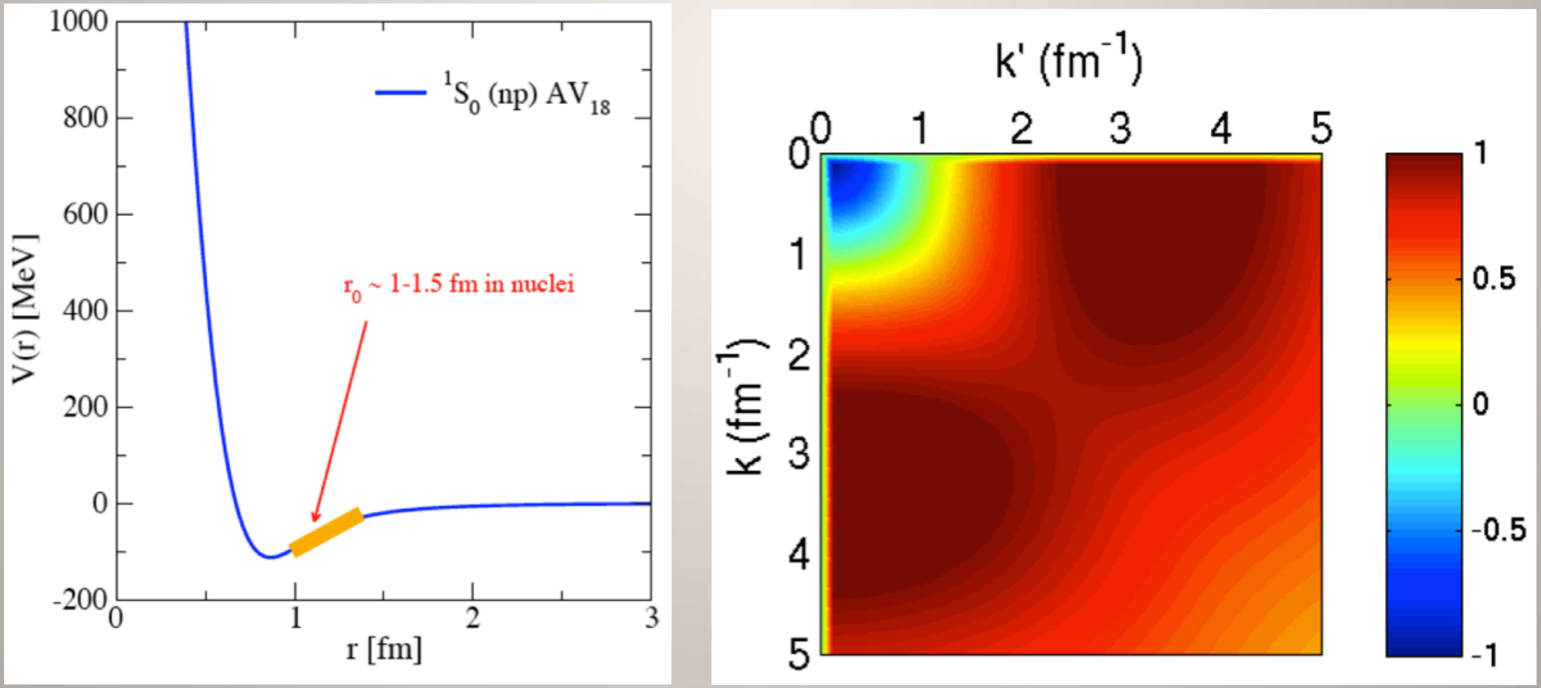
  - n^th^ iteration computes 2n^th^ moment
  - Eigenvalues converge to extreme (largest and smallest) values
  - ~ 100-200 iterations needed for 10 eigenvalues (even for 10^9 states)

- Typically we use M-scheme:
  - Total M_J, M_T=(Z-N)/2 and parity conserved

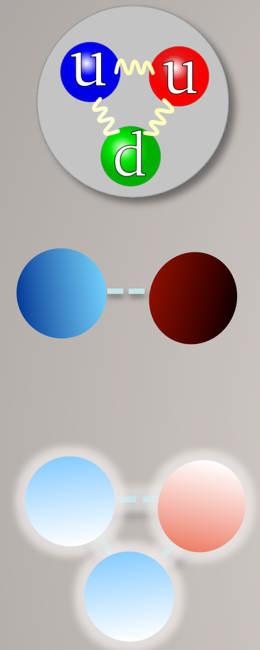
TRIUMF

Accurate NN potentials are hard to use

- Repulsive core of nuclear force introduces coupling to high momenta
  - Very large model spaces are required to reach convergent solution of the nuclear many-body problem



From QCD to nuclei



Low-energy QCD

↓

NN+3N interactions from chiral EFT

…or accurate meson-exchange potentials

↓

Unitary/similarity transformations

Identity or SRG or OLS or UCOM … Softens NN, induces 3N

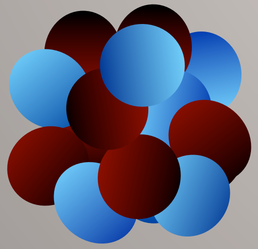
↓

$$H|\Psi\rangle = E|\Psi\rangle$$

Many-Body methods

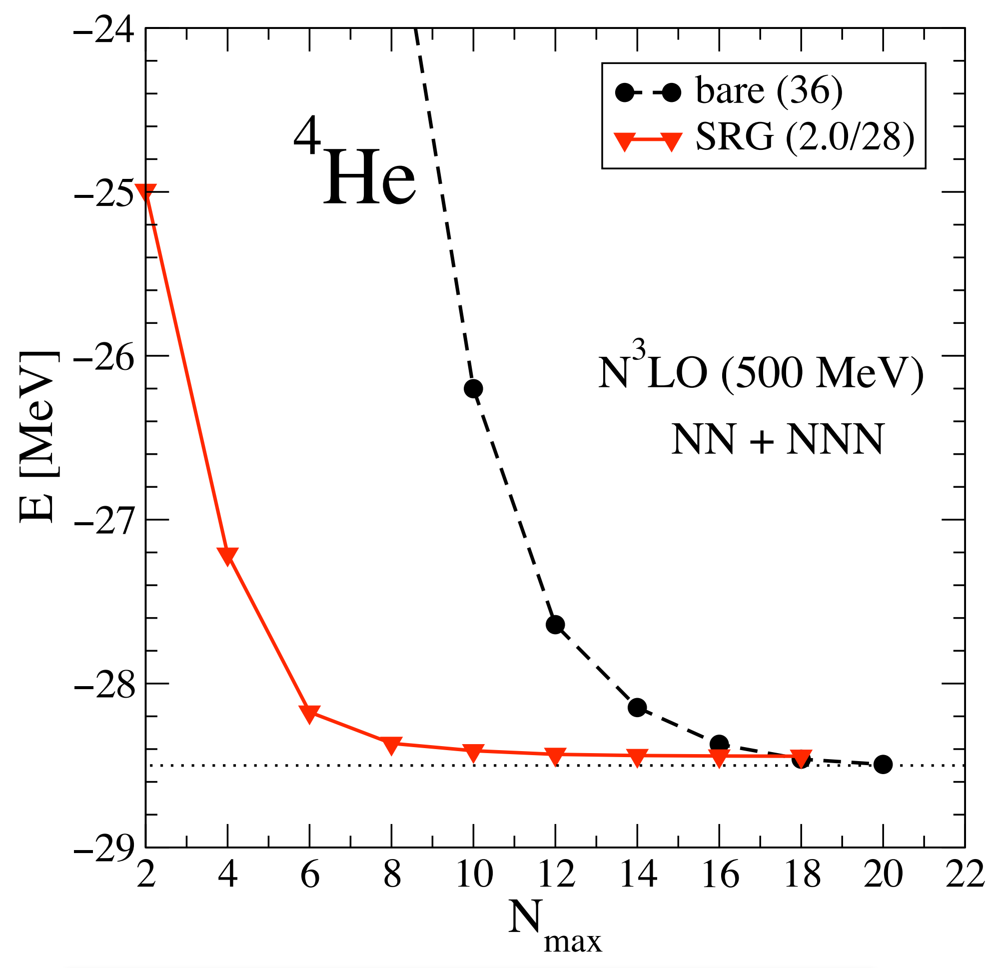
NCSM, NCSM/RGM, CCM, GFMC, HH, Nuclear Lattice EFT…

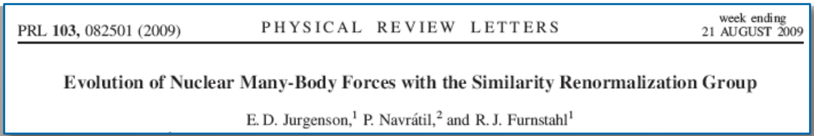
↓



Nuclear structure and reactions

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

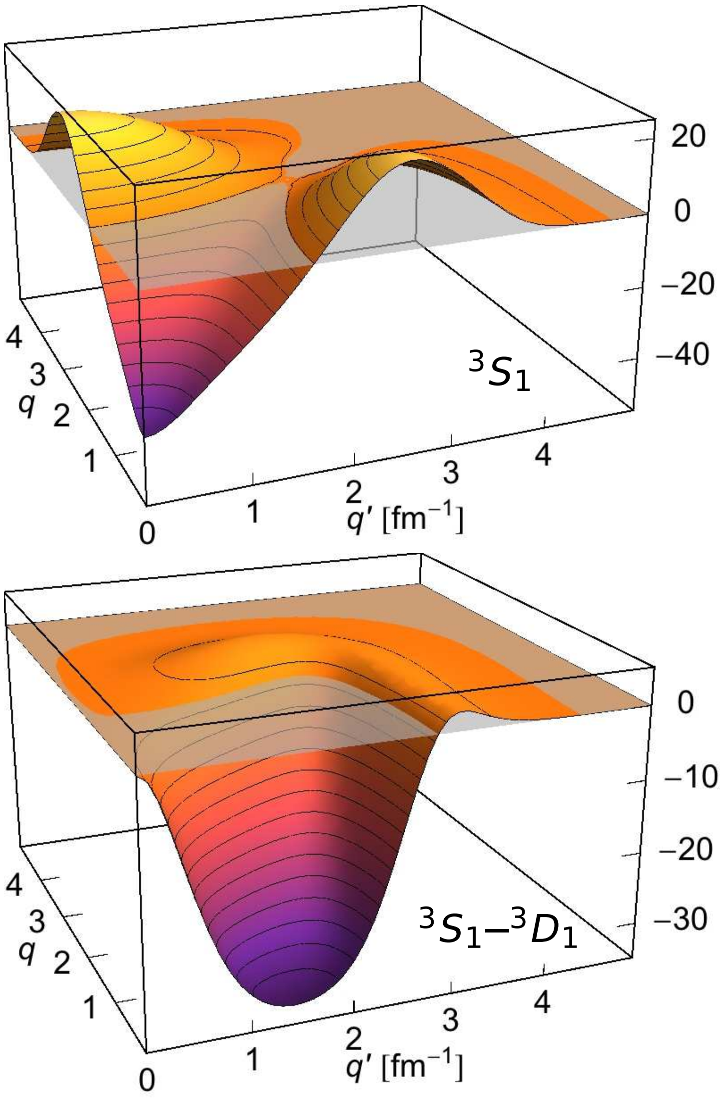
- Bare interaction (black line)
  - Strong short-range correlations
    - Large basis needed
- SRG evolved effective interaction (red line)
  - Unitary transformation

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

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

Why similarity renormalization?

momentum-space matrix elements

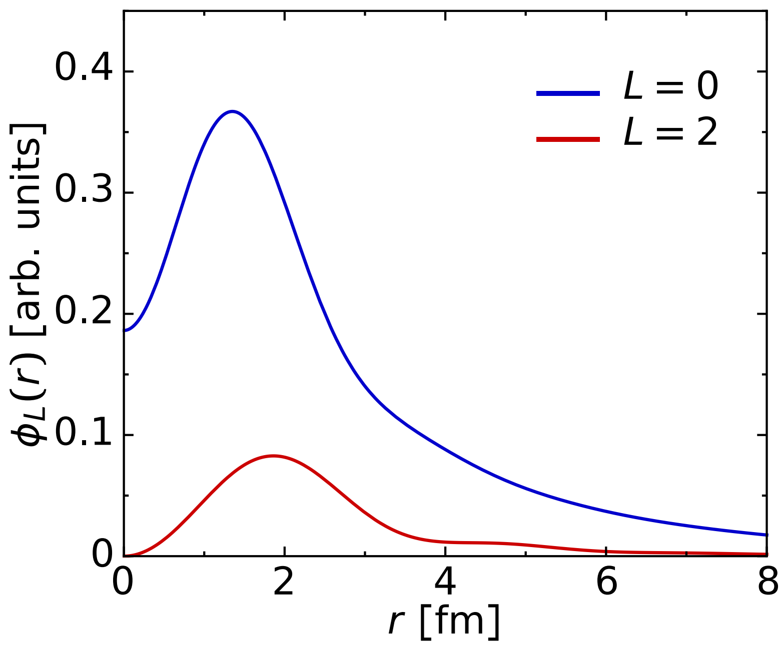


chiral N^{3}LO

Entem & Machleidt, 500 MeV

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

deuteron wave-function



Similarity Renormalization Group (SRG) evolution

- Continuous transformation driving Hamiltonian to band-diagonal form with respect to a chosen basis
- Unitary transformation $H_\alpha = U_\alpha H U_\alpha^+$ $\quad U_\alpha U_\alpha^+ = U_\alpha^+ U_\alpha = 1$

$$\frac{dH_\alpha}{d\alpha} = \frac{dU_\alpha}{d\alpha} H U_\alpha^+ + U_\alpha H \frac{dU_\alpha^+}{d\alpha} = \frac{dU_\alpha}{d\alpha} U_\alpha^+ U_\alpha H U_\alpha^+ + U_\alpha H U_\alpha^+ U_\alpha \frac{dU_\alpha^+}{d\alpha}$$

$$= \frac{dU_\alpha}{d\alpha} U_\alpha^+ H_\alpha + H_\alpha U_\alpha \frac{dU_\alpha^+}{d\alpha} = \left[\eta_\alpha, H_\alpha\right]$$

$$\eta_\alpha \equiv \frac{dU_\alpha}{d\alpha} U_\alpha^+ = -\eta_\alpha^+$$

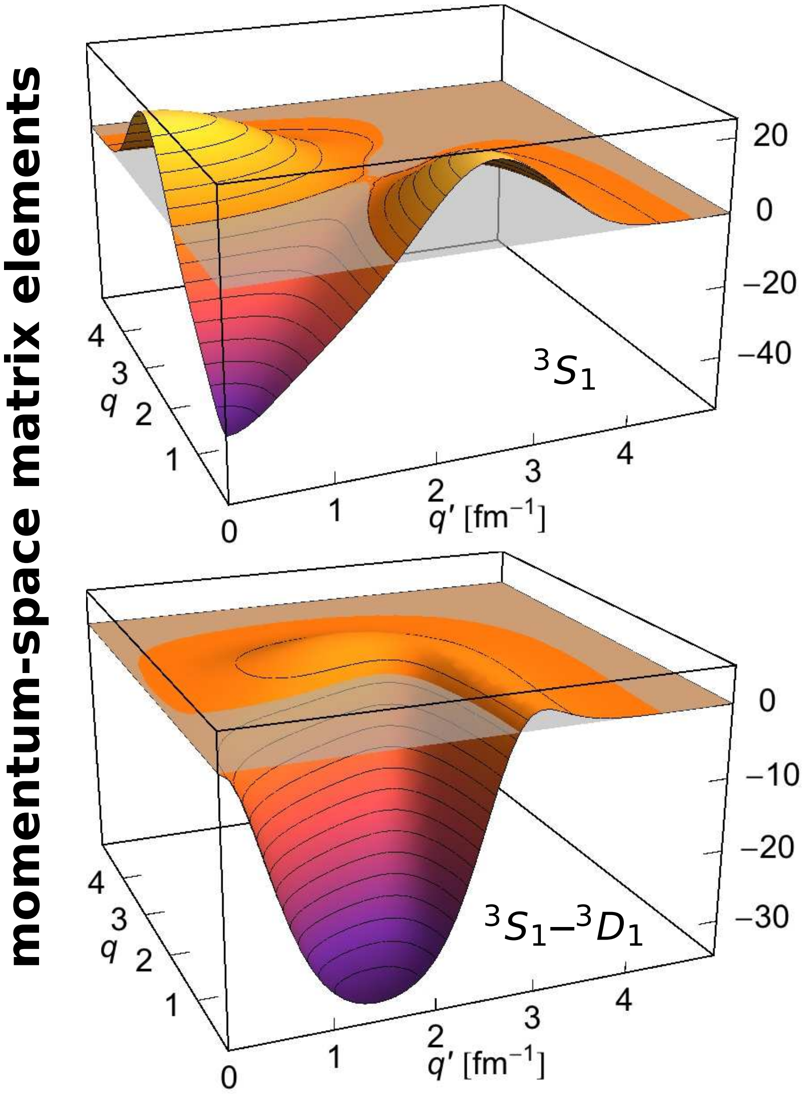
anti-Hermitian generator

- Setting $\eta_\alpha = \left[G_\alpha, H_\alpha\right]$ with Hermitian G_α

$$\frac{dH_\alpha}{d\alpha} = \left[\left[G_\alpha, H_\alpha\right], H_\alpha\right]$$

- Customary choice in nuclear physics $G_\alpha = T$ …kinetic energy operator
  - band-diagonal in momentum space plane-wave basis
- Initial condition $H_{\alpha=0} = H_{\lambda=\infty} = H$ $\quad \lambda^2 = 1/\sqrt{\alpha}$

SRG evolution in two-nucleon space

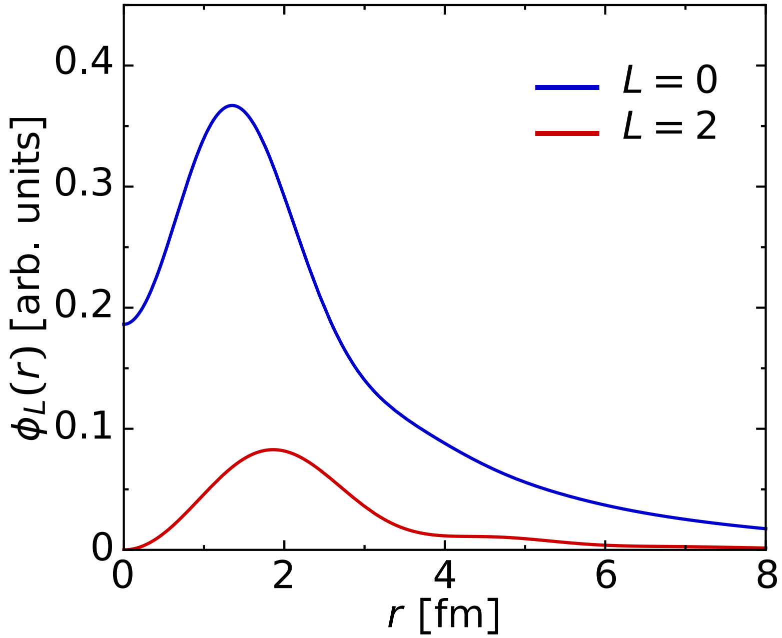


$\alpha = 0.000\,\mathrm{fm}^4$

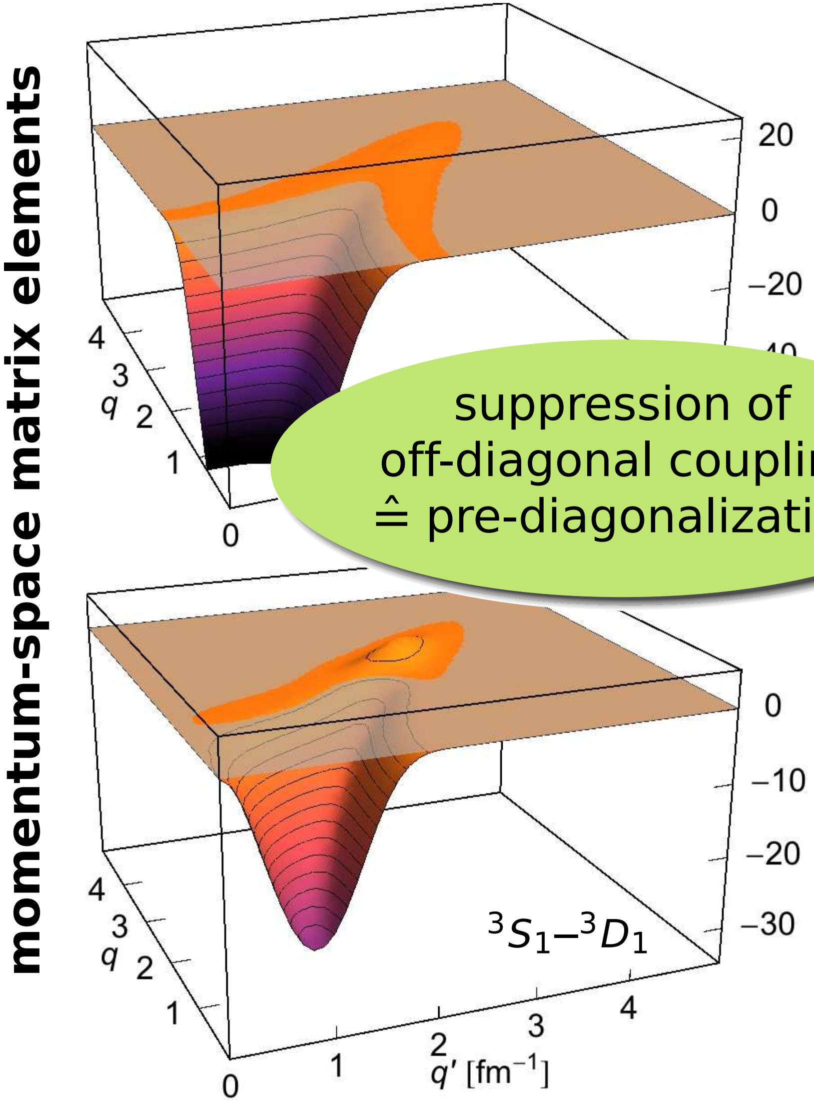
$\Lambda = \infty\,\mathrm{fm}^{-1}$

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

deuteron wave-function



SRG evolution in two-nucleon space



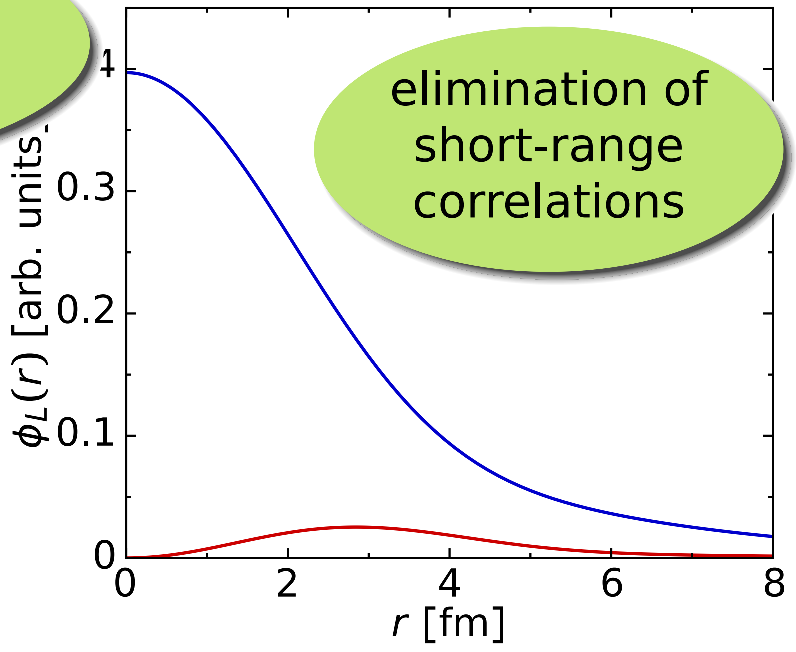
suppression of
off-diagonal coupling
≙ pre-diagonalization

$\alpha = 0.320\,\mathrm{fm}^4$

$\Lambda = 1.33\,\mathrm{fm}^{-1}$

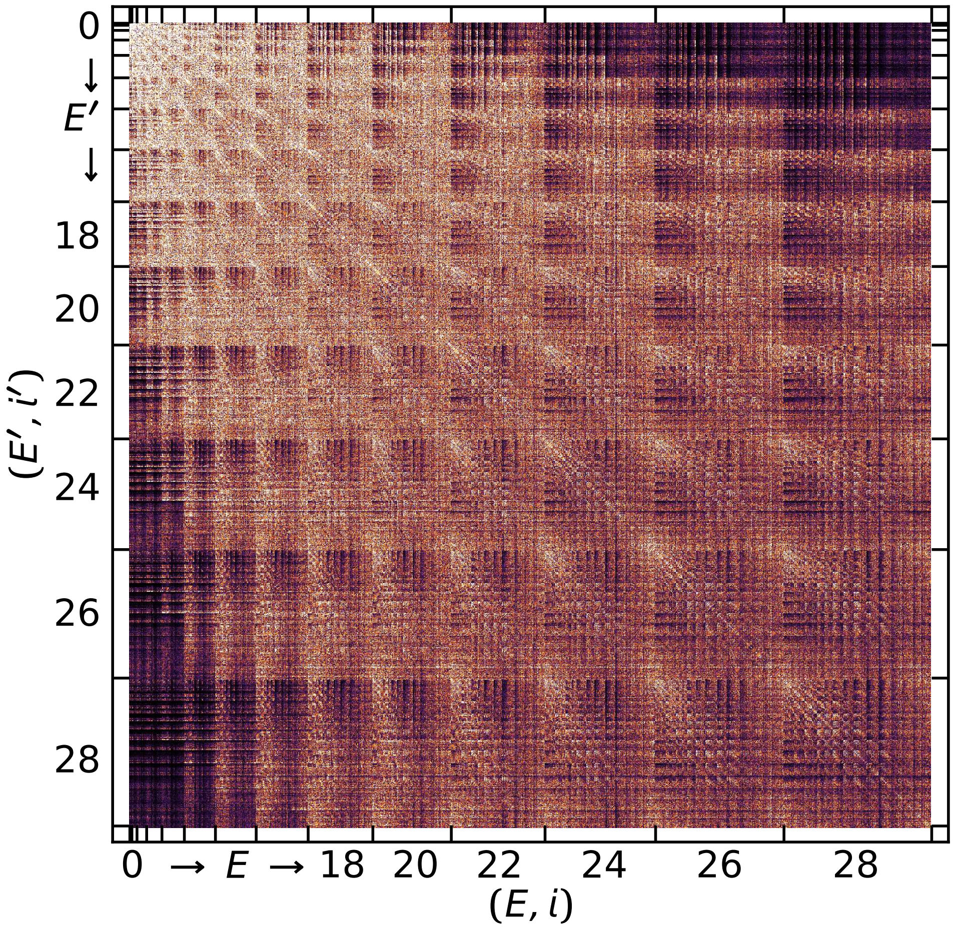
$J^\pi = 1^+, T = 0$

deuteron wave-function



elimination of
short-range
correlations

SRG evolution in three-nucleon space

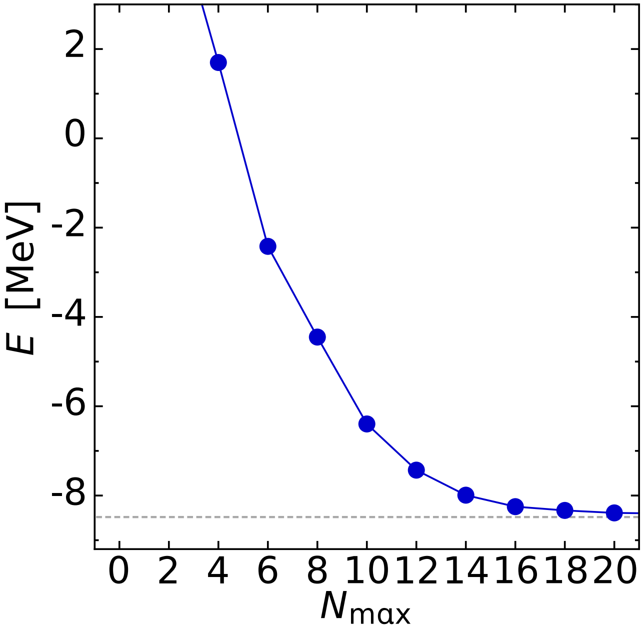


3B-Jacobi HO matrix elements

$\alpha = 0.000\,\mathrm{fm}^4$

$\Lambda = \infty\,\mathrm{fm}^{-1}$

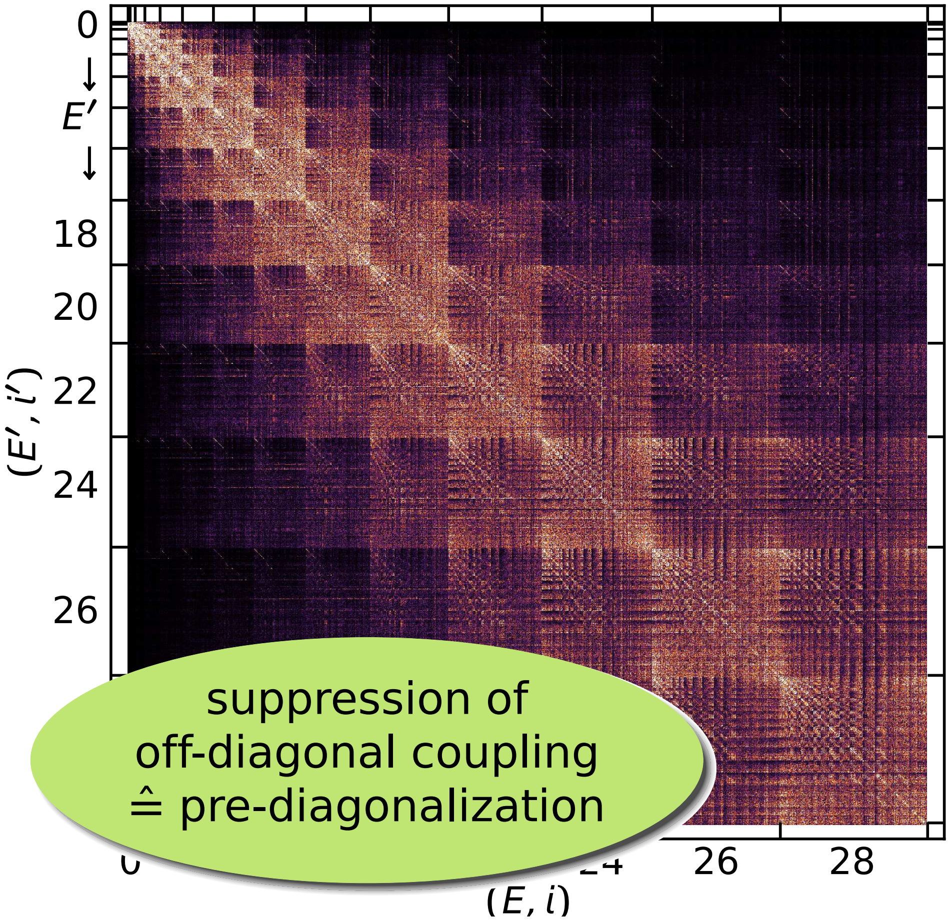
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\mathrm{MeV}$



NCSM ground state ^{3}H

SRG evolution in three-nucleon space

3B-Jacobi HO matrix elements



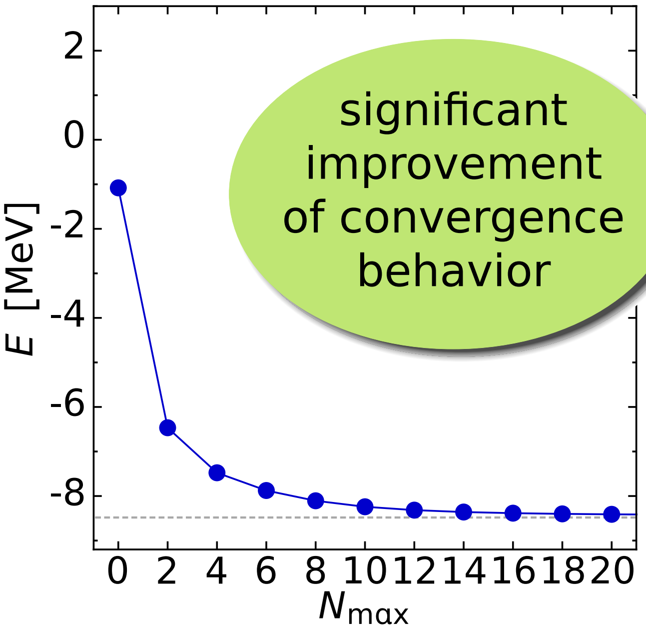
suppression of
off-diagonal coupling
≙ pre-diagonalization

$\alpha = 0.320\,\mathrm{fm}^4$

$\Lambda = 1.33\,\mathrm{fm}^{-1}$

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\mathrm{MeV}$

NCSM ground state ^{3}H



significant
improvement
of convergence
behavior

TRIUMF

SRG evolution for *A*-nucleon system

- Evolution induces many-nucleon terms (up to *A*)

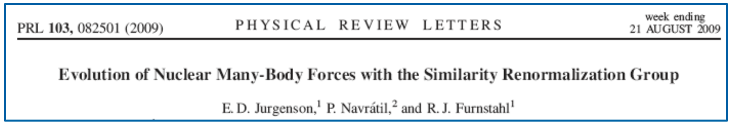
$$\tilde{H}_\alpha = \tilde{H}_\alpha^{[1]} + \tilde{H}_\alpha^{[2]} + \tilde{H}_\alpha^{[3]} + \tilde{H}_\alpha^{[4]} + \ldots + \tilde{H}_\alpha^{[A]}$$

- In actual calculations so far only terms up to $\tilde{H}_\alpha^{[3]}$ kept

- Three types of SRG-evolved Hamiltonians used
  - **NN only**: Start with initial T+V_{NN} and keep $\tilde{H}_\alpha^{[1]} + \tilde{H}_\alpha^{[2]}$
  - **NN+3N-induced**: Start with initial T+V_{NN} and keep $\tilde{H}_\alpha^{[1]} + \tilde{H}_\alpha^{[2]} + \tilde{H}_\alpha^{[3]}$
  - **NN+3N-full**: Start with initial T+V_{NN}+V_{NNN} and keep $\tilde{H}_\alpha^{[1]} + \tilde{H}_\alpha^{[2]} + \tilde{H}_\alpha^{[3]}$

α variation (Λ variation) provides a diagnostic tool
to asses the contribution of omitted many-body terms,
tests the unitarity of the SRG transformation

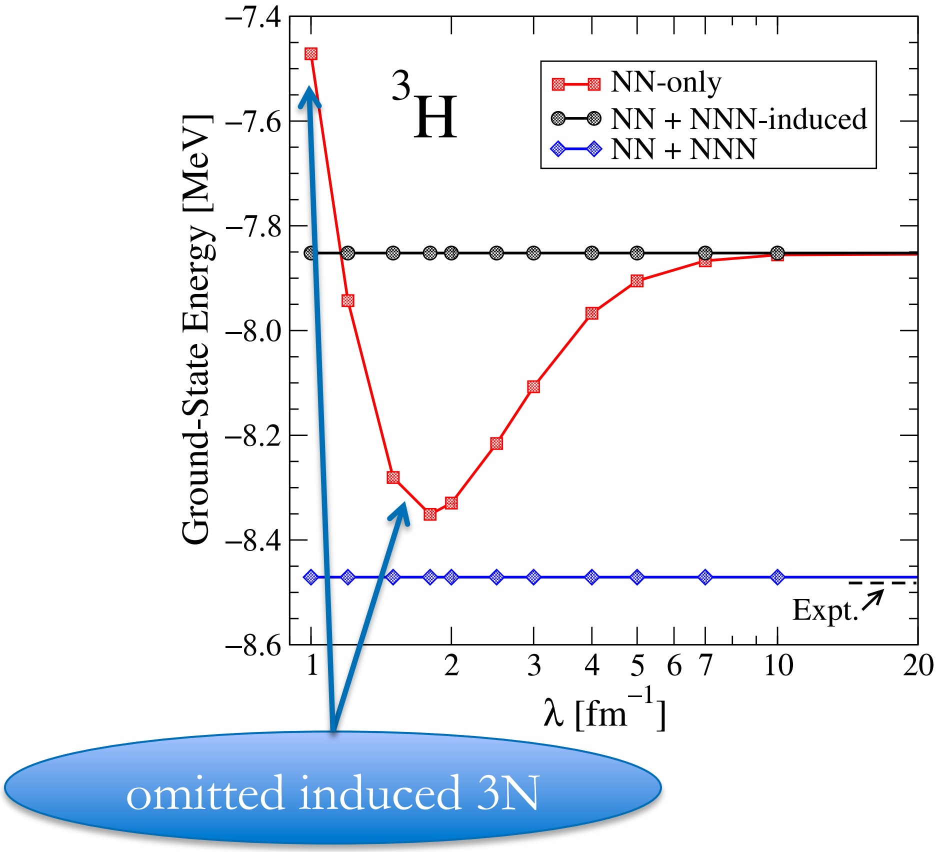
SRG evolution: ^{3}H and ^{4}He



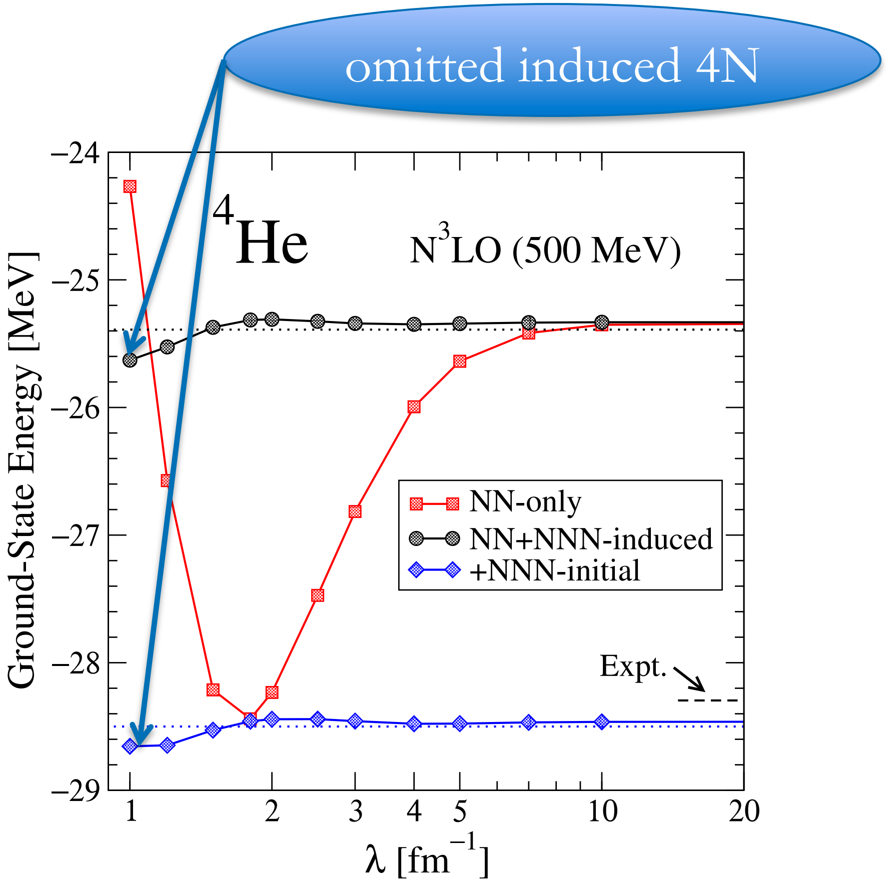
PRL **103,** 082501 (2009) PHYSICAL REVIEW LETTERS week ending 21 AUGUST 2009

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

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



omitted induced 3N

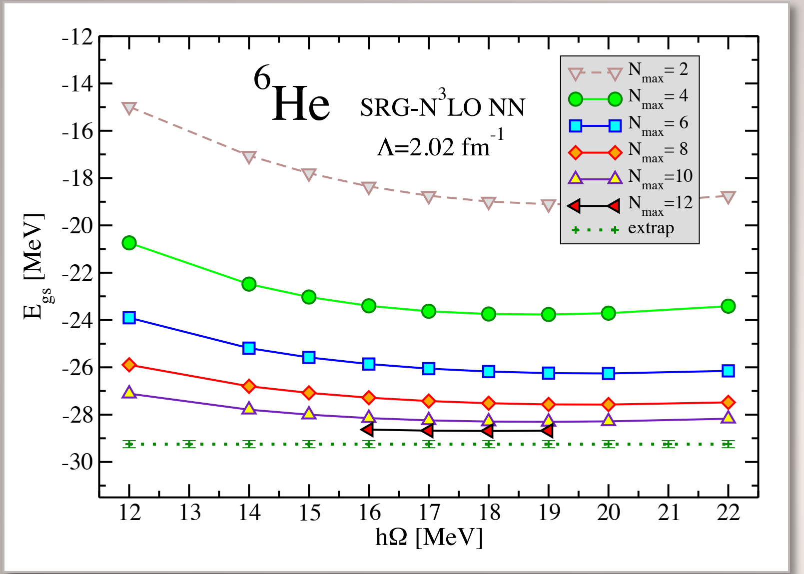


omitted induced 4N

Ab initio calculations (NCSM, in this case)
used also for SRG evolution of NNN force (in HO basis)

TRIUMF

NCSM calculations of ^{6}He g.s. energy



Dependence on:

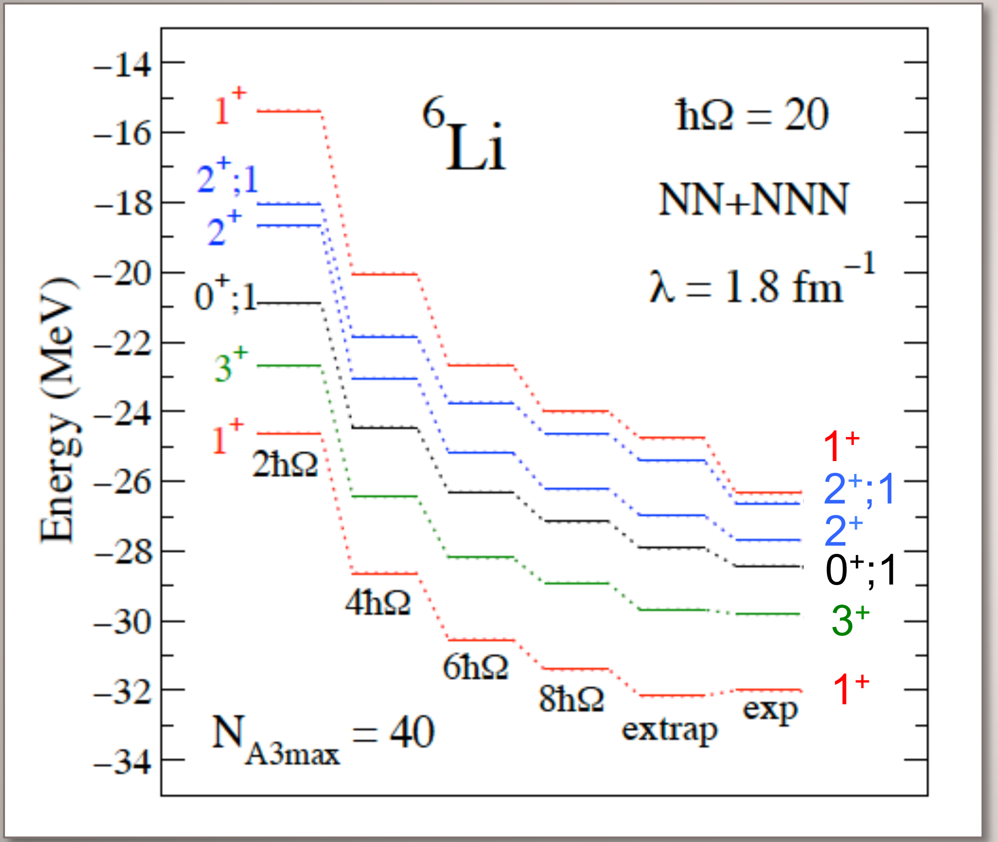
Basis size – N_{max}

HO frequency – hΩ

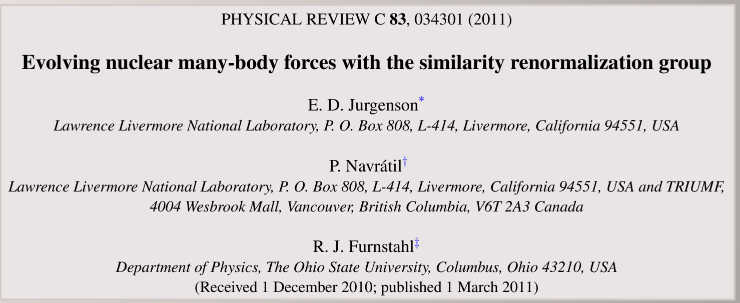
- Soft SRG evolved NN potential
- ✓ N_{max} convergence OK
- ✓ Extrapolation feasible

$E_{g.s.}$ [MeV]	^{4}He	^{6}He
NCSM N_{max}=12	-28.05	-28.63
NCSM extrap.	-28.22(1)	-29.25(15)
Expt.	-28.30	-29.27

^{6}Li from chiral EFT interactions: Ground-state & excitation energies



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



PHYSICAL REVIEW C **83**, 034301 (2011)

Evolving nuclear many-body forces with the similarity renormalization group

E. D. Jurgenson[*]
Lawrence Livermore National Laboratory, P. O. Box 808, L-414, Livermore, California 94551, USA

P. Navrátil[†]
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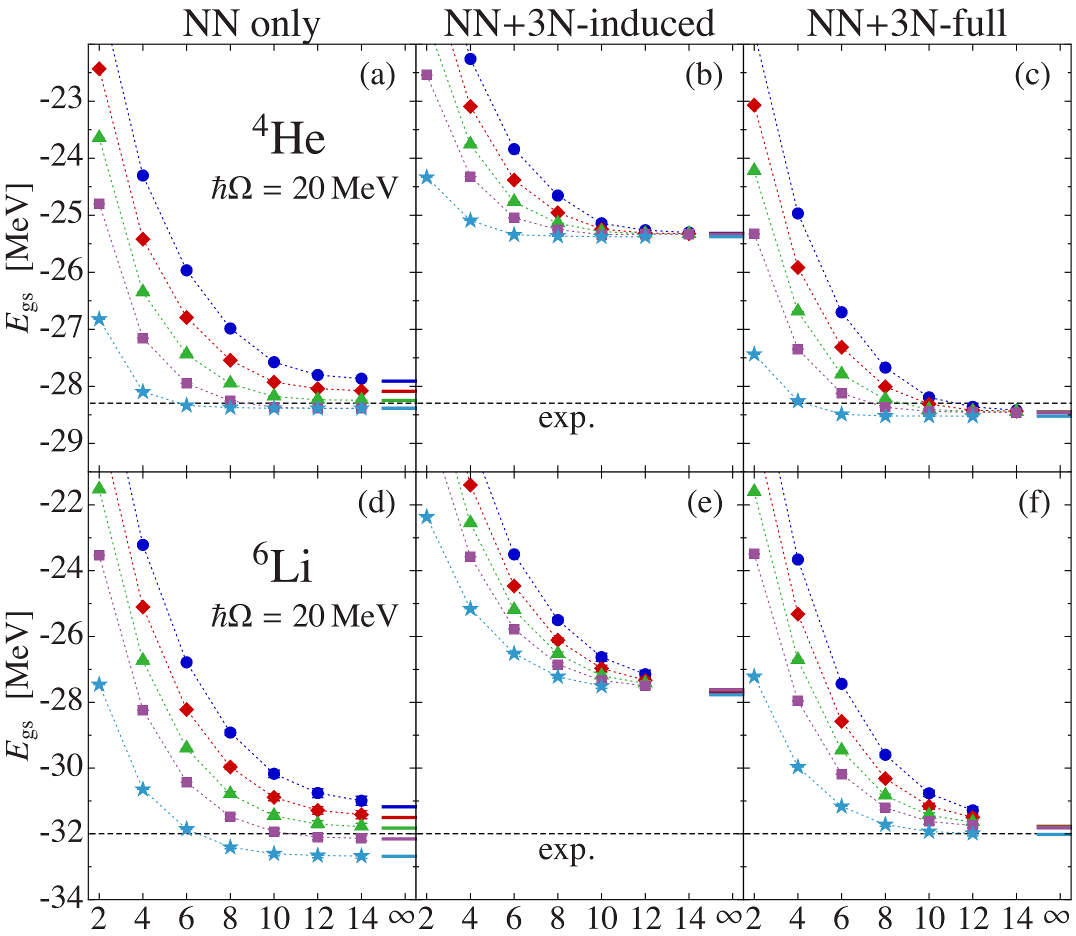
Department of Physics, The Ohio State University, Columbus, Ohio 43210, USA
(Received 1 December 2010; published 1 March 2011)

SRG with 2- plus 3-body: Good convergence, extrapolation to infinite basis space possible

Light nuclei with SRG evolved interactions



- Fast convergence
- Significant 3N induced interaction
- No 4N induced interaction


PRL **107,** 072501 (2011) PHYSICAL REVIEW LETTERS week ending 12 AUGUST 2011

Similarity-Transformed Chiral *NN* + 3*N* Interactions for the *Ab Initio* Description of ^{12}C and ^{16}O

Robert Roth,[1,*] Joachim Langhammer,[1] Angelo Calci,[1] Sven Binder,[1] and Petr Navrátil[2,3]

● $\alpha = 0.04\,\mathrm{fm}^4$ $\Lambda = 2.24\,\mathrm{fm}^{-1}$

◆ $\alpha = 0.05\,\mathrm{fm}^4$ $\Lambda = 2.11\,\mathrm{fm}^{-1}$

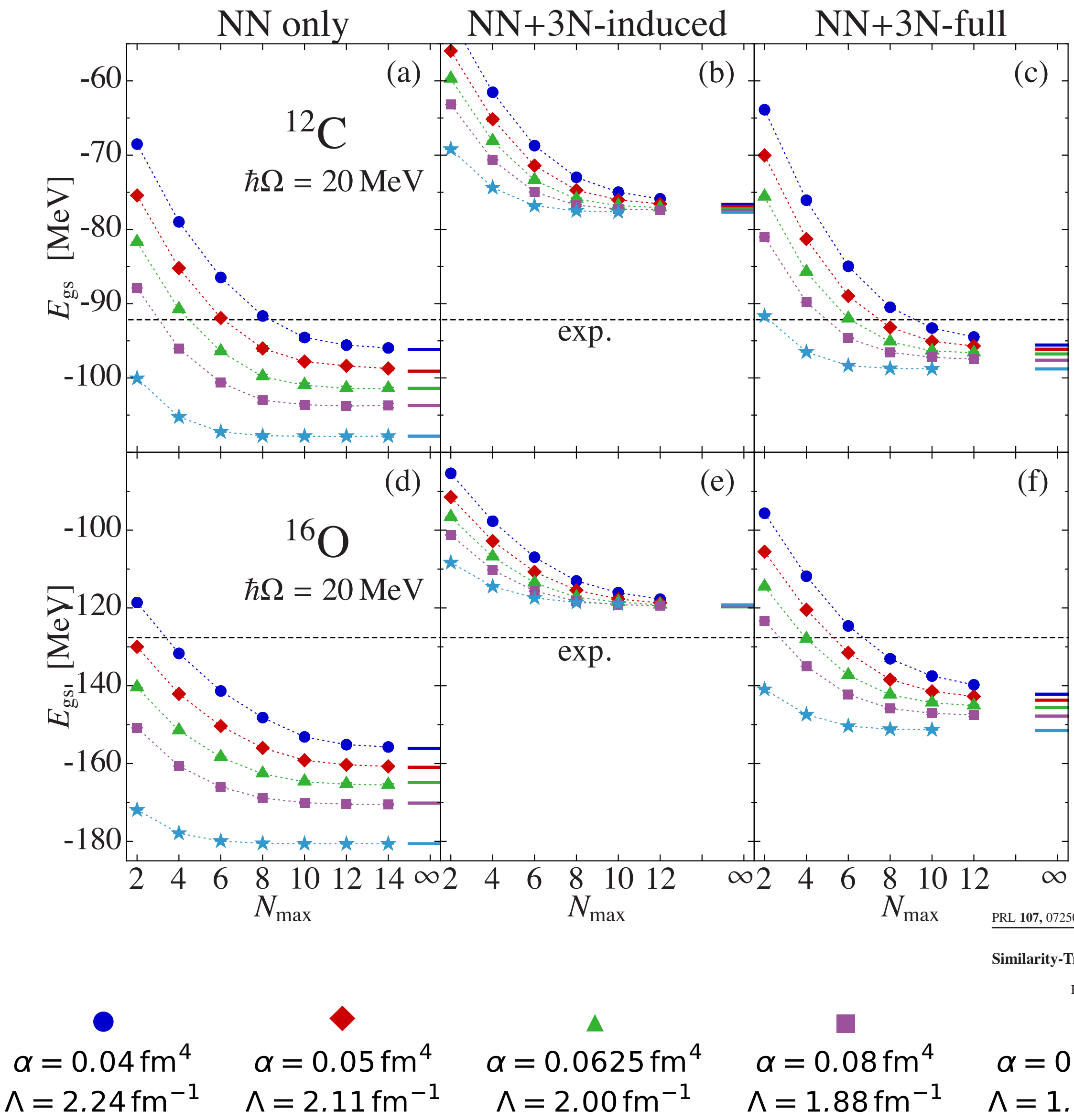
▲ $\alpha = 0.0625\,\mathrm{fm}^4$ $\Lambda = 2.00\,\mathrm{fm}^{-1}$

■ $\alpha = 0.08\,\mathrm{fm}^4$ $\Lambda = 1.88\,\mathrm{fm}^{-1}$

★ $\alpha = 0.16\,\mathrm{fm}^4$ $\Lambda = 1.58\,\mathrm{fm}^{-1}$

TRIUMF

Heavier p-shell nuclei with SRG evolved interactions



- Fast convergence
- Significant 3N induced interaction
- 4N induced interaction when chiral 3N included

4N induced suppressed by lowering the chiral 3N cutoff to 400 MeV

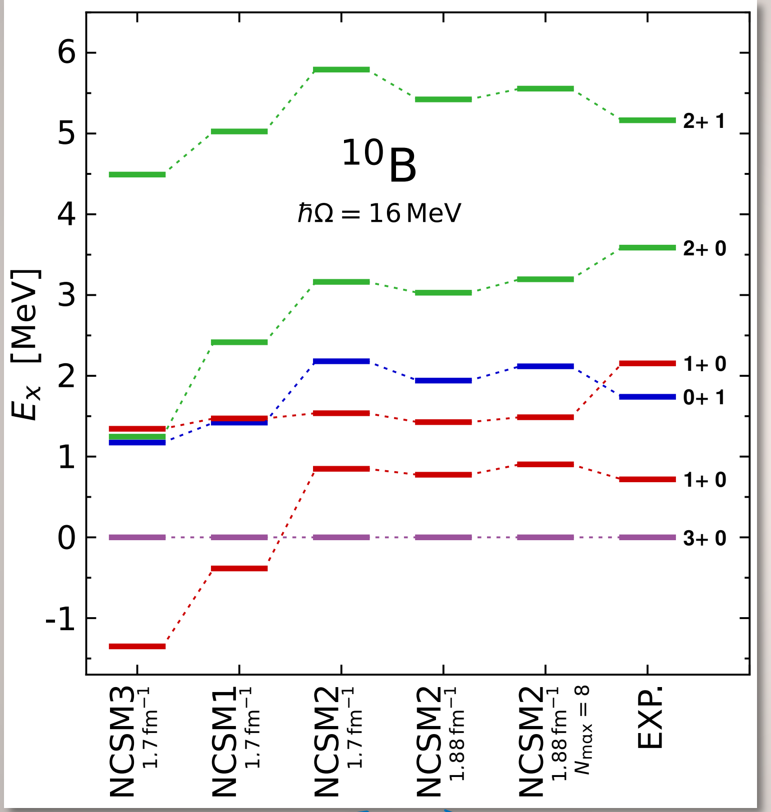
PRL **107,** 072501 (2011) PHYSICAL REVIEW LETTERS week ending 12 AUGUST 2011

Similarity-Transformed Chiral *NN* + 3*N* Interactions for the *Ab Initio* Description of ^{12}C and ^{16}O

Robert Roth,[1,*] Joachim Langhammer,[1] Angelo Calci,[1] Sven Binder,[1] and Petr Navrátil[2,3]

TRIUMF

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



PHYSICAL REVIEW C **86**, 054609 (2012)

Microscopic two-nucleon overlaps and knockout reactions from ^{12}C

E. C. Simpson,[1] P. Navrátil,[2] R. Roth,[3] and J. A. Tostevin[1,4]

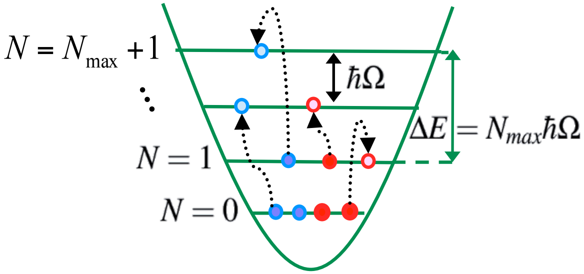
chiral NN

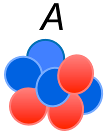
chiral NN+3N(400)

chiral NN+3N(500)

No-core shell model

- No-core shell model (NCSM)
  - *A*-nucleon wave function expansion in the harmonic-oscillator (HO) basis
  - short- and medium range correlations
  - Bound-states, narrow resonances





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

$$\Psi^{(A)} = \sum_\lambda c_\lambda \left|^{(A)} \, , \lambda\right\rangle$$

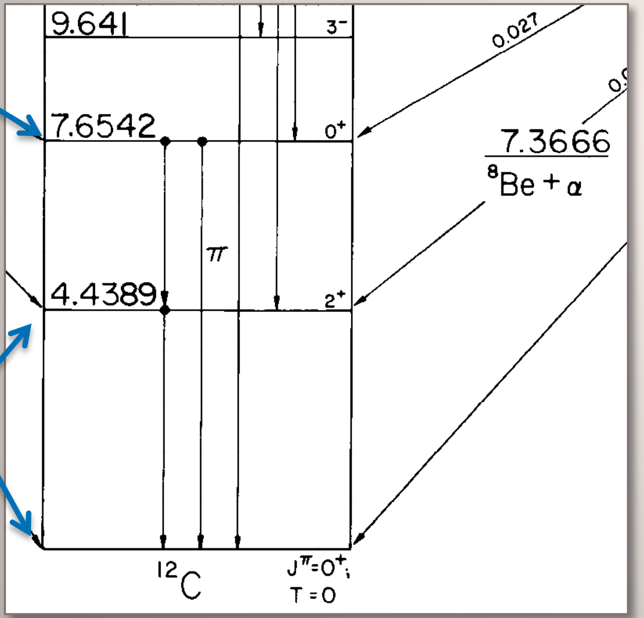
Unknowns

Light & medium mass nuclei from first principles

- Nuclear **structure** and **reaction** theory for light nuclei cannot be uncoupled
  - Well-bound nuclei, e.g. ^{12}C, have low-lying **cluster-dominated resonances**
  - Bound states of exotic nuclei, e.g. ^{11}Be, manifest **many-nucleon correlations**

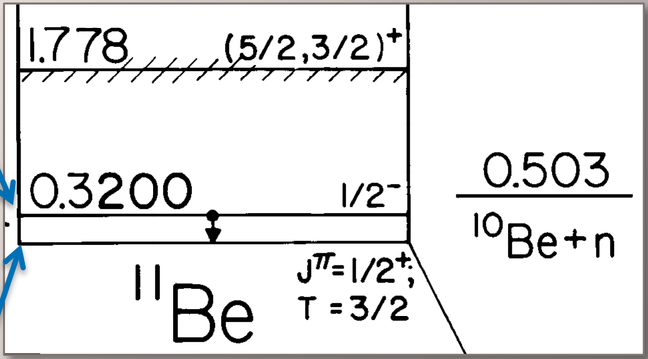
Hoyle state: α-cluster resonance with *p*-shell components

p-shell states

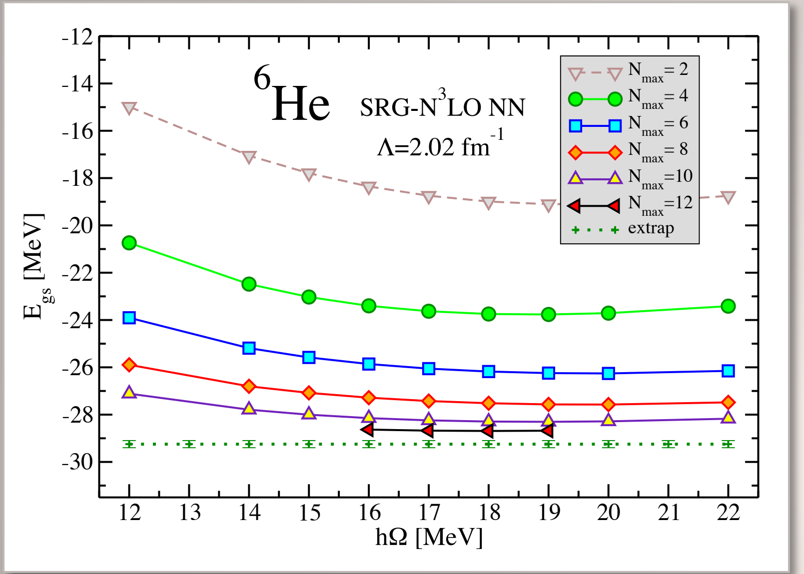


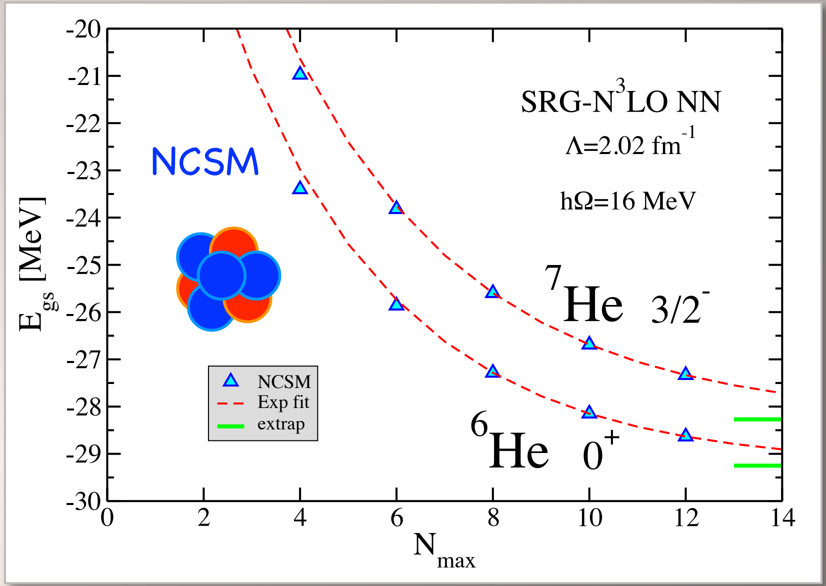
p-shell state with extended tail

^{10}Be$_{gs}$ + (*l=0*) *n* with significant ^{10}Be* components



NCSM calculations of ^{6}He and ^{7}He g.s. energies

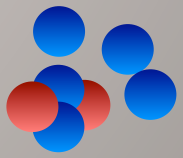




$E_{g.s.}$ [MeV]	^{4}He	^{6}He	^{7}He
NCSM N_{max}=12	-28.05	-28.63	-27.33
NCSM extrap.	-28.22(1)	-29.25(15)	-28.27(25)
Expt.	-28.30	-29.27	-28.84

- Soft SRG evolved NN potential
- ✓ N_{max} convergence OK
- ✓ Extrapolation feasible

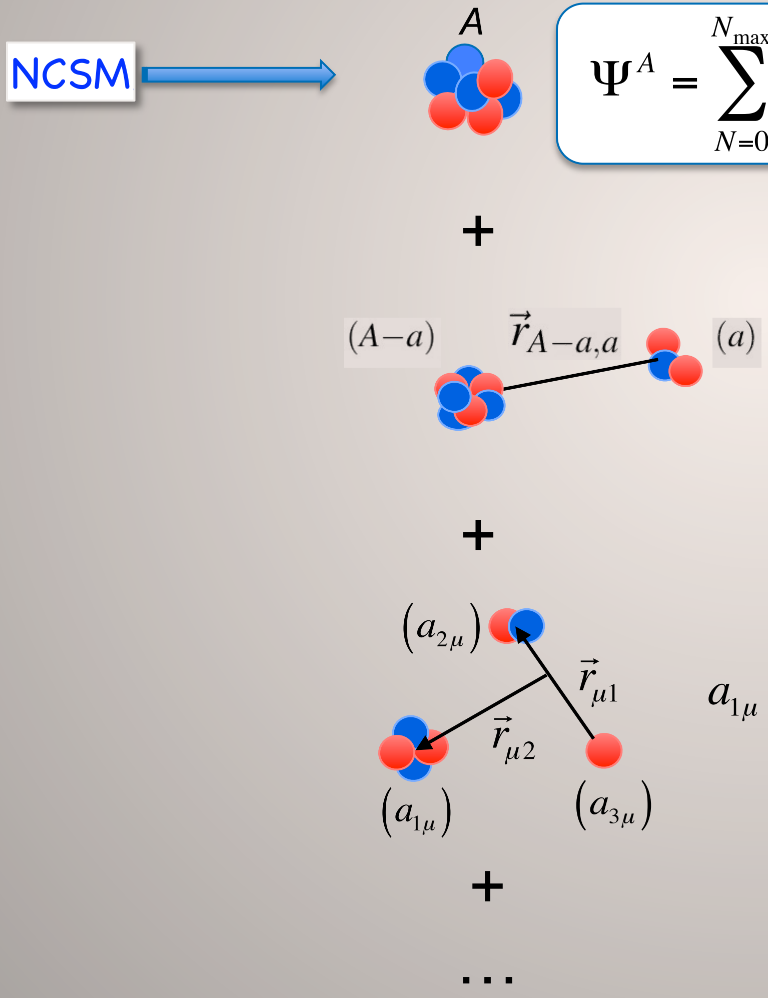
- ^{7}He unbound
  - Expt. E_{th}=+0.430(3) MeV: NCSM E_{th}≈ +1 MeV
  - Expt. width 0.182(5) MeV: **NCSM no information about the width**



^{7}He unbound

Extending no-core shell model beyond bound states

Include more many nucleon correlations…



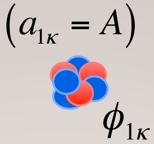
$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

…using the Resonating Group Method (RGM) ideas

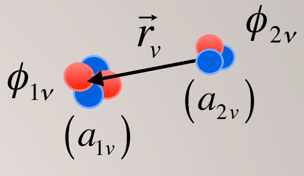
$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

Trial function: generalized cluster wave function

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



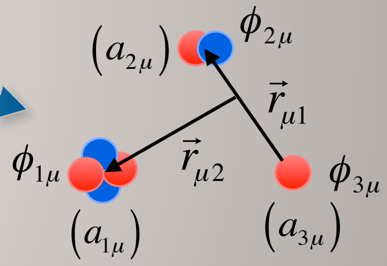
$$+ \sum_{\nu} \hat{A}_{\nu} \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right) \phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_{\nu}(\vec{r}_{\nu})$$



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

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

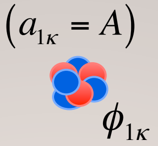
$$+ \cdots$$



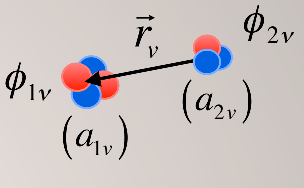
$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

Trial function: generalized cluster wave function

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



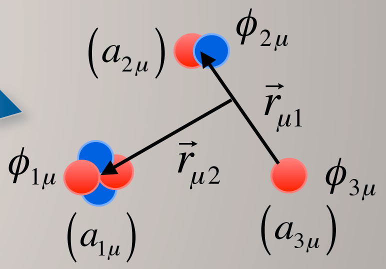
$$+\sum_{\nu} \hat{A}_{\nu} \boxed{\phi_{1\nu}}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\boxed{\phi_{2\nu}}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_{\nu}(\vec{r}_{\nu})$$



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

$$+\sum_{\mu} \hat{A}_{\mu} \boxed{\phi_{1\mu}}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\boxed{\phi_{2\mu}}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\boxed{\phi_{3\mu}}\left(\left\{\vec{\xi}_{3\mu}\right\}\right) G_{\mu}(\vec{r}_{\mu1}, \vec{r}_{\mu2})$$

$$+ \cdots$$

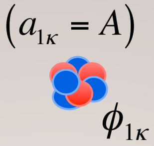


$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

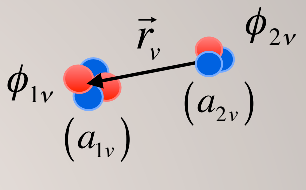
- ϕ : antisymmetric cluster wave functions
  - {ξ}: Translationally invariant internal coordinates (Jacobi relative coordinates)
  - These are known, they are an input

Trial function: generalized cluster wave function

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



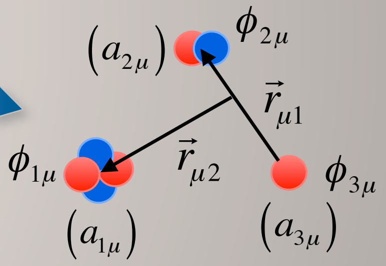
$$+ \sum_{\nu} \boxed{\hat{A}_{\nu}} \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right) \phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_{\nu}(\vec{r}_{\nu})$$



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

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

$$+ \cdots$$



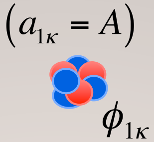
$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

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

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

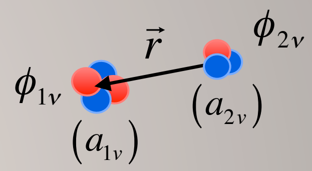
Trial function: generalized cluster wave function

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



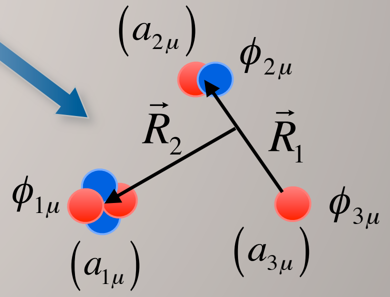
$$+\sum_{\nu} \int \boxed{g_\nu(\vec{r}\,)}\, \hat{A}_\nu \left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r} - \vec{r}_\nu)\right] d\vec{r}$$

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



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

$$+ \cdots$$

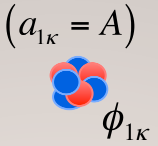


$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$

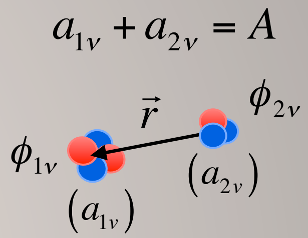
- $\boldsymbol{c}$, $\boldsymbol{g}$ and $\boldsymbol{G}$: discrete and continuous linear variational amplitudes
  - Unknowns to be determined

Trial function: generalized cluster wave function

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

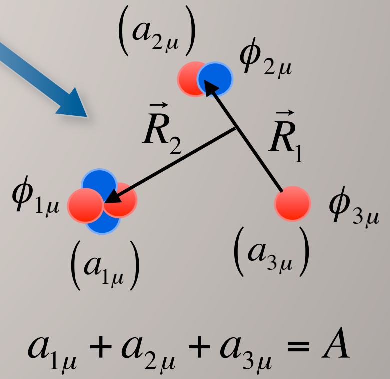


$$+\sum_{\nu} \int g_\nu(\vec{r}\,)\ \hat{A}_\nu \boxed{\left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r} - \vec{r}_\nu)\right]} d\vec{r}$$



$$+\sum_{\mu} \iint G_\mu(\vec{R}_1,\vec{R}_2)\ \hat{A}_\mu \boxed{\left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)\delta(\vec{R}_1 - \vec{R}_{\mu1})\delta(\vec{R}_2 - \vec{R}_{\mu2})\right]} d\vec{R}_1 d\vec{R}_2$$

$$+\ \cdots$$



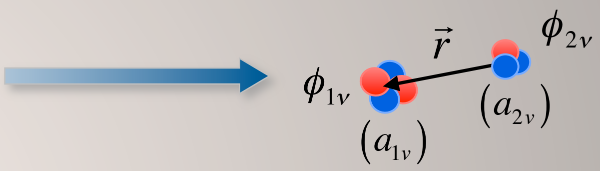
- Discrete and continuous set of basis functions
  - Non-orthogonal
  - Over-complete

Binary cluster wave function

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

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

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

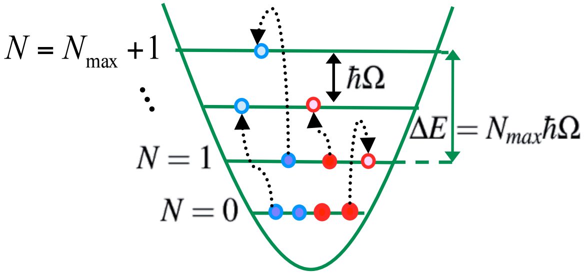


$$\cancel{+ \sum_{\mu} \iint G_{\mu}(\vec{R}_1,\vec{R}_2)\ \hat{A}_{\mu}\left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)\delta(\vec{R}_1-\vec{R}_{\mu 1})\delta(\vec{R}_2-\vec{R}_{\mu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

$$+ \cdots$$

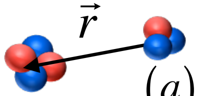
- In practice: function space limited by using relatively simple forms of Ψ chosen according to physical intuition and energetical arguments
  - Most common: expansion over binary-cluster basis

No-core shell model with RGM



- No-core shell model (NCSM)
  - *A*-nucleon wave function expansion in the harmonic-oscillator (HO) basis
  - short- and medium range correlations
  - Bound-states, narrow resonances

- NCSM with Resonating Group Method (NCSM/RGM)
  - cluster expansion
  - proper asymptotic behavior
  - long-range correlations



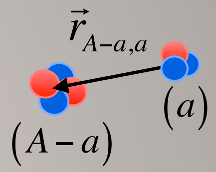
$$\Psi^{(A)} = \sum_{\nu} \int d\vec{r}\; \gamma_{\nu}(\vec{r}\,)\; \hat{A}_{\nu} \left| \underset{(A-a)}{} \;\; \overset{\vec{r}}{} \;\; \underset{(a)}{} \,, \nu \right\rangle$$

Unknowns

Binary cluster Resonating Group Method

- Working in partial waves ($\nu \equiv \left\{A-a\ \alpha_1 I_1^{\pi_1} T_1; a\ \alpha_2 I_2^{\pi_2} T_2; s\ell\right\}$)

$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \hat{A}_\nu \left[\left(\underbrace{\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle}_{\text{Target}}\underbrace{\left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle}_{\text{Projectile}}\right)^{(sT)} Y_\ell(\hat{r}_{A-a,a})\right]^{(J^\pi T)} \frac{g_\nu^{J^\pi T}(r_{A-a,a})}{r_{A-a,a}}$$



- Introduce a dummy variable $\vec{r}$ with the help of the delta function

$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \int \frac{g_\nu^{J^\pi T}(r)}{r} \hat{A}_\nu \left[\left(\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle\left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle\right)^{(sT)} Y_\ell(\hat{r})\right]^{(J^\pi T)} \delta(\vec{r}-\vec{r}_{A-a,a})\ r^2 dr\, d\hat{r}$$

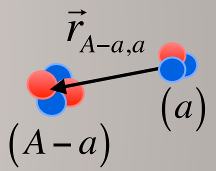
  - Allows to bring the wave function of the relative motion in front of the antisymmetrizer

Binary cluster Resonating Group Method

$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \int \frac{g_\nu^{J^\pi T}(r)}{r}\, \hat{A}_\nu \left[\left(\left| A-a\ \alpha_1 I_1^{\pi_1} T_1 \right\rangle \left| a\ \alpha_2 I_2^{\pi_2} T_2 \right\rangle \right)^{(sT)} Y_\ell(\hat{r}) \right]^{(J^\pi T)} \delta(\vec{r} - \vec{r}_{A-a,a})\; r^2 dr\, d\hat{r}$$

- Now introduce partial wave expansion of delta function

$$\delta(\vec{r} - \vec{r}_{A-a,a}) = \sum_{\lambda\mu} \frac{\delta(r - r_{A-a,a})}{r r_{A-a,a}} Y^*_{\lambda\mu}(\hat{r}) Y_{\lambda\mu}(\hat{r}_{A-a,a})$$



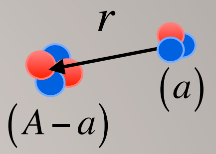
- After integration in the solid angle one obtains:

$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \int \frac{g_\nu^{J^\pi T}(r)}{r}\, \hat{A}_\nu \underbrace{\left[\left(\left| A-a\ \alpha_1 I_1^{\pi_1} T_1 \right\rangle \left| a\ \alpha_2 I_2^{\pi_2} T_2 \right\rangle \right)^{(sT)} Y_\ell(\hat{r}_{A-a,a}) \right]^{(J^\pi T)} \frac{\delta(r - r_{A-a,a})}{r r_{A-a,a}}}_{\left|\Phi^{J^\pi T}_{\nu r}\right\rangle}\; r^2 dr$$

(Jacobi) channel basis

Binary cluster RGM equations

- Trial wave function: $\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \int \frac{g_\nu^{J^\pi T}(r)}{r} \hat{A}_\nu \left|\Phi^{J^\pi T}_{\nu r}\right\rangle r^2 dr$



- Projecting the Schrödinger equation on the channel basis yields:

$$\sum_\nu \int \Big[\underbrace{H^{J^\pi T}_{\nu'\nu}(r',r)}_{\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} H \hat{A}_\nu \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle} - E \ \underbrace{N^{J^\pi T}_{\nu'\nu}(r',r)}_{\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} \hat{A}_\nu \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle} \Big] \frac{g_\nu^{J^\pi T}(r)}{r} \ r^2 \, dr = 0$$

Hamiltonian kernel

Overlap (or norm) kernel

- Breakdown of approach:
  1. Build channel basis states from input target and projectile wave functions
  2. Calculate Hamiltonian and norm kernels
  3. Solve RGM equations: find unknown relative motion wave functions
     - Bound-state / scattering boundary conditions

How to calculate the RGM kernels?

- Depends on chosen target and projectile intrinsic wave functions
  - NCSM/RGM approach: use eigenstates of the $(A\text{-}a)$- and a-body intrinsic Hamiltonians obtained within the NCSM approach
- Note : $H_{\text{int}}^{(A)} = T_{rel}(r) + V_{rel}(r) + \bar{V}_{Coul}(r) + H_{\text{int}}^{(A-a)} + H_{\text{int}}^{(a)}$
  - Relative kinetic energy
  - Relative interaction: sum of all interactions between nucleons belonging to different clusters (minus average Coulomb interaction)
    - Example for single-nucleon projectile (a = 1): $V_{rel}(r) = \sum_{i=1}^{A-1} \underbrace{V_{iA}^{2b}}_{} + \sum_{i<j=1}^{A-1} V_{ijA}^{3b} - \bar{V}_{Coul}(r)$

      nuclear + point-Coulomb
  - Average Coulomb interaction $\bar{V}_{Coul}(r) = \frac{Z_{1\nu}Z_{2\nu}e^2}{r}$
  - $(A\text{-}a)$- and a-body intrinsic Hamiltonians (same interaction everywhere!)

$$H_{\text{int}}^{(A-a)} \left| A-a\ \alpha_1 I_1^{\pi_1} T_1 \right\rangle = \varepsilon_{\alpha_1}^{I_1^{\pi_1}T} \left| A-a\ \alpha_1 I_1^{\pi_1} T_1 \right\rangle \qquad H_{\text{int}}^{(a)} \left| a\ \alpha_2 I_2^{\pi_2} T_2 \right\rangle = \varepsilon_{\alpha_2}^{I_2^{\pi_2}T} \left| a\ \alpha_2 I_2^{\pi_2} T_2 \right\rangle$$

How to calculate the RGM kernels?

- Since we are using NCSM wave functions, it is convenient to introduce Jacobi channel states in the HO space

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

- Note :
  - The coordinate space channel states are given by

$$\left|\Phi^{J^\pi T}_{\nu r}\right\rangle = \sum_n R_{n\ell}(r)\left|\Phi^{J^\pi T}_{\nu n}\right\rangle$$

    - We used the closure properties of HO radial wave functions

Trick #1

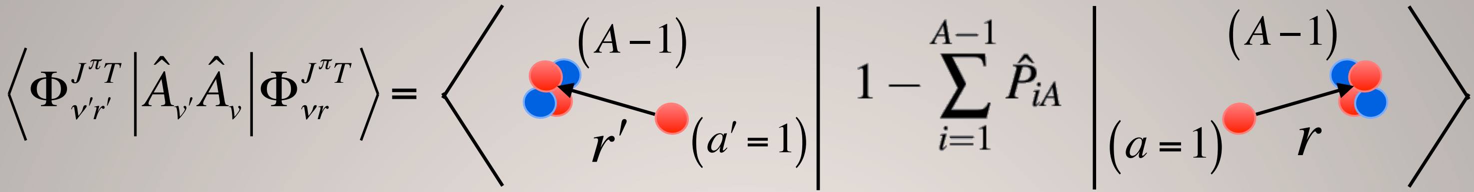
$$\frac{\delta(r-r_{A-a,a})}{r\,r_{A-a,a}} = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

Note that this is OK,
in particular when the sum
is truncated,
ONLY for localized
parts of the kernels

  - We call them Jacobi channel states because they describe only the internal motion
    - Target and projectile wave functions are both translational invariant NCSM eigenstates calculated in the Jacobi coordinate basis

Norm kernel (Pauli principle)

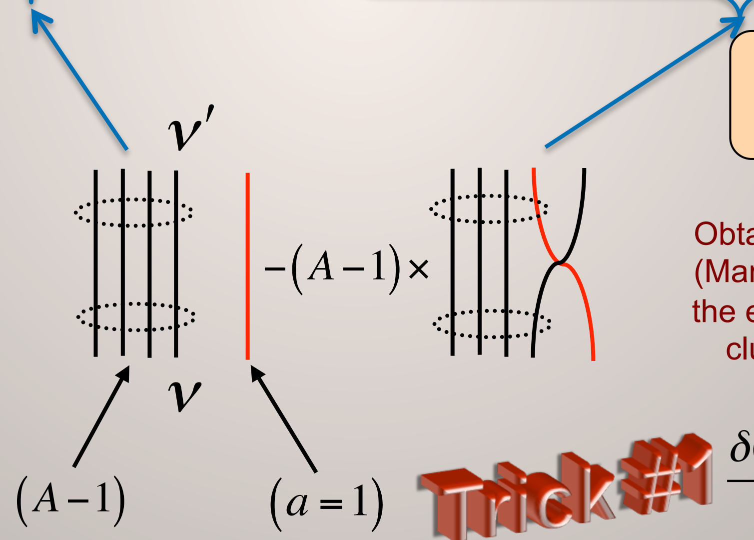
Single-nucleon projectile



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

$$N^{J^\pi T}_{\nu'\nu}(r',r) = \underbrace{\delta_{\nu'\nu}\frac{\delta(r'-r)}{r'r}} - \underbrace{(A-1)\sum_{n'n} R_{n'\ell'}(r')R_{n\ell}(r)\left\langle \Phi^{J^\pi T}_{\nu' n'} \middle| \hat{P}_{A-1,A} \middle| \Phi^{J^\pi T}_{\nu n}\right\rangle}$$

$${}_{\mathrm{SD}}\left\langle \psi^{(A-1)}_{\mu_1} \middle| a^{+} a \middle| \psi^{(A-1)}_{\nu_1}\right\rangle_{\mathrm{SD}}$$



Direct term:
Treated exactly!
(in the full space)

Exchange term:
Obtained in the model space!
(Many-body correction due to the exchange part of the inter-cluster antisymmetrizer)

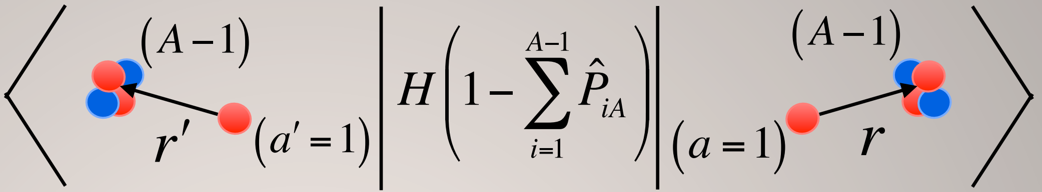
Trick #1

$$\frac{\delta(r-r_{A-a,a})}{r\,r_{A-a,a}} = \sum_n R_{n\ell}(r)R_{n\ell}(r_{A-a,a})$$

Trick #2 Target wave functions expanded in the SD basis, the CM motion exactly removed

Hamiltonian kernel (projectile-target potentials)

Single-nucleon projectile



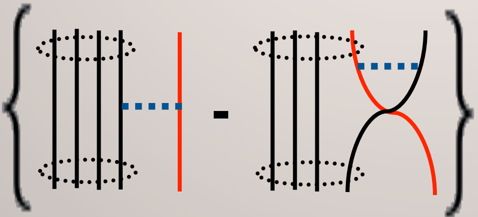
$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} H \hat{A}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left\langle (A-1) \; r' \; (a'=1) \right| H\left(1-\sum_{i=1}^{A-1}\hat{P}_{iA}\right) \left| (a=1) \; r \; (A-1) \right\rangle$$

$$H^{J^\pi T}_{\nu'\nu}(r',r) = \left[T_{rel}(r) + \bar{V}_{Coul}(r) + \varepsilon^{I_1'^{\pi_1'} T_1'}_{\alpha_1'}\right] N^{J^\pi T}_{\nu'\nu}(r',r)$$

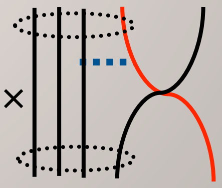
$$+ (A-1)\sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \middle| V_{A-1,A}\left(1-\hat{P}_{A-1,A}\right) \middle| \Phi^{J^\pi T}_{\nu n} \right\rangle$$

$$- (A-1)(A-2)\sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \middle| \hat{P}_{A-1,A} V_{A-2,A-1} \middle| \Phi^{J^\pi T}_{\nu n} \right\rangle$$

$+(A-1)\times$



$-(A-1)(A-2)\times$



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

Exchange potential:
in the model space

Introduce SD channel states in the HO space

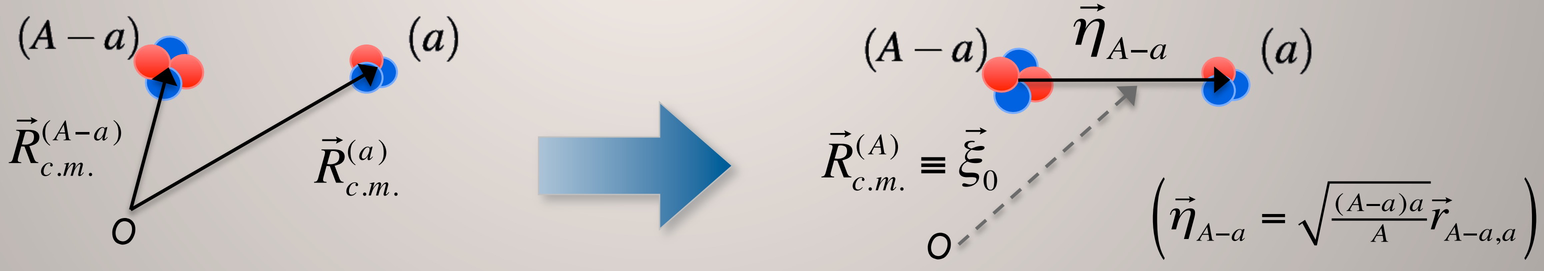
- Define SD channel states in which the eigenstates of the heaviest of the two clusters (target) are described by a SD wave function:

$$\left|\Phi^{J^\pi T}_{\nu n}\right\rangle_{SD} = \left[\left(\underbrace{\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle_{SD}}_{\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle \varphi_{00}\left(\underbrace{\vec R^{(A-a)}_{c.m.}}\right)} \left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle\right)^{(sT)} Y_\ell\left(\underbrace{\hat R^{(a)}_{c.m.}}\right)\right]^{(J^\pi T)} R_{n\ell}\left(\underbrace{R^{(a)}_{c.m.}}\right)$$

Vector proportional to the c.m. coordinate of the *A*-*a* nucleons

Vector proportional to the c.m. coordinate of the *a* nucleons

Trick #2



$$\left(\vec\eta_{A-a} = \sqrt{\tfrac{(A-a)a}{A}}\,\vec r_{A-a,a}\right)$$

$$\left(\varphi_{00}\left(\vec R^{(A-a)}_{c.m.}\right)\varphi_{n\ell}\left(\vec R^{(a)}_{c.m.}\right)\right)^{\ell} = \sum_{n_r\ell_r,NL}\left\langle 00,n\ell,\ell\middle|n_r\ell_r,NL,\ell\right\rangle_{d=\frac{a}{A-a}}\left(\varphi_{n_r\ell_r}\left(\vec\eta_{A-a}\right)\varphi_{NL}\left(\vec\xi_0\right)\right)^{\ell}$$

Translational invariant matrix elements from SD ones

- More in detail:

$$\left|\Phi^{J^\pi T}_{\nu n}\right\rangle_{SD} = \sum_{n_r\ell_r,NL,J_r} \hat{\ell}\hat{J}_r(-1)^{s+\ell_r+L+J} \begin{Bmatrix} s & \ell_r & J_r \\ L & J & \ell \end{Bmatrix} \langle 00,n\ell,\ell|n_r\ell_r,NL,\ell\rangle_{d=\frac{a}{A-a}} \left[\left|\Phi^{J_r^{\pi_r}T}_{\nu_r n_r}\right\rangle \varphi_{NL}(\vec{\xi}_0)\right]^{(J^\pi T)}$$

- The spurious motion of the c.m. is mixed with the intrinsic motion

$$\boxed{{}_{SD}\left\langle\Phi^{J^\pi T}_{\nu' n'}\middle|\hat{O}\middle|\Phi^{J^\pi T}_{\nu n}\right\rangle_{SD}} = \sum_{n'_r\ell'_r,n_r\ell_r,J_r} \left\langle\Phi^{J_r^{\pi_r}T}_{\nu'_r n'_r}\middle|\hat{O}\middle|\Phi^{J_r^{\pi_r}T}_{\nu_r n_r}\right\rangle$$

Interested in this

Trick #2

$$\boxed{\begin{aligned}&\times\sum_{NL}\hat{\ell}\hat{\ell}'\hat{J}_r^2(-1)^{s+\ell-s'-\ell'}\begin{Bmatrix} s & \ell_r & J_r \\ L & J & \ell \end{Bmatrix}\begin{Bmatrix} s' & \ell'_r & J_r \\ L & J & \ell' \end{Bmatrix}\\ &\times\langle 00,n\ell,\ell|n_r\ell_r,NL,\ell\rangle_{d=\frac{a}{A-a}}\langle 00,n'\ell',\ell'|n'_r\ell'_r,NL,\ell'\rangle_{d'=\frac{a'}{A-a'}}\end{aligned}}$$

Calculate these

Matrix that can be inverted

- Translational invariance preserved (exactly!) also with SD channels
- Transformation is general: same for different A's or different a's

Is the SD channel basis advantageous?

- SD to Jacobi transformation is general and exact
- Can use powerful second quantization representation
  - Matrix elements of translational invariant operators can be expressed in terms of matrix elements of density operators on the target eigenstates
  - For example, for $a = a' = 1$

$$
{}_{SD}\left\langle \Phi^{J^\pi T}_{\nu' n'} \right| P_{A-1,A} \left| \Phi^{J^\pi T}_{\nu n} \right\rangle_{SD} = \frac{1}{A-1} \sum_{jj'K\tau} \hat{s}\hat{s}'\hat{j}\hat{j}'\hat{K}\hat{\tau} (-1)^{I_1'+j'+J} (-1)^{T_1+\frac{1}{2}+T}
$$

Trick #2

$$
\times \begin{Bmatrix} I_1 & \frac{1}{2} & s \\ \ell & J & j \end{Bmatrix} \begin{Bmatrix} I_1' & \frac{1}{2} & s' \\ \ell' & J & j' \end{Bmatrix} \begin{Bmatrix} I_1 & K & I_1' \\ j' & J & j \end{Bmatrix} \begin{Bmatrix} T_1 & \tau & T_1' \\ \frac{1}{2} & T & \frac{1}{2} \end{Bmatrix}
$$

One-body density matrix elements

$$
\times \boxed{ {}_{SD}\left\langle A-1\ \alpha_1' I_1'^{\pi_1'} T_1' \right\| \left(a^+_{n\ell j\frac{1}{2}} \tilde{a}_{n'\ell' j'\frac{1}{2}} \right)^{(K\tau)} \left\| A-1\ \alpha_1 I_1^{\pi_1} T_1 \right\rangle_{SD} }
$$

- Given a, a', matrix elements are also general (same for different A's)

Solving the NCSM/RGM equations

- There are other technical details
  - Because of the norm kernel, the radial wave functions solutions of the RGM equation are not Schrödinger wave functions
  - However, the RGM equations can be orthogonalized

$$\sum_{\nu'}\int dr' r'^2 \left[N^{-\frac{1}{2}} H N^{-\frac{1}{2}}\right]_{\nu\nu'}(r,r')\frac{u_{\nu'}(r')}{r'} = E\,\frac{u_\nu(r)}{r}$$

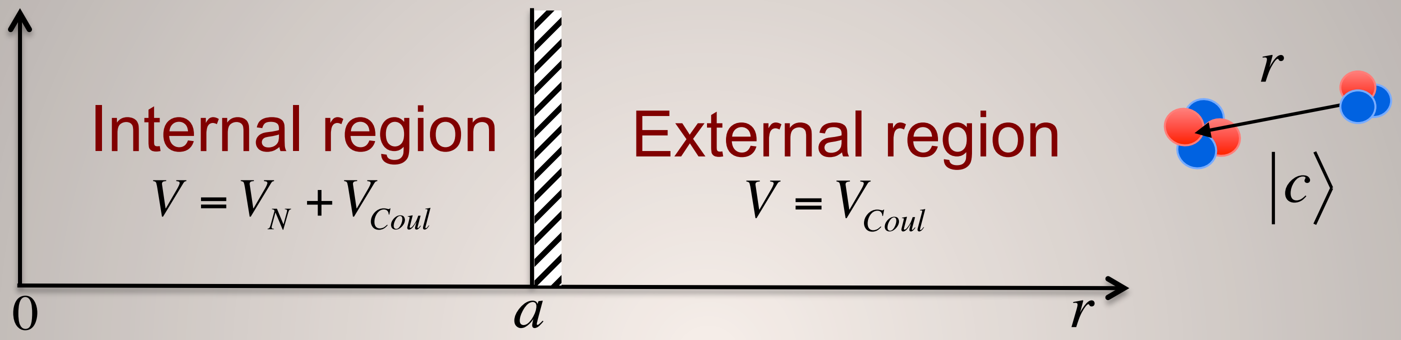
  - This procedure is explained in Phys. Rev. C 79, 044606 (2009)

- In the end, one is left with a set of integral-differential coupled channel equations with a non-local potential of the type:

$$\left[T_{rel}(r)+\bar{V}_{Coul}(r)-(E-\varepsilon_{\alpha_1}-\varepsilon_{\alpha_2})\right]u_\nu(r)+\sum_{\nu'}\int dr' r'\ W_{\nu\nu'}(r,r')\ u_{\nu'}(r')=0$$

Microscopic *R*-matrix theory

- Separation into “internal” and “external” regions at the channel radius a

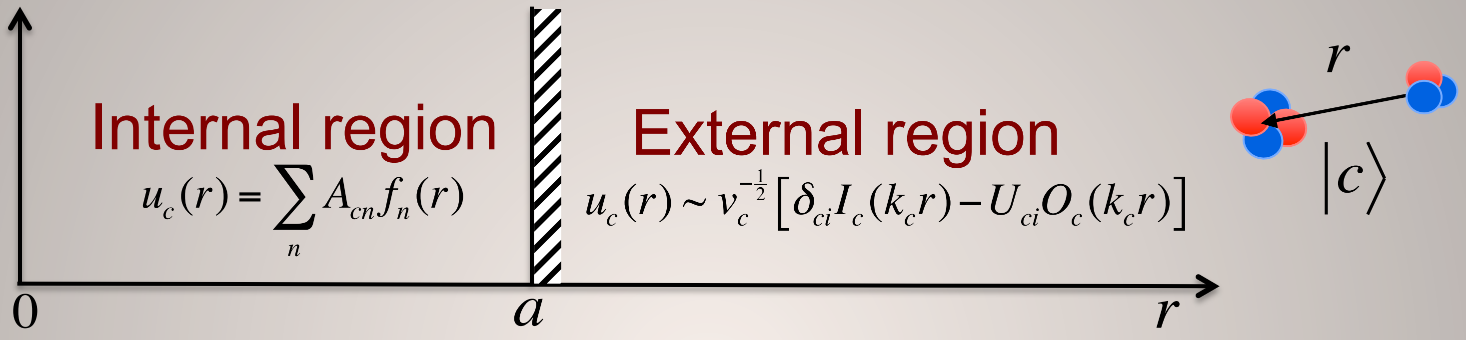


  - This is achieved through the Bloch operator: $L_c = \frac{\hbar^2}{2\mu_c}\delta(r-a)\left(\frac{d}{dr} - \frac{B_c}{r}\right)$
  - System of Bloch-Schrödinger equations:

$$\left[\hat{T}_{rel}(r) + L_c + \overline{V}_{Coul}(r) - (E - E_c)\right]u_c(r) + \sum_{c'} \int dr'\, r' W_{cc'}(r,r') u_{c'}(r') = L_c u_c(r)$$

Microscopic *R*-matrix theory

- Separation into “internal” and “external” regions at the channel radius a



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  - System of Bloch-Schrödinger equations:

$$\left[\hat{T}_{rel}(r) + L_c + \overline{V}_{Coul}(r) - (E - E_c)\right]u_c(r) + \sum_{c'}\int dr' r' W_{cc'}(r,r')u_{c'}(r') = L_c u_c(r)$$

  - Internal region: expansion on square-integrable basis $u_c(r) = \sum_n A_{cn} f_n(r)$
  - External region: asymptotic form for large r

$$u_c(r) \sim C_c W(k_c r) \quad \text{or} \quad u_c(r) \sim v_c^{-\frac{1}{2}}\left[\delta_{ci} I_c(k_c r) - \underset{\text{Scattering matrix}}{U_{ci}} O_c(k_c r)\right]$$

Bound state

Scattering state

To find the Scattering matrix

- After projection on the basis $f_n(r)$:

$$\sum_{c'n'}[C_{cn,c'n'} - (E-E_c)\delta_{cn,c'n'}]A_{c'n'} = \frac{\hbar^2 k_c}{2\mu_c v_c^{1/2}}\langle f_n|L_c|I_c\delta_{ci} - U_{ci}O_c\rangle$$

$$\boxed{\langle f_n|\hat{T}_{rel}(r) + L_c + \overline{V}_{Coul}(r)|f_{n'}\rangle\delta_{cc'} + \langle f_n|W_{cc'}(r,r')|f_{n'}\rangle}$$

1. Solve for A_{cn}
2. Match internal and external solutions at channel radius, a

$$\sum_{c'} R_{cc'}\frac{k_{c'}a}{\sqrt{\mu_{c'}v_{c'}}}[I'_{c'}(k_{c'}a)\delta_{ci} - U_{c'i}O'_{c'}(k_{c'}a)] = \frac{1}{\sqrt{\mu_c v_c}}[I_c(k_c a)\delta_{ci} - U_{ci}O_c(k_c a)]$$

Lagrange basis associated with Lagrange mesh:

$$\{ax_n \in [0,a]\}$$

$$\int_0^1 g(x)dx \approx \sum_{n=1}^{N}\lambda_n g(x_n)$$

$$\int_0^a f_n(r)f_{n'}(r)dr \approx \delta_{nn'}$$

- In the process introduce *R*-matrix, projection of the Green’s function operator on the channel-surface functions

$$R_{cc'} = \sum_{nn'}\frac{\hbar}{\sqrt{2\mu_c a}} f_n(a)[C - EI]^{-1}_{cn,c'n'}\frac{\hbar}{\sqrt{2\mu_{c'}a}} f_{n'}(a)$$

To find the Scattering matrix

3. Solve equation with respect to the scattering matrix U

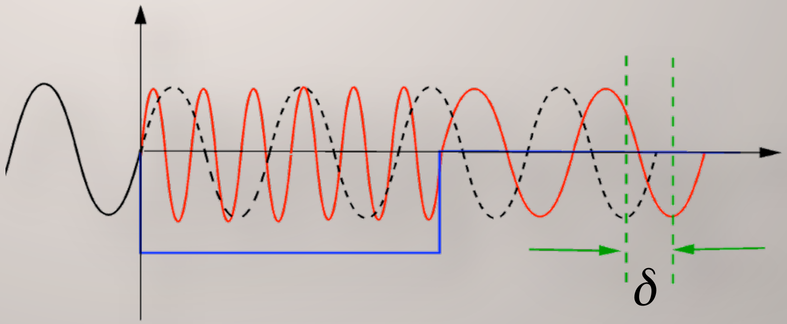
$$\sum_{c'} R_{cc'} \frac{k_{c'}a}{\sqrt{\mu_{c'}v_{c'}}}\left[I'_{c'}(k_{c'}a)\delta_{ci} - \boxed{U_{c'i}}\, O'_{c'}(k_{c'}a)\right] = \frac{1}{\sqrt{\mu_c v_c}}\left[I_c(k_ca)\delta_{ci} - \boxed{U_{ci}}\, O_c(k_ca)\right]$$

4. You can demonstrate that the solution is given by:

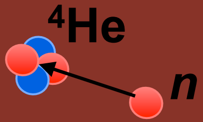
$$U = Z^{-1}Z^{*}, \qquad Z_{cc'} = \left(k_{c'}a\right)^{-1}\left[O_c(k_ca)\delta_{cc'} - k_{c'}a\, R_{cc'}\; O'_{c'}(k_{c'}a)\right]$$

- Scattering phase shifts are extracted from the scattering matrix elements

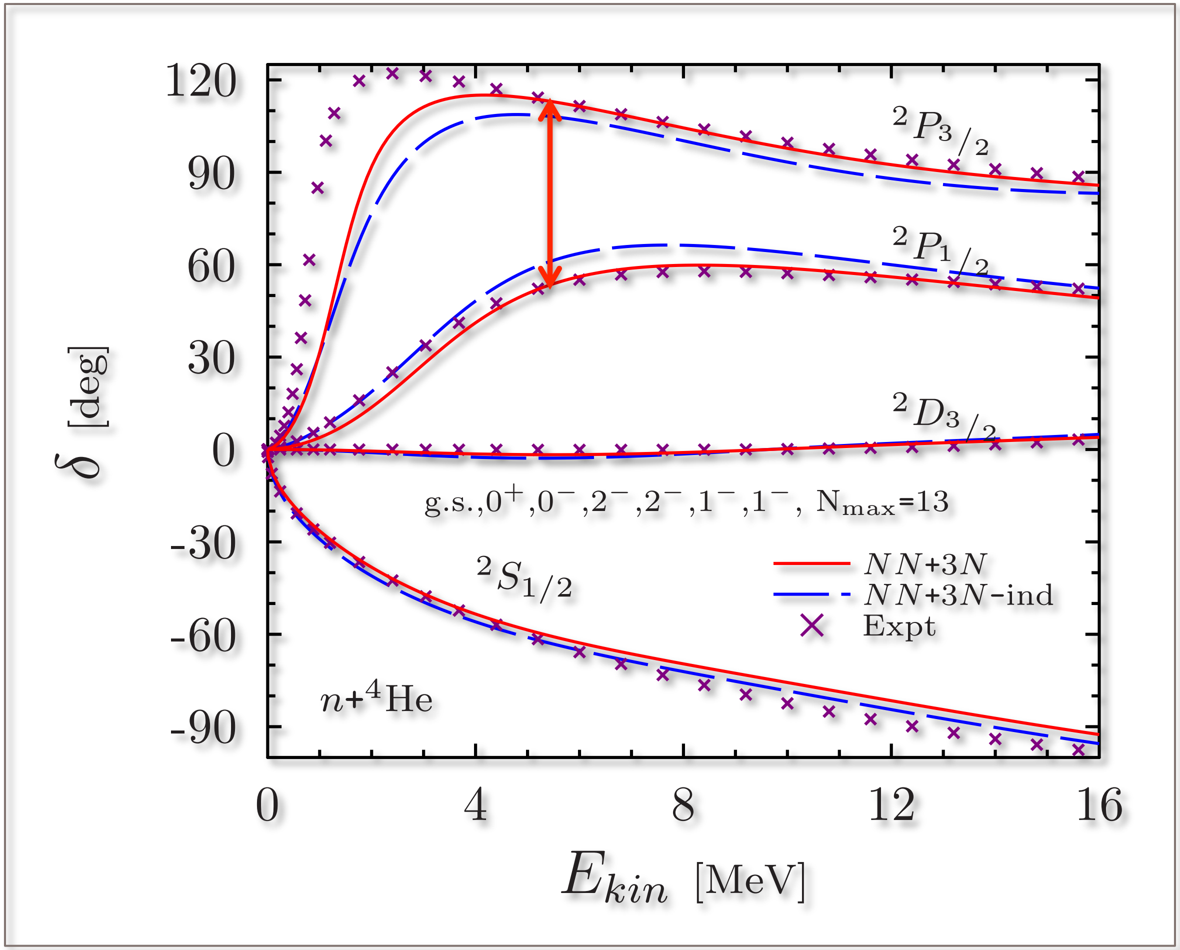
$$U = \exp(2i\delta)$$



TRIUMF

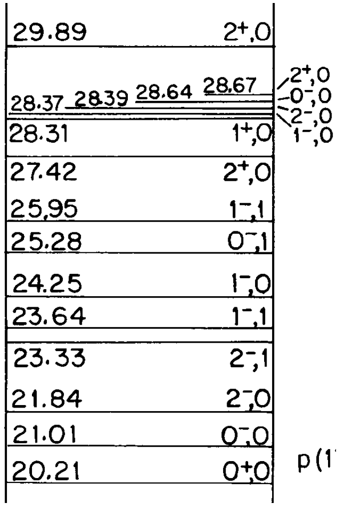


n-^{4}He scattering within the NCSM/RGM

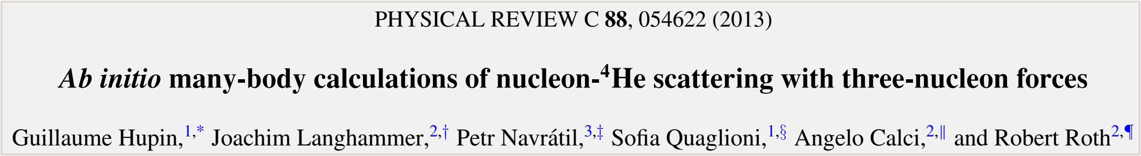


chiral NN+NNN(500)
chiral NN+NNN-induced
SRG λ=2 fm^{-1}
HO N$_{max}$=13, hΩ=20 MeV

^{4}He g.s. and 6 excited states



29.89	2^+,0
28.37 28.39 28.64 28.67	2^+,0 0^-,0 2^-,0 1^-,0
28.31	1^+,0
27.42	2^+,0
25.95	1^-,1
25.28	0^-,1
24.25	1^-,0
23.64	1^-,1
23.33	2^-,1
21.84	2^-,0
21.01	0^-,0
20.21	0^+,0



PHYSICAL REVIEW C **88**, 054622 (2013)

***Ab initio* many-body calculations of nucleon-^{4}He scattering with three-nucleon forces**

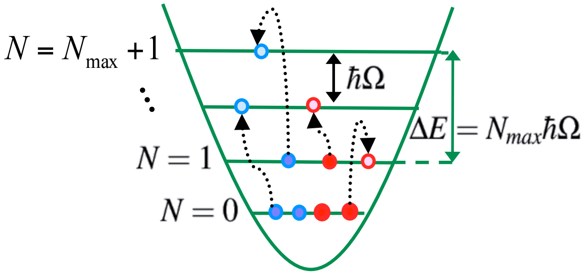
Guillaume Hupin,[1,*] Joachim Langhammer,[2,†] Petr Navrátil,[3,‡] Sofia Quaglioni,[1,§] Angelo Calci,[2,∥] and Robert Roth[2,¶]

A larger splitting between the *P*-waves obtained with the chiral NN+NNN interaction

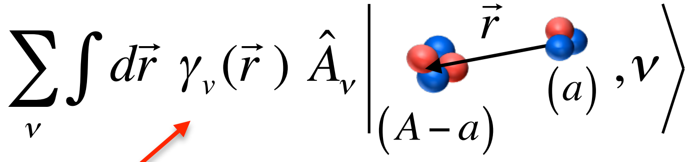
The 3/2$^-$ resonance still off:
Interaction or **CONVERGENCE?**

No-core shell model with RGM

- No-core shell model (NCSM)
  - *A*-nucleon wave function expansion in the harmonic-oscillator (HO) basis
  - short- and medium range correlations
  - Bound-states, narrow resonances



- NCSM with Resonating Group Method (NCSM/RGM)
  - cluster expansion
  - proper asymptotic behavior
  - long-range correlations

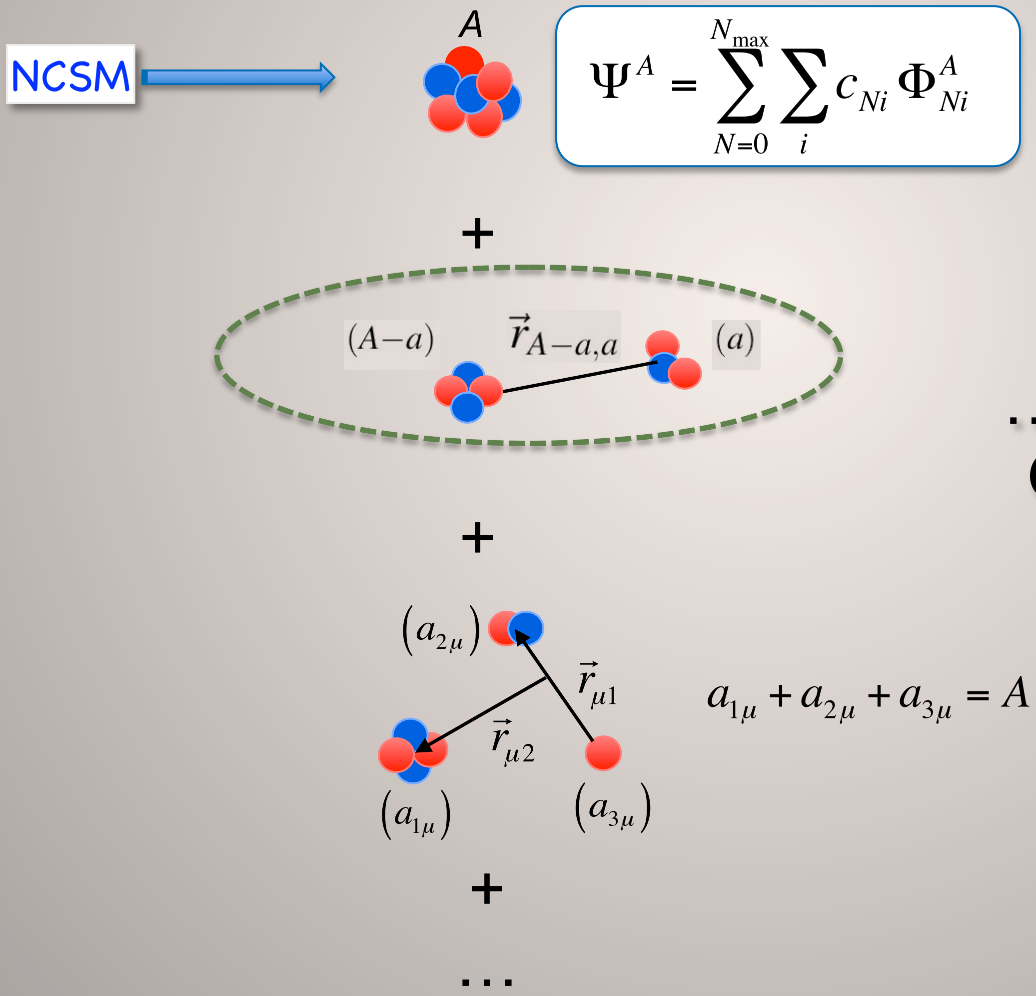


$$\Psi^{(A)} = \sum_{\nu} \int d\vec{r}\ \gamma_\nu(\vec{r}\,)\ \hat{A}_\nu \left| \ _{(A-a)} \xrightarrow{\vec{r}} \ _{(a)} , \nu \right\rangle$$

Unknowns

Extending no-core shell model beyond bound states

Include more many nucleon correlations…



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

+

+

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

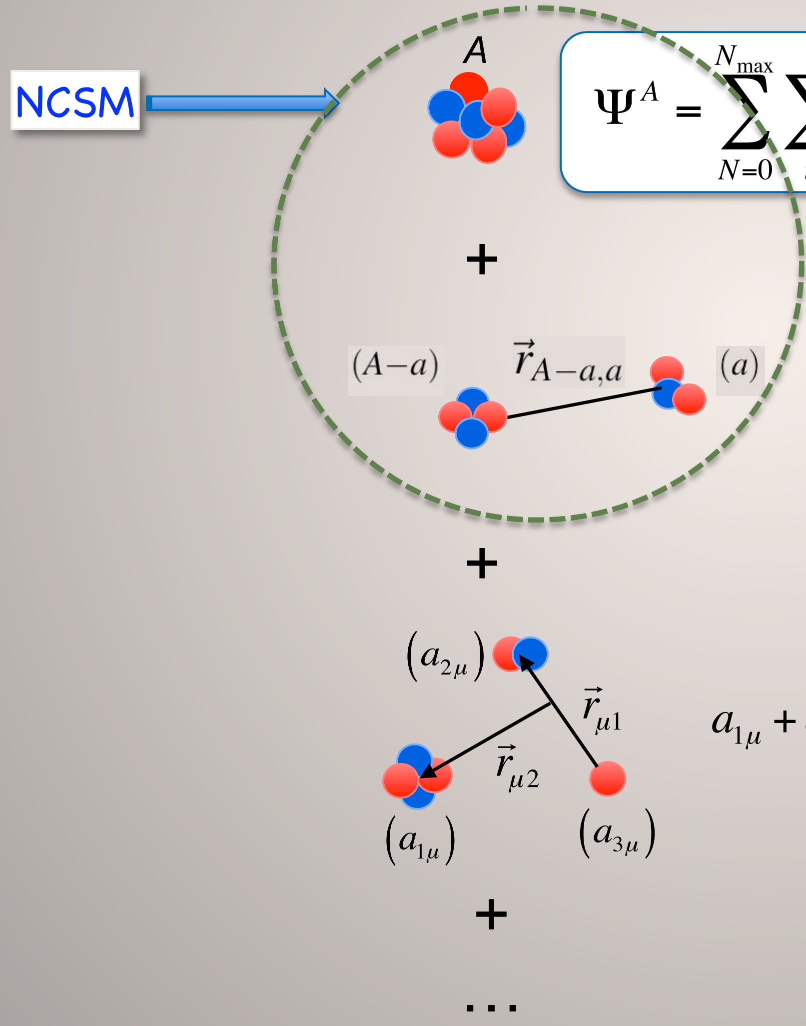
+

…

…using the Resonating Group Method (RGM) ideas

Extending no-core shell model beyond bound states

Include more many nucleon correlations…



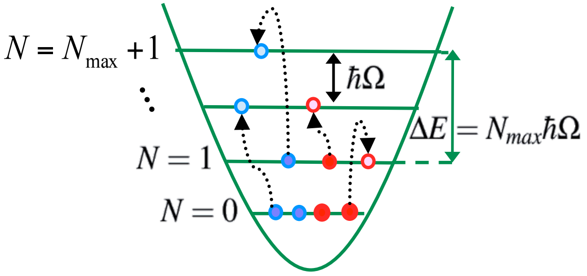
$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

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

…using the Resonating Group Method (RGM) ideas

Unified approach to bound & continuum states; to nuclear structure & reactions

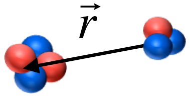
- *Ab initio* no-core shell model
  - Short- and medium range correlations
  - Bound-states, narrow resonances



Harmonic oscillator basis

NCSM

- …with resonating group method
  - Bound & scattering states, reactions
  - Cluster dynamics, long-range correlations

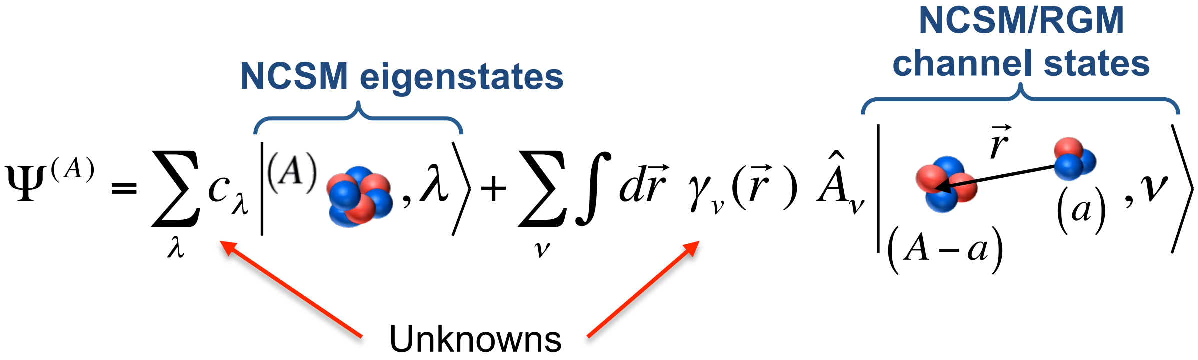


NCSM/RGM

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

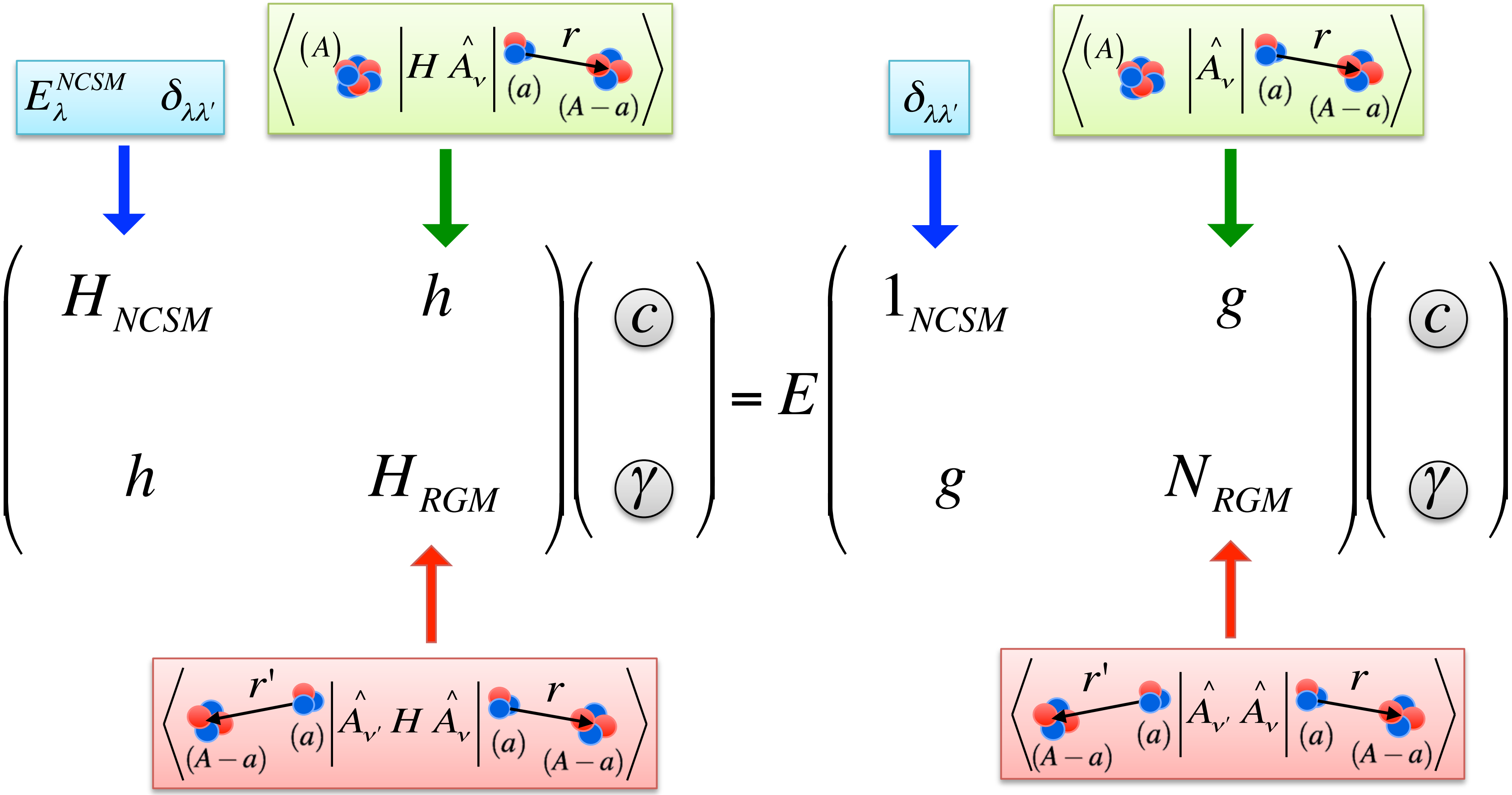
- Most efficient: *ab initio* no-core shell model with continuum

NCSMC



$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \overbrace{\left| {}^{(A)}\, , \lambda \right\rangle}^{\text{NCSM eigenstates}} + \sum_{\nu} \int d\vec{r}\, \gamma_{\nu}(\vec{r}\,)\, \hat{A}_{\nu} \overbrace{\left| {}_{(A-a)} \quad \vec{r} \quad {}_{(a)}\, , \nu \right\rangle}^{\text{NCSM/RGM channel states}}$$

Coupled NCSMC equations



$$E_\lambda^{NCSM}\ \delta_{\lambda\lambda'}$$

$$\left\langle {}^{(A)} \middle| H\,\hat{A}_\nu \middle| \underset{(a)}{} \overset{r}{\longrightarrow} \underset{(A-a)}{} \right\rangle$$

$$\delta_{\lambda\lambda'}$$

$$\left\langle {}^{(A)} \middle| \hat{A}_\nu \middle| \underset{(a)}{} \overset{r}{\longrightarrow} \underset{(A-a)}{} \right\rangle$$

$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix} = E \begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix}$$

$$\left\langle \underset{(A-a)}{} \overset{r'}{\longleftarrow} \underset{(a)}{} \middle| \hat{A}_{\nu'}\, H\, \hat{A}_\nu \middle| \underset{(a)}{} \overset{r}{\longrightarrow} \underset{(A-a)}{} \right\rangle$$

$$\left\langle \underset{(A-a)}{} \overset{r'}{\longleftarrow} \underset{(a)}{} \middle| \hat{A}_{\nu'}\, \hat{A}_\nu \middle| \underset{(a)}{} \overset{r}{\longrightarrow} \underset{(A-a)}{} \right\rangle$$

Scattering matrix (and observables) from matching solutions to known asymptotic with microscopic *R*-matrix on Lagrange mesh

NCSMC formalism

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

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 *h* from SD wave functions:

$$\left\langle A\lambda J^\pi T \middle| V_{3N} \middle| \mathcal{A}_\nu \Phi^{J^\pi T}_{\nu r} \right\rangle \propto {}_{SD}\!\left\langle A\,\lambda\,J^\pi M\,TM_T \middle| V_{3N} \mathcal{A} \left[\left| A-1\alpha_1 I_1 T_1 \right\rangle_{SD} \varphi_{nlj}(A) \right]^{(J^\pi T)}_{MM_T} \right. =$$

$$\sum_{\beta M_1 m} \tfrac{1}{12} (I_1 M_1 jm \,|\, JM)(T_1 M_{T_1} \, \tfrac{1}{2} m_t \,|\, TM_T) \left\langle \beta_{A-2} \beta_{A-1} \beta_A \middle| V_{3N} \middle| \beta'_{A-2}\, \beta'_{A-1}\, nljm \tfrac{1}{2} m_t \right\rangle$$

$$\times \, {}_{SD}\!\left\langle A\,\lambda\,J^\pi M\,TM_T \middle| a^+_{\beta_A} a^+_{\beta_A - 1} a^+_{\beta_A - 2} a_{\beta'_{A-2}} a_{\beta'_{A-1}} \middle| A-1\alpha_1\, I_1 M_1\, T_1\, M_{T_1} \right\rangle_{SD}$$

NCSMC formalism

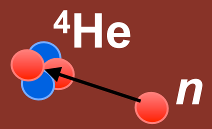
- Calculation of *h* from SD wave functions:

$$\left\langle A\lambda J^{\pi}T\right|V_{3N}\left|\mathcal{A}_{\nu}\Phi_{\nu r}^{J^{\pi}T}\right\rangle \propto {}_{SD}\left\langle A\,\lambda\,J^{\pi}M\,TM_{T}\right|V_{3N}\mathcal{A}\left[\left|A-1\alpha_{1}I_{1}T_{1}\right\rangle_{SD}\,\varphi_{nlj}(A)\right]_{MM_{T}}^{(J^{\pi}T)} =$$

$$\sum_{\beta M_1 m}\tfrac{1}{12}(I_1M_1jm\,|\,JM)(T_1M_{T_1}\,{}^1\!/\!{}_2\,m_t\,|\,TM_T)\left\langle\beta_{A-2}\beta_{A-1}\beta_A\right|V_{3N}\left|\beta'_{A-2}\,\beta'_{A-1}\,nljm\,{}^1\!/\!{}_2\,m_t\right\rangle$$

$$\times\;{}_{SD}\left\langle A\,\lambda\,J^{\pi}M\,TM_{T}\right|a^{+}_{\beta_A}a^{+}_{\beta_{A}-1}a^{+}_{\beta_{A}-2}a_{\beta'_{A-2}}a_{\beta'_{A-1}}\left|A-1\alpha_{1}\,I_{1}M_{1}\,T_{1}\,M_{T_1}\right\rangle_{SD}$$

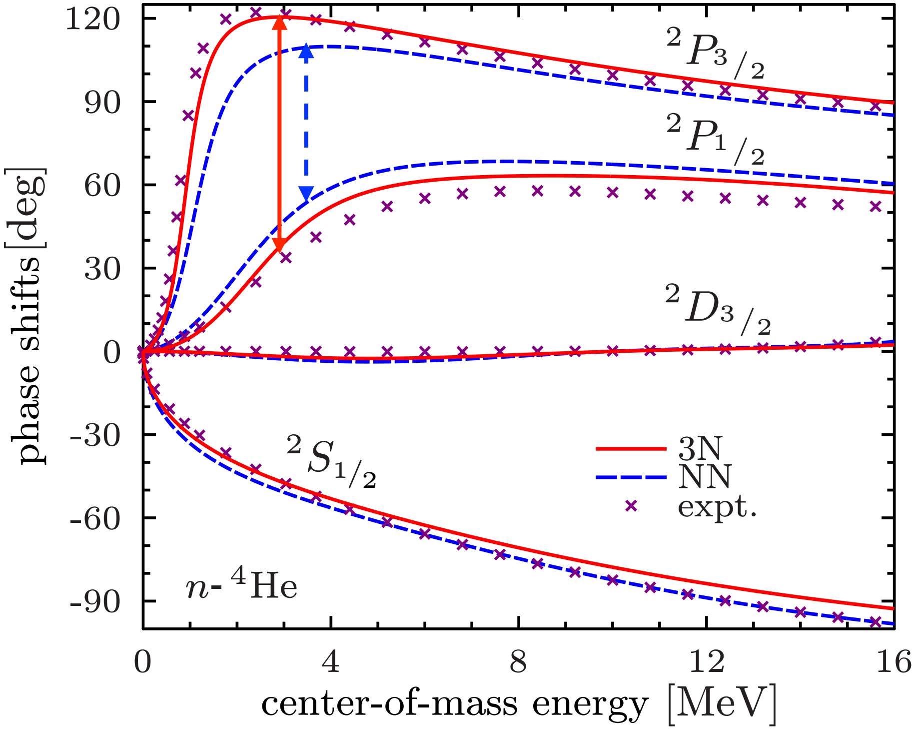
- Tricky part: Sums over M_1, M_{T1}
  - Need target eigenvectors for all M's:
  - Use raising and lowering $J_{\pm}$ and $T_{\pm}$ acting on $\left|A-1\alpha_{1}\,I_{1}M_{1}\,T_{1}M_{T_1}\right\rangle_{SD}$ with M_1=0 for even *A* or 1/2 for odd *A*

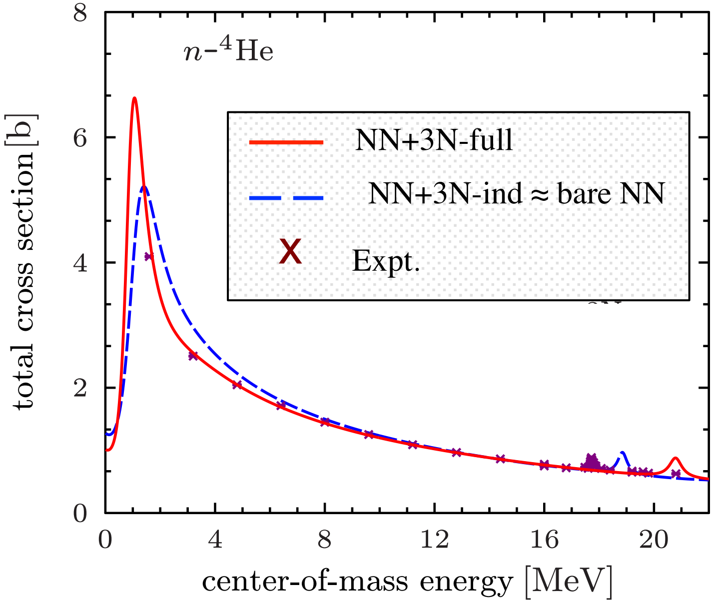


n-^{4}He scattering within NCSMC

n-^{4}He scattering phase-shifts for chiral NN and NN+3N potential

Total n-^{4}He cross section with NN and NN+3N potentials





3N force enhances 1/2$^-$ ←→ 3/2$^-$ splitting: Essential at low energies!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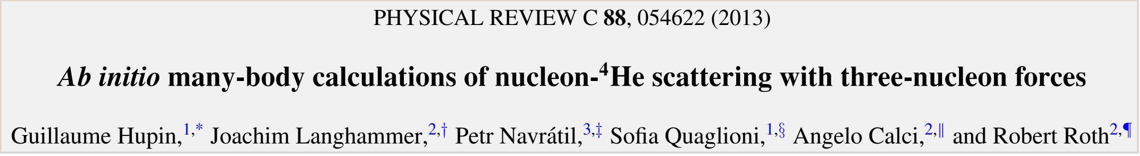
Invited Comment

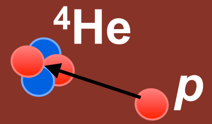
Unified *ab initio* approaches to nuclear structure and reactions

Petr Navrátil[1], Sofia Quaglioni[2], Guillaume Hupin[3,4], Carolina Romero-Redondo[2] and Angelo Calci[1]


PHYSICAL REVIEW C **88**, 054622 (2013)

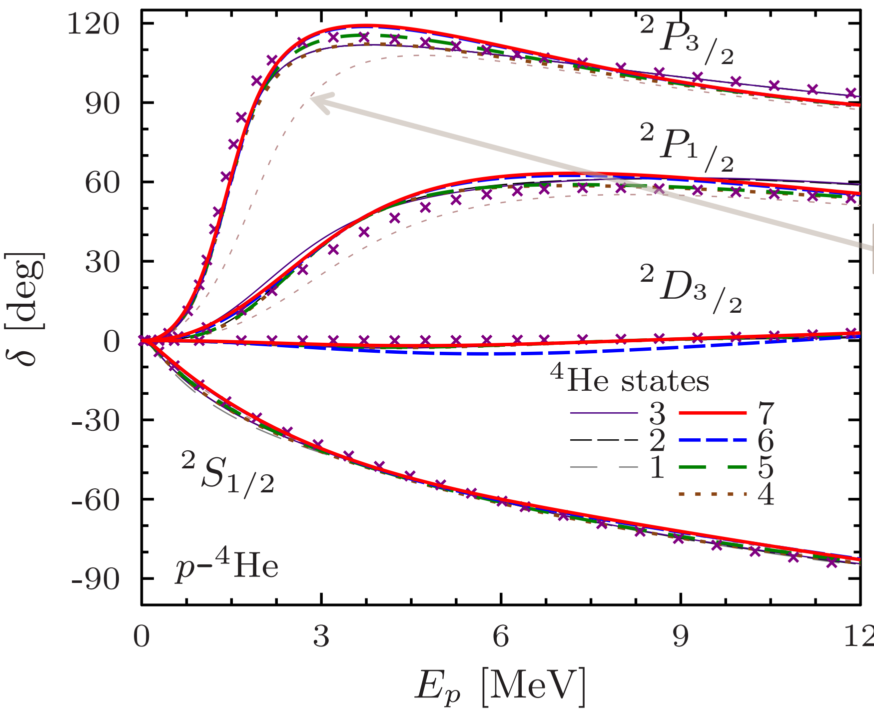
***Ab initio* many-body calculations of nucleon-^{4}He scattering with three-nucleon forces**

Guillaume Hupin,[1,*] Joachim Langhammer,[2,†] Petr Navrátil,[3,‡] Sofia Quaglioni,[1,§] Angelo Calci,[2,∥] and Robert Roth[2,¶]

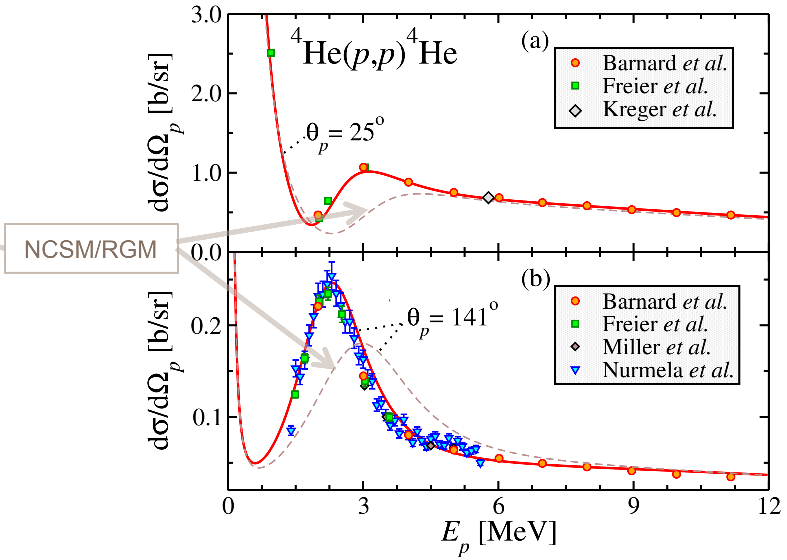


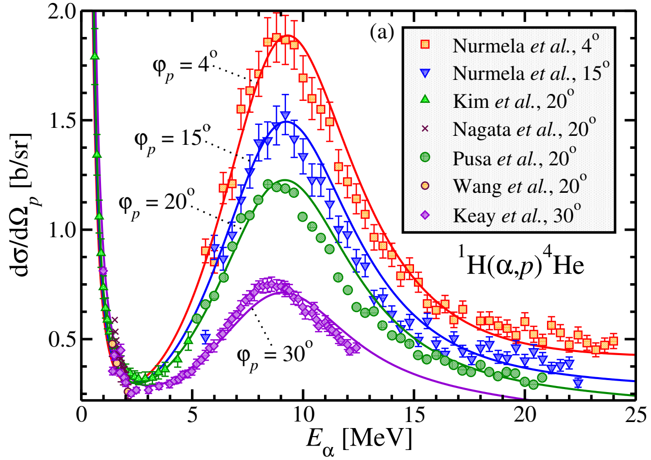
p-^{4}He scattering within NCSMC

p-^{4}He scattering phase-shifts for NN+3N potential: Convergence



Differential p-^{4}He cross section with NN+3N potentials





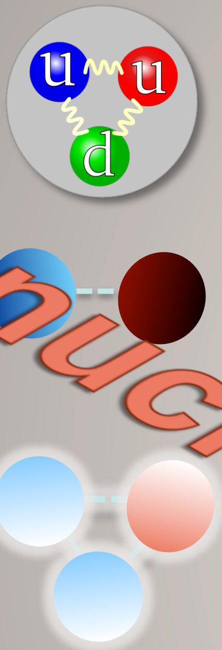
Predictive power in the 3/2$^-$ resonance region:
Applications to material science

PHYSICAL REVIEW C **90**, 061601(R) (2014)

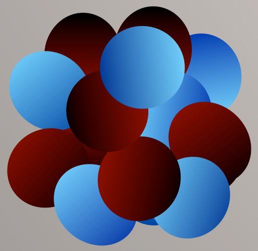
Predictive theory for elastic scattering and recoil of protons from ^{4}He

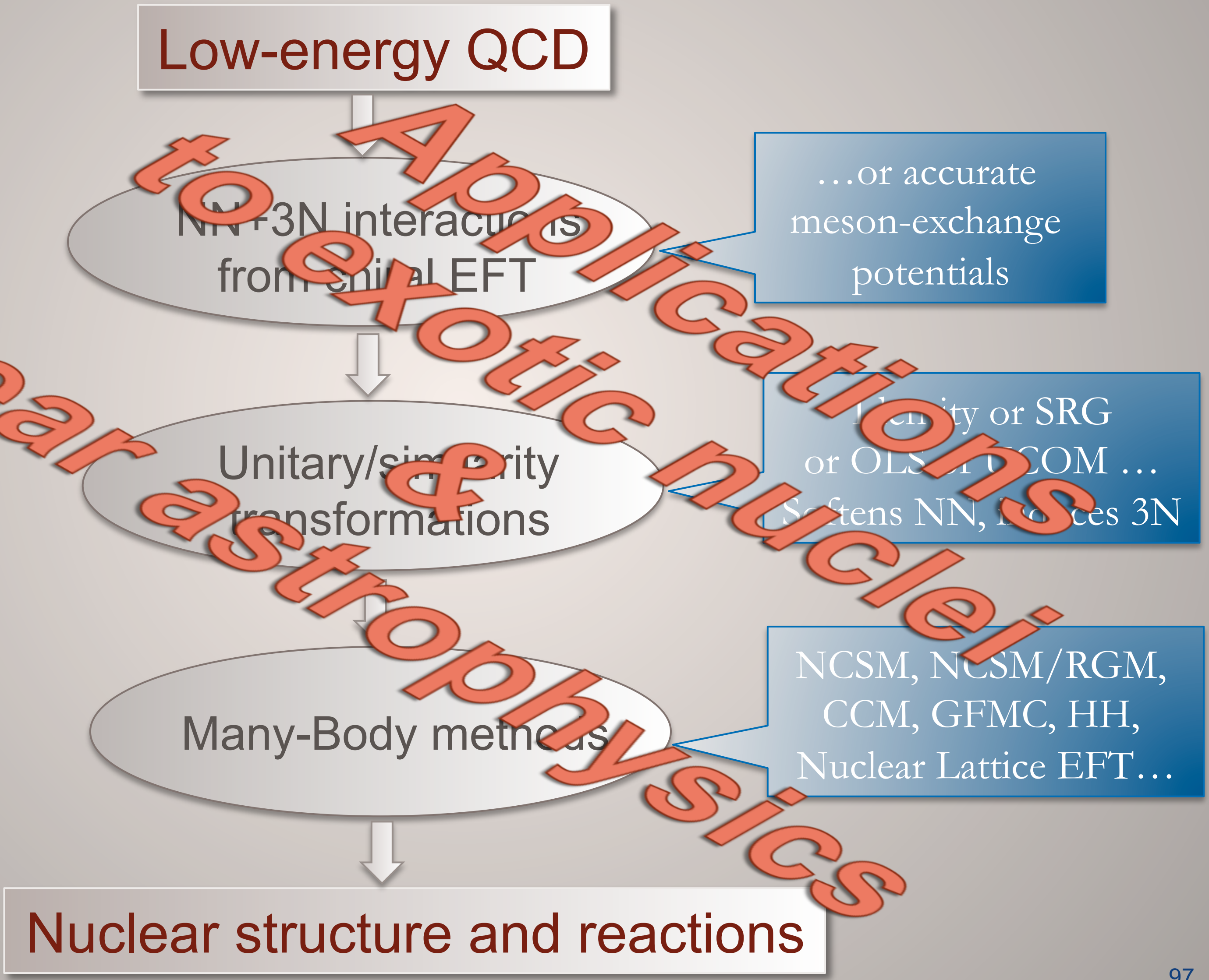
Guillaume Hupin,[1,*] Sofia Quaglioni,[1,†] and Petr Navrátil[2,‡]

From QCD to nuclei



$$H|\Psi\rangle = E|\Psi\rangle$$





Low-energy QCD

NN+3N interactions from chiral EFT

…or accurate meson-exchange potentials

Unitary/similarity transformations

Identity or SRG or OLS or UCOM … Softens NN, induces 3N

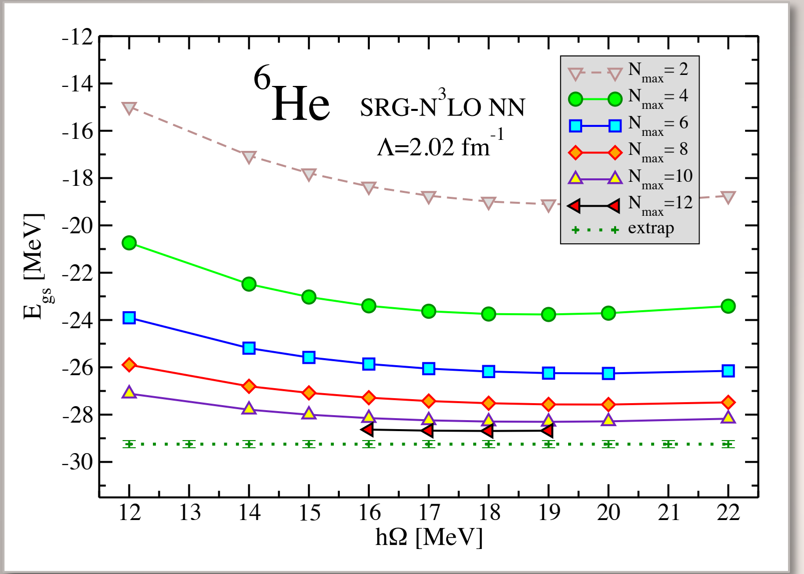
Many-Body methods

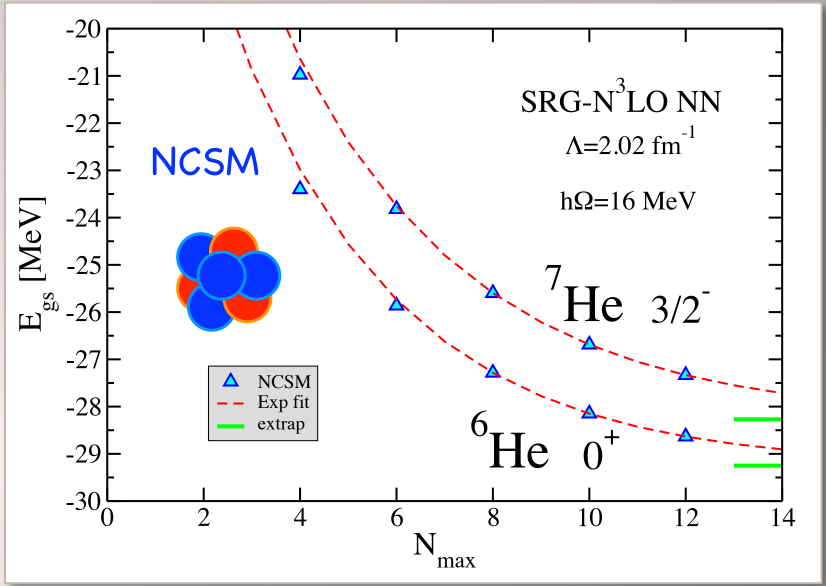
NCSM, NCSM/RGM, CCM, GFMC, HH, Nuclear Lattice EFT…

Nuclear structure and reactions

Applications to exotic nuclei & nuclear astrophysics

NCSM calculations of ^{6}He and ^{7}He g.s. energies

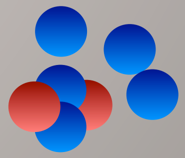




$E_{\rm g.s.}$ [MeV]	^{4}He	^{6}He	^{7}He
NCSM $N_{\rm max}$=12	-28.05	-28.63	-27.33
NCSM extrap.	-28.22(1)	-29.25(15)	-28.27(25)
Expt.	-28.30	-29.27	-28.84

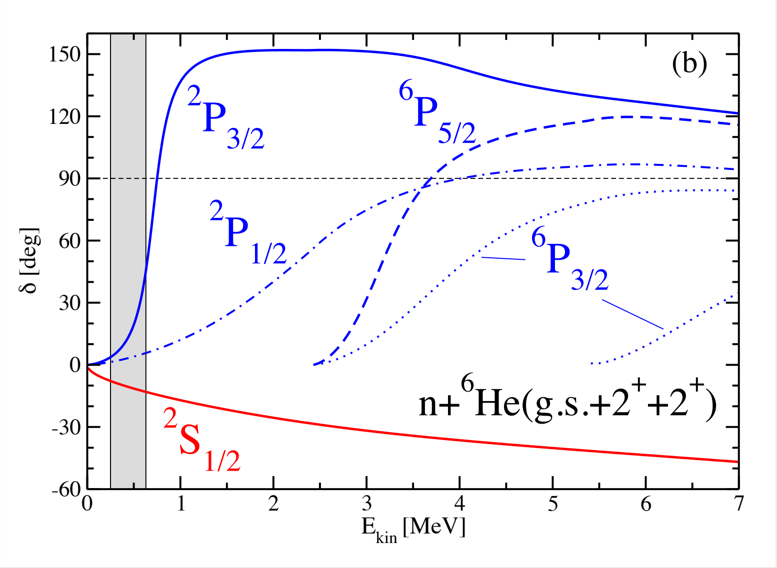
- Soft SRG evolved NN potential
- ✓ N_{max} convergence OK
- ✓ Extrapolation feasible

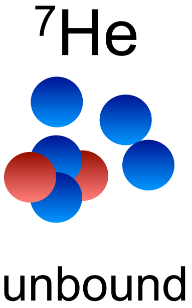
- ^{7}He unbound
  - Expt. E_{th}=+0.430(3) MeV: NCSM E_{th}≈ +1 MeV
  - Expt. width 0.182(5) MeV: **NCSM no information about the width**



^{7}He unbound

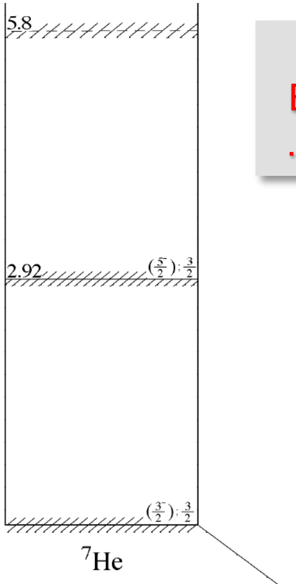
NCSM with continuum: ^{7}He ↔ ^{6}He+*n*

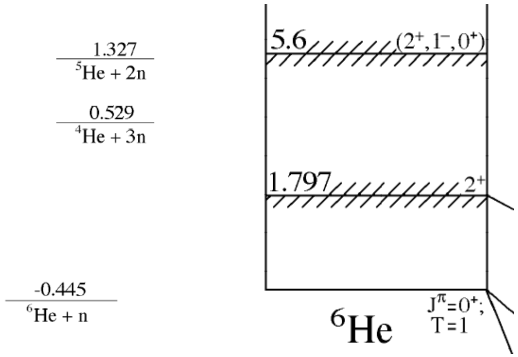




J^π	experiment E_R	Γ	Ref.	NCSMC E_R	Γ
$3/2^-$	0.430(3)	0.182(5)	[2]	0.71	0.30
$5/2^-$	3.35(10)	1.99(17)	[40]	3.13	1.07
$1/2^-$	3.03(10)	2	[11]	2.39	2.89
	3.53	10	[15]		
	1.0(1)	0.75(8)	[5]		

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

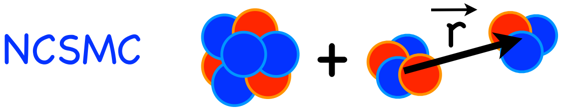




Experimental controversy:
Existence of low-lying 1/2$^-$ state
… not seen in these calculations

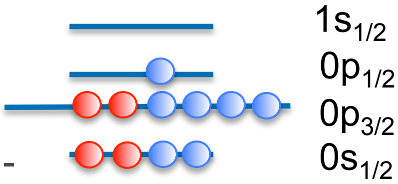
$$\Gamma = \left.\frac{2}{\partial\delta(E_{kin})/\partial E_{kin}}\right|_{E_{kin}=E_R}$$

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



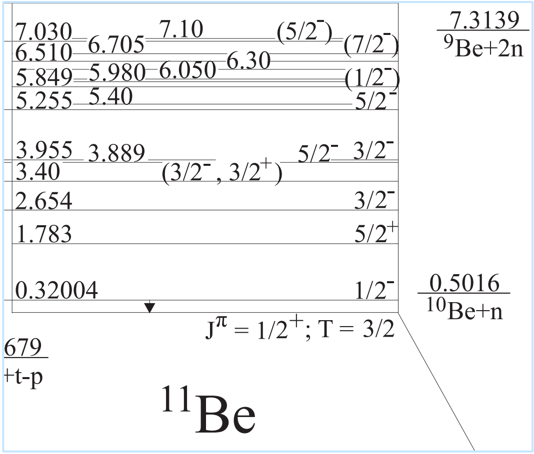
S. Baroni, P. N., and S. Quaglioni,
PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

Neutron-rich halo nucleus ^{11}Be



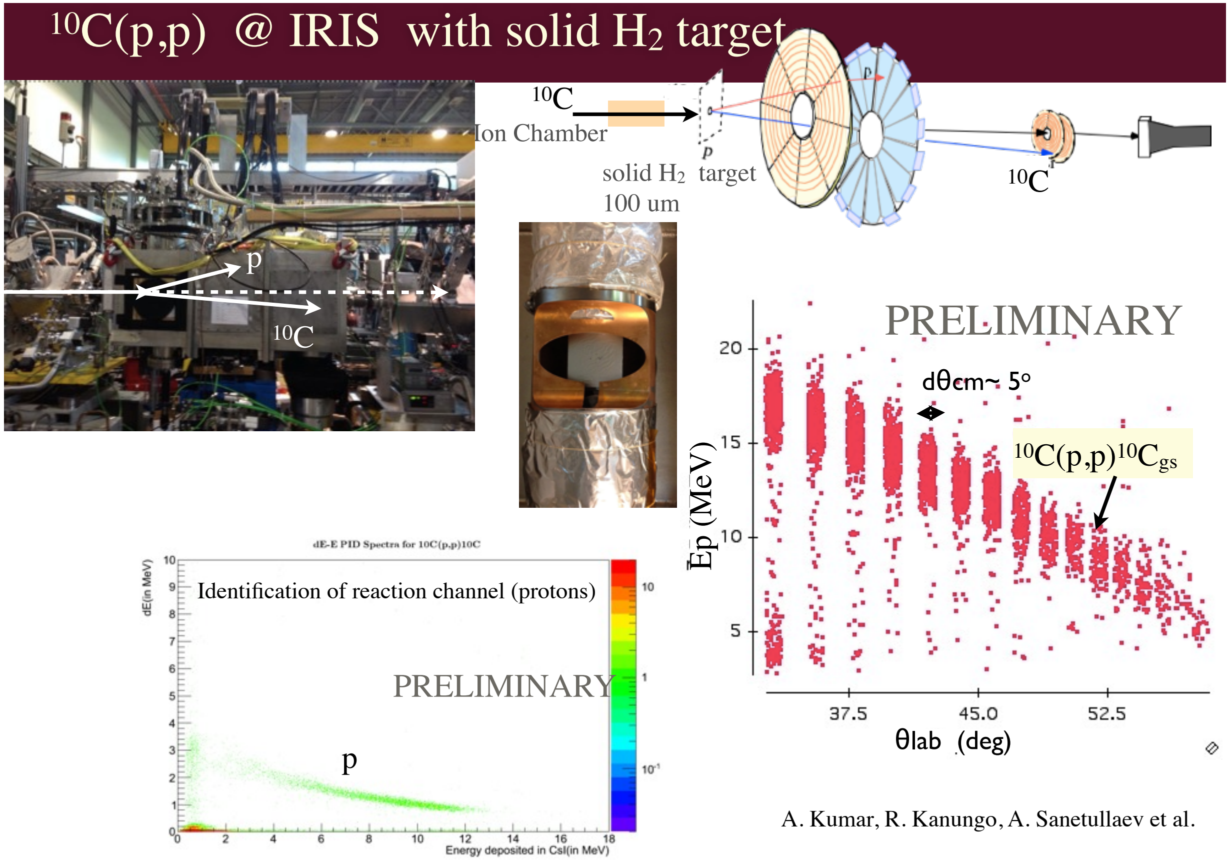
- Z=4, N=7
  - – In the shell model picture g.s. expected to be $J^{\pi}=1/2^-$
    - Z=6, N=7 ^{13}C and Z=8, N=7 ^{15}O have $J^{\pi}=1/2^-$ g.s.
  - – In reality, ^{11}Be g.s. is **$J^{\pi}=1/2^+$** - parity inversion
  - – Very weakly bound: E_{th}=-0.5 MeV
    - Halo state – dominated by ^{10}Be-n in the *S*-wave
  - – The $1/2^-$ state also bound – only by 180 keV

- Can we describe ^{11}Be in *ab initio* calculations?
  - – Continuum must be included
  - – Does the 3N interaction play a role in the parity inversion?



$^{10}C(p,p)$ @ IRIS with solid H_2 target

- New experiment at TRIUMF with the novel IRIS solid H_2 target
  - First re-accelerated ^{10}C beam at TRIUMF
  - $^{10}C(p,p)$ angular distributions measured at E_{CM} ~ 4.16 MeV and 4.4 MeV



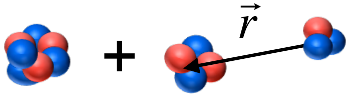
$^{10}C(p,p)$ @ IRIS with solid H_2 target

A. Kumar, R. Kanungo, A. Sanetullaev et al.

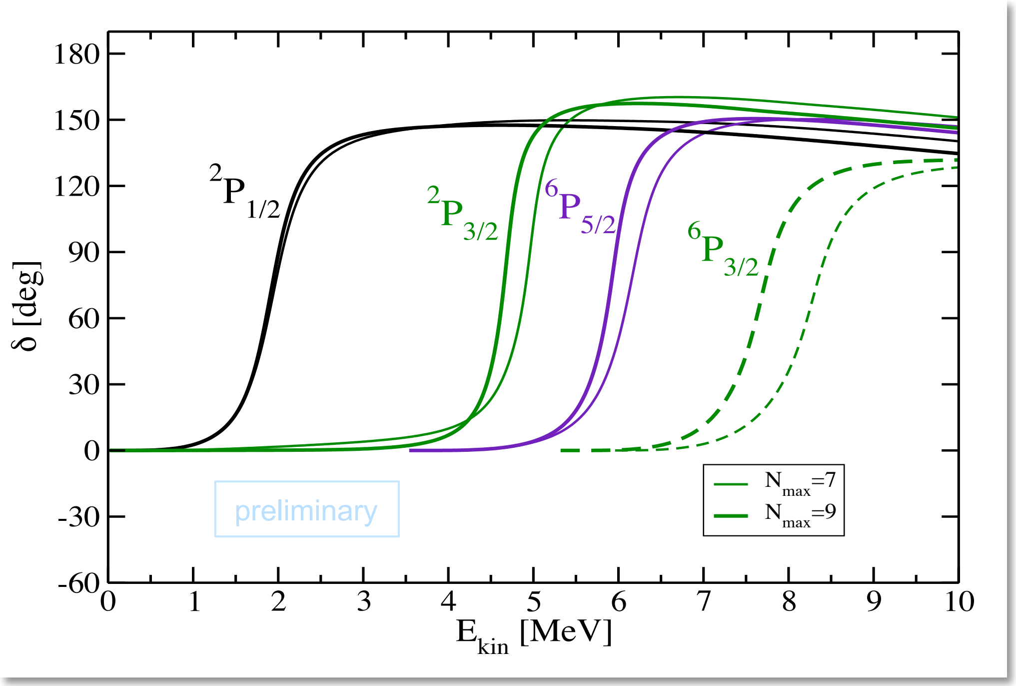
IRIS collaboration:
A. Kumar, R. Kanungo,
A. Sanetullaev *et al.*

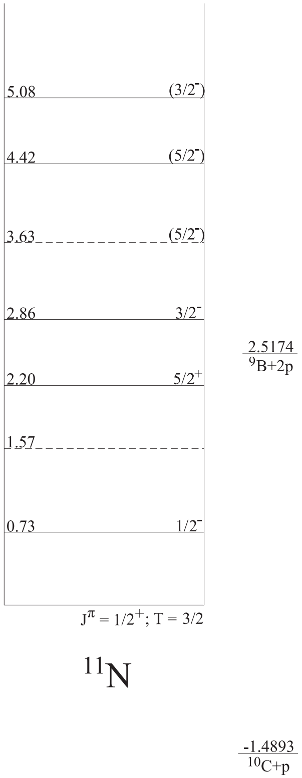
p+^{10}C scattering: structure of ^{11}N resonances

- NCSMC calculations with **chiral NN+3N** (N^{3}LO NN+N^{2}LO 3NF400, NNLOsat)
  - p-^{10}C + ^{11}N
    - ^{10}C: 0^+, 2^+, 2^+ NCSM eigenstates
    - ^{11}N: ≥4 π = -1 and ≥3 π = +1 NCSM eigenstates



chiral NN+3NF400

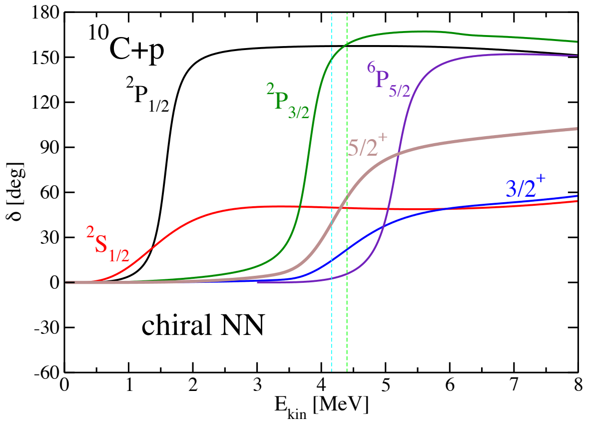


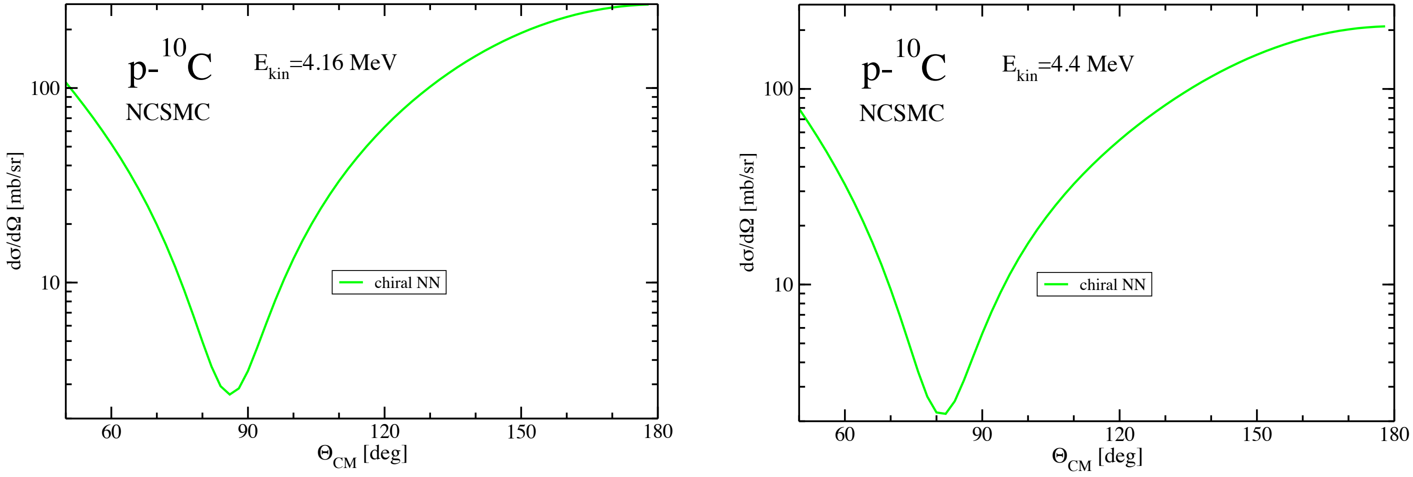


A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth *et al* with IRIS collaboration, in preparation

TRIUMF

p+^{10}C scattering: structure of ^{11}N resonances





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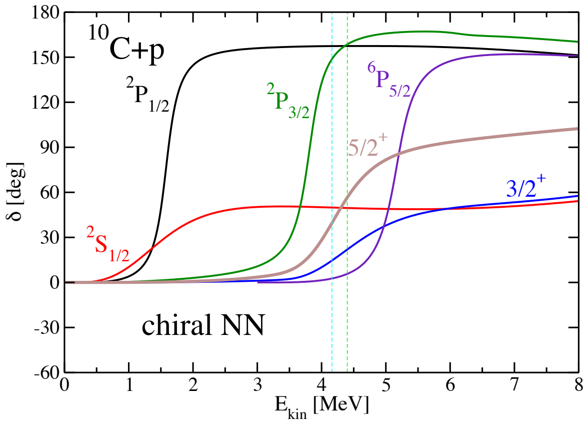
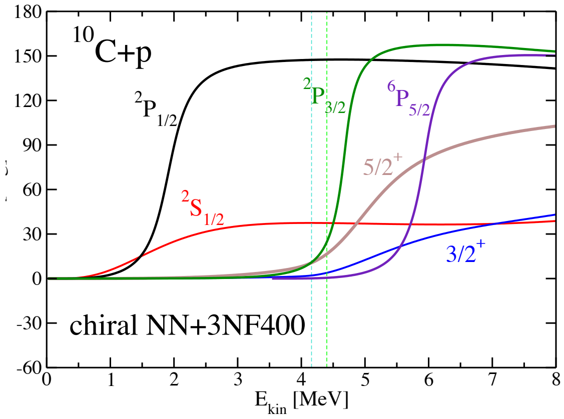
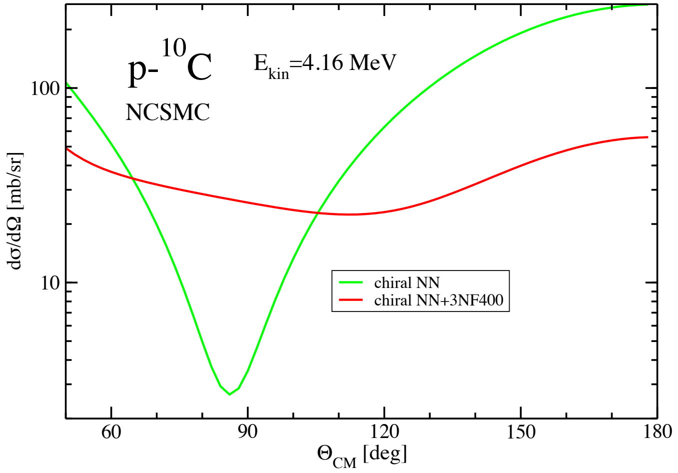
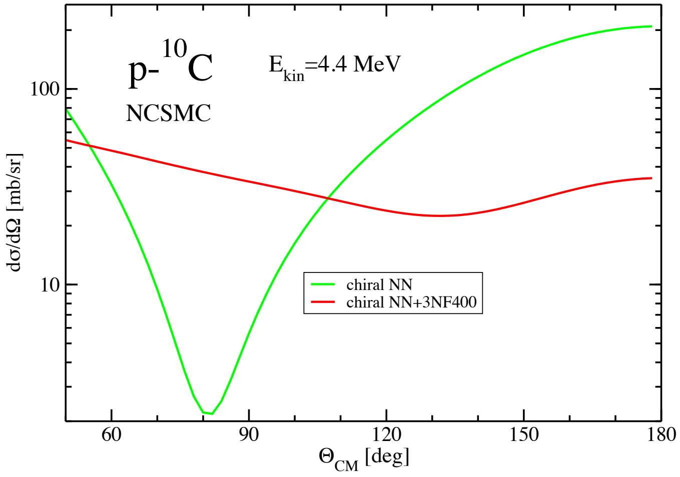
TRIUMF

p+^{10}C scattering: structure of ^{11}N resonances





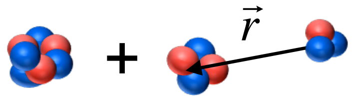


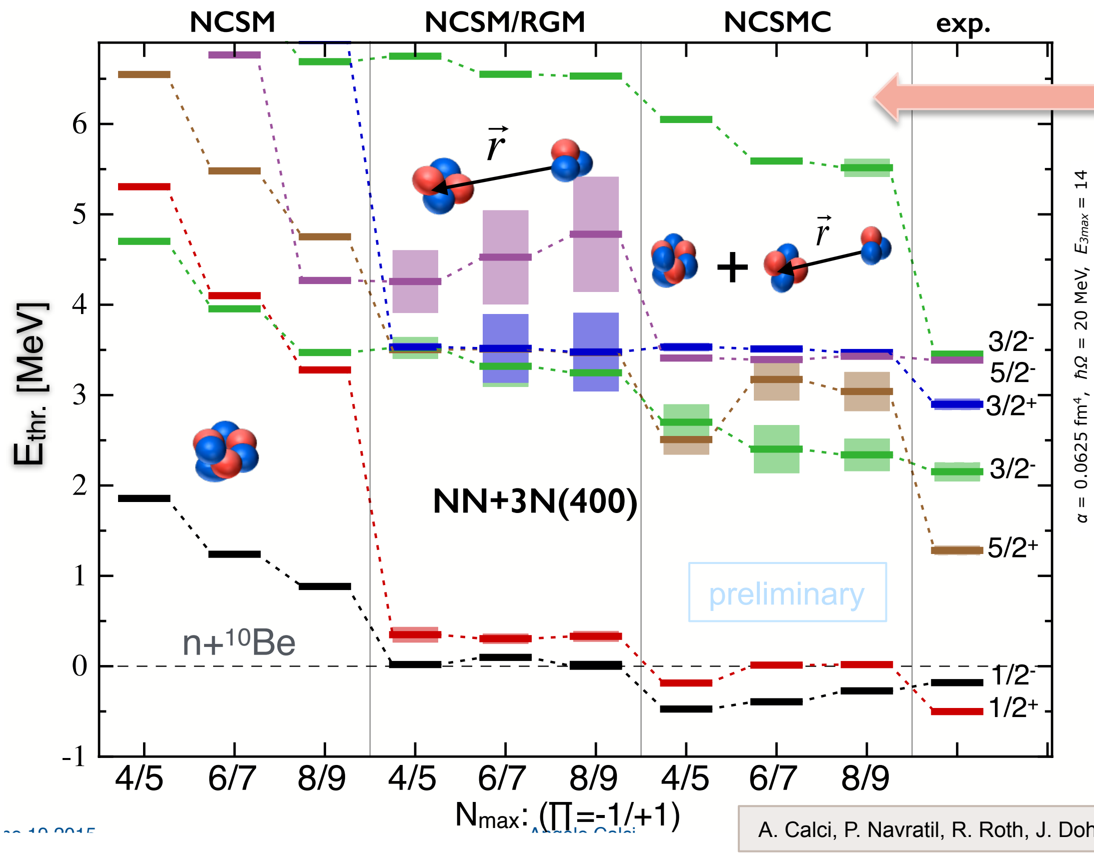


A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth *et al* with IRIS collaboration, in preparation

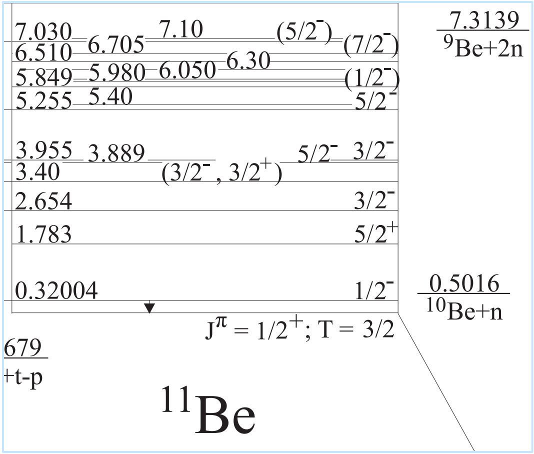
Structure of ^{11}Be from chiral NN+3N forces

- NCSMC calculations **including chiral 3N** (N^{3}LO NN+N^{2}LO 3NF400)
  - n-^{10}Be + ^{11}Be
    - ^{10}Be: 0$^+$, 2$^+$, 2$^+$ NCSM eigenstates
    - ^{11}Be: ≥6 π = -1 and ≥3 π = +1 NCSM eigenstates



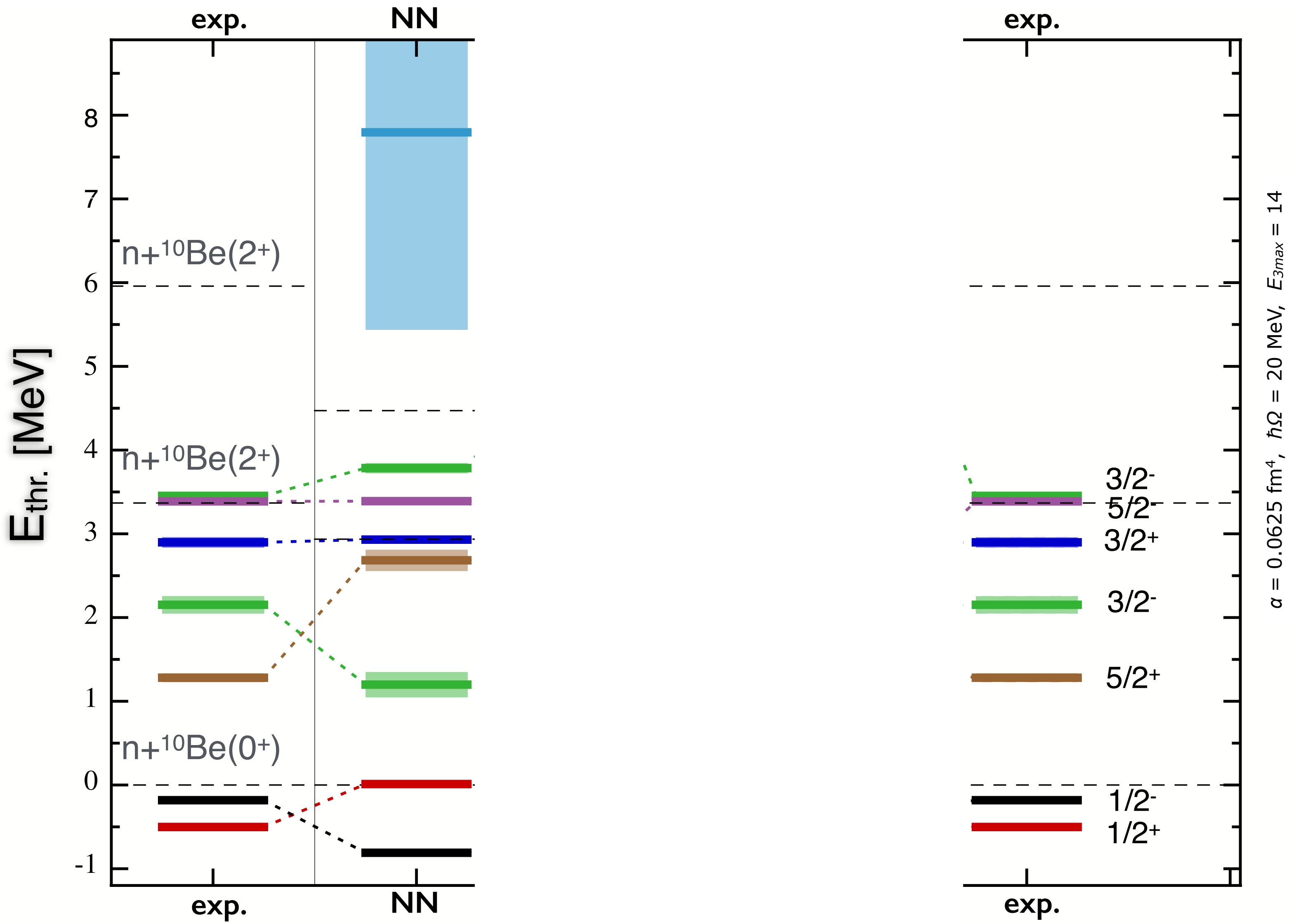


Continuum effects



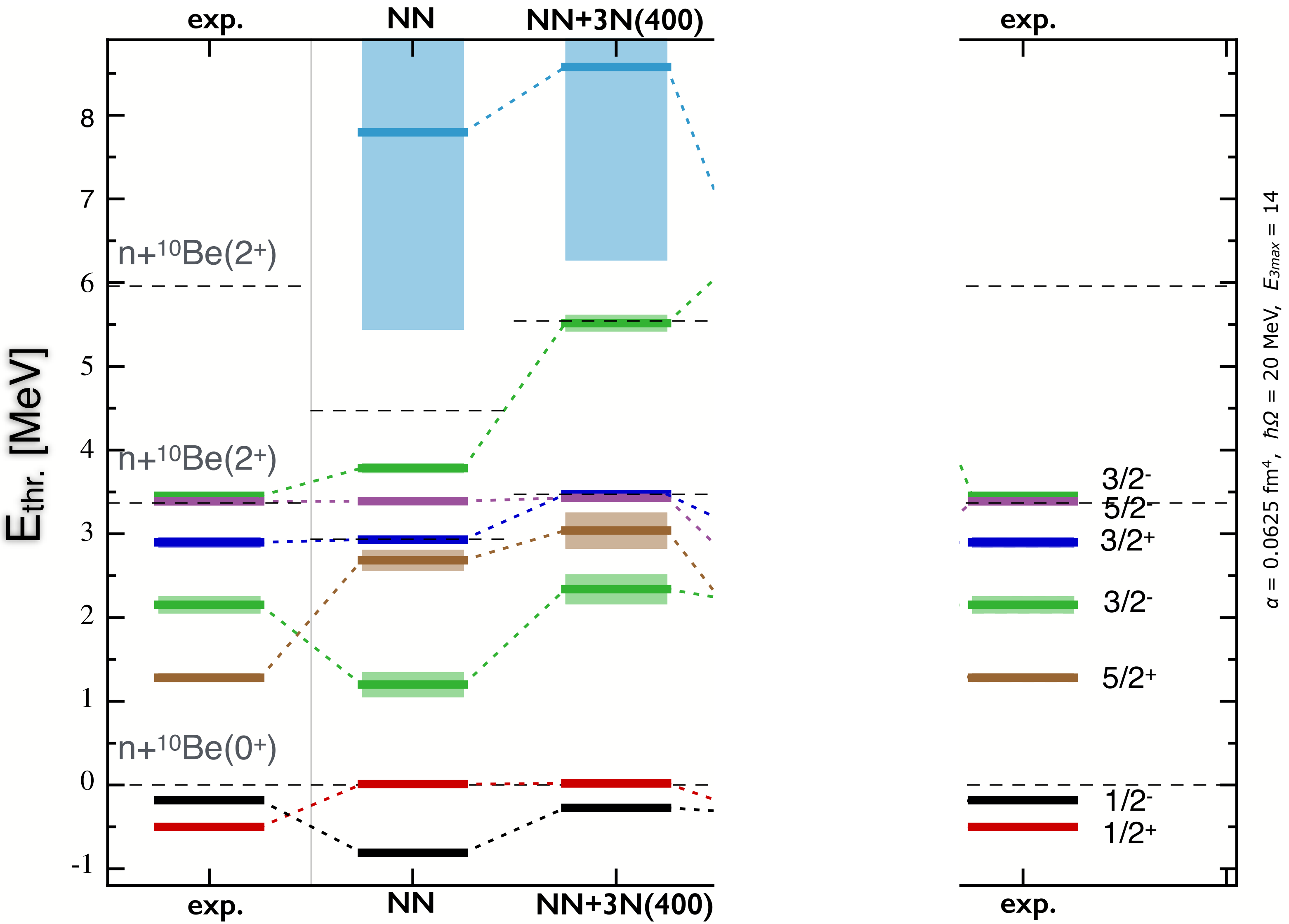
A. Calci, P. Navratil, R. Roth, J. Dohet-Eraly, S. Quaglioni, G. Hupin, arXiv: 1608.03318

^{11}Be within NCSMC: Discrimination among chiral nuclear forces



A. Calci, P. Navratil, R. Roth, J. Dohet-Eraly, S. Quaglioni, G. Hupin, arXiv: 1608.03318

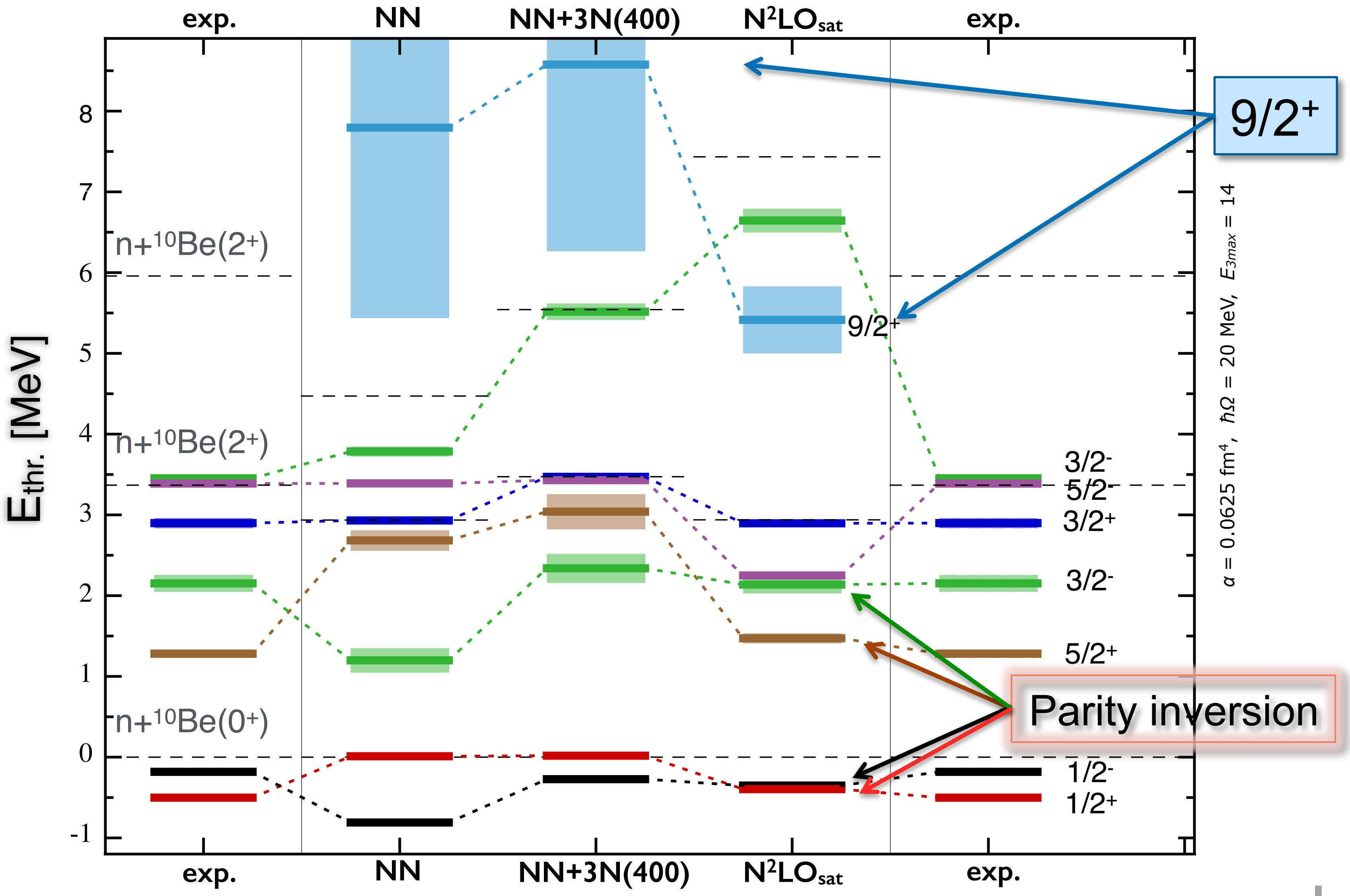
^{11}Be within NCSMC: Discrimination among chiral nuclear forces



A. Calci, P. Navratil, R. Roth, J. Dohet-Eraly, S. Quaglioni, G. Hupin, arXiv: 1608.03318

TRIUMF

^{11}Be within NCSMC: Discrimination among chiral nuclear forces

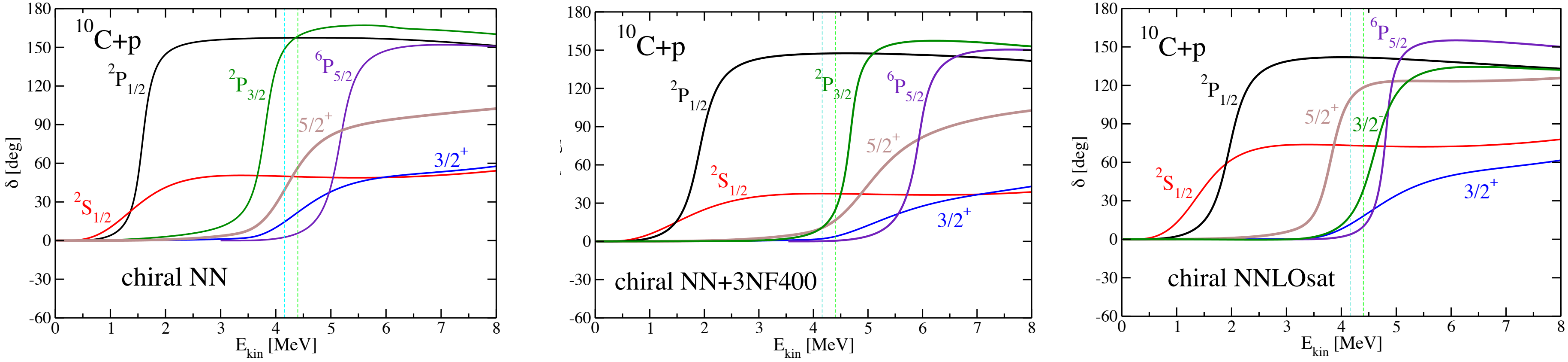


$9/2^+$

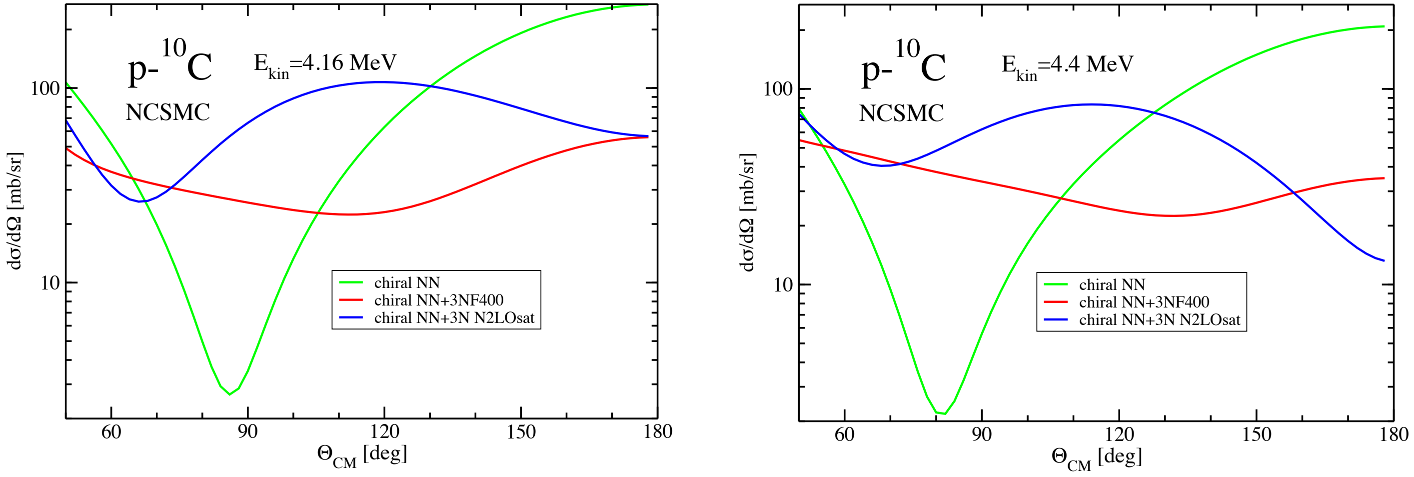
Parity inversion

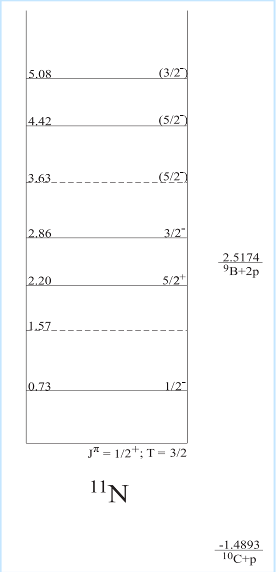
A. Calci, P. Navratil, R. Roth, J. Dohet-Eraly, S. Quaglioni, G. Hupin, arXiv: 1608.03318

p+^{10}C scattering: structure of ^{11}N resonances



Discrimination among chiral nuclear forces

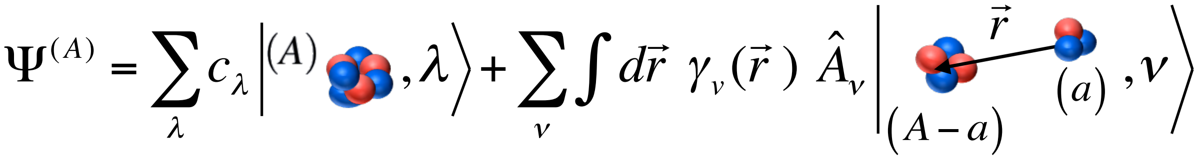




A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth *et al* with IRIS collaboration, in preparation

TRIUMF

NCSMC wave function



$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left|^{(A)} , \lambda \right\rangle + \sum_{\nu} \int d\vec{r}\; \gamma_{\nu}(\vec{r}\,)\; \hat{A}_{\nu} \left|_{(A-a)} \overset{\vec{r}}{\longleftarrow} (a) , \nu \right\rangle$$

$$\left|\Psi_A^{J^\pi T}\right\rangle = \sum_{\lambda} |A\lambda J^\pi T\rangle \left[\sum_{\lambda'} (N^{-\frac{1}{2}})^{\lambda\lambda'} \bar{c}_{\lambda'} + \sum_{\nu'} \int dr'\, r'^2 (N^{-\frac{1}{2}})^{\lambda}_{\nu' r'} \frac{\bar{\chi}_{\nu'}(r')}{r'} \right]$$

$$+ \sum_{\nu\nu'} \int dr\, r^2 \int dr'\, r'^2 \hat{\mathcal{A}}_{\nu} \left|\Phi_{\nu r}^{J^\pi T}\right\rangle \mathcal{N}_{\nu\nu'}^{-\frac{1}{2}}(r, r') \left[\sum_{\lambda'} (N^{-\frac{1}{2}})^{\lambda'}_{\nu' r'} \bar{c}_{\lambda'} + \sum_{\nu''} \int dr''\, r''^2 (N^{-\frac{1}{2}})_{\nu' r' \nu'' r''} \frac{\bar{\chi}_{\nu''}(r'')}{r''} \right].$$

Asymptotic behavior $r \longrightarrow \infty$:

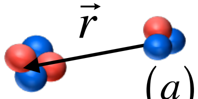
$$\bar{\chi}_{\nu}(r) \sim C_{\nu} W(k_{\nu} r) \qquad \bar{\chi}_{\nu}(r) \sim \mathrm{v}_{\nu}^{-\frac{1}{2}} \left[\delta_{\nu i} I_{\nu}(k_{\nu} r) - U_{\nu i} O_{\nu}(k_{\nu} r) \right]$$

Bound state

Scattering state

Scattering matrix

E1 transitions in NCSMC



$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| {}^{(A)} , \lambda \right\rangle + \sum_{\nu} \int d\vec{r} \; \gamma_{\nu}(\vec{r}\,) \; \hat{A}_{\nu} \left| \; \overset{\vec{r}}{} \; {}_{(A-a)} \; (a) \; , \nu \right\rangle$$

$$\begin{aligned} \vec{E}1 = e \sum_{i=1}^{A-a} \frac{1+\tau_i^{(3)}}{2} \left(\vec{r}_i - \vec{R}^{(A-a)}_{\rm c.m.} \right) \\ + e \sum_{j=A-a+1}^{A} \frac{1+\tau_j^{(3)}}{2} \left(\vec{r}_i - \vec{R}^{(a)}_{\rm c.m.} \right) \\ + e \frac{Z_{(A-a)} a - Z_{(a)} (A-a)}{A} \vec{r}_{A-a,a} \, . \end{aligned}$$

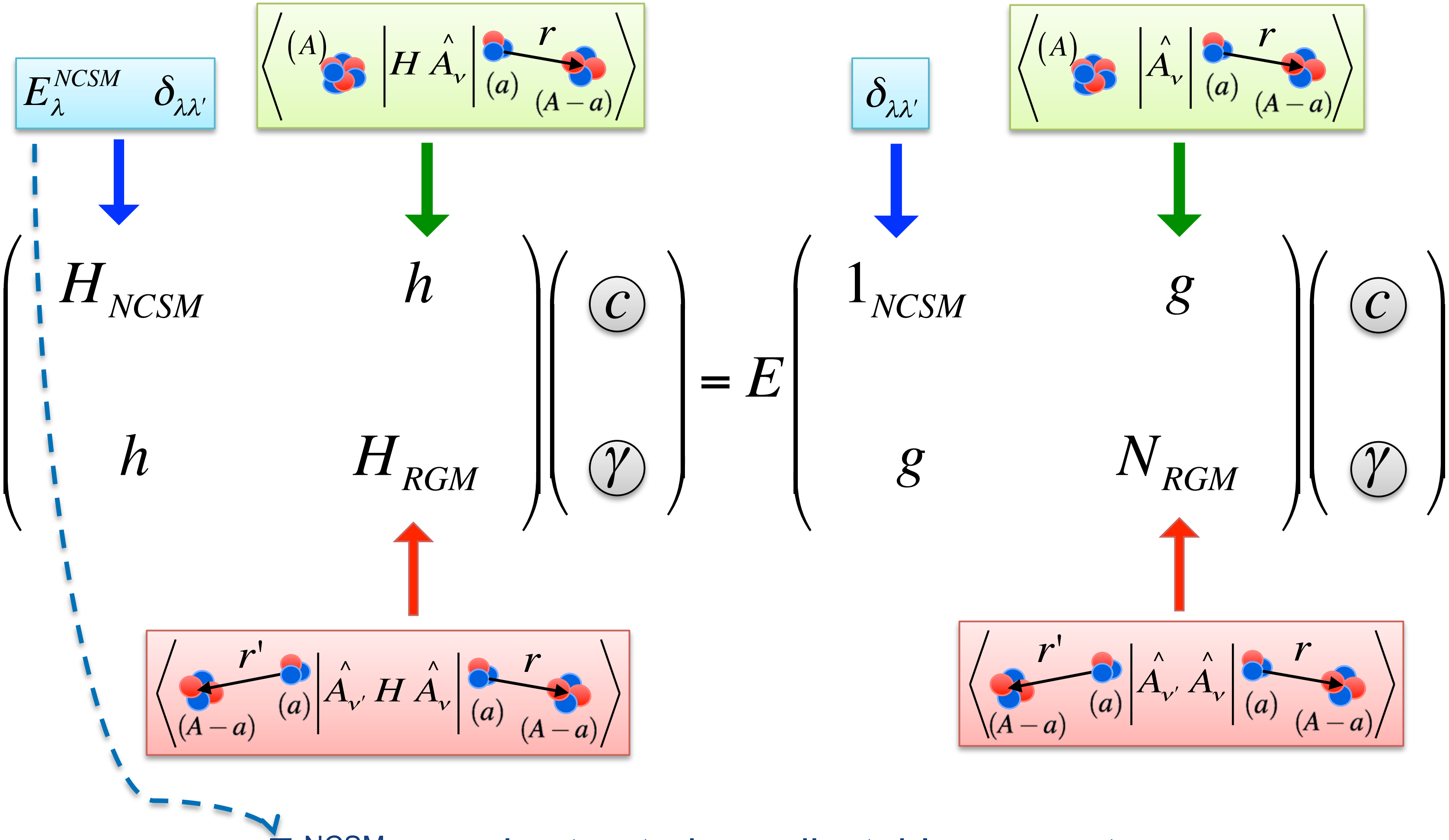
$$\mathcal{M}^E_{1\mu} = e \sum_{j=1}^{A} \frac{1+\tau_j^{(3)}}{2} \left| \vec{r}_j - \vec{R}^{(A)}_{\rm c.m.} \right| Y_{1\mu}(\widehat{r_j - R^{(A)}_{\rm c.m.}})$$

$$\begin{aligned} \mathcal{B}^{E1}_{fi} = & \sum_{\lambda\lambda'} c^{*f}_{\lambda'} \langle A\lambda' J_f^{\pi_f} T_f || \mathcal{M}^E_1 || A\lambda J_i^{\pi_i} T_i \rangle \, c^i_{\lambda} \\ & + \sum_{\lambda'\nu} \int dr r^2 \, c^{*f}_{\lambda'} \langle A\lambda' J_f^{\pi_f} T_f || \mathcal{M}^E_1 \hat{\mathcal{A}}_{\nu} || \Phi^i_{\nu r} \rangle \, \frac{\gamma^i_{\nu}(r)}{r} \\ & + \sum_{\lambda\nu'} \int dr' r'^2 \frac{\gamma^{*f}_{\nu'}(r')}{r'} \langle \Phi^f_{\nu' r'} || \hat{\mathcal{A}}_{\nu'} \mathcal{M}^E_1 || A\lambda J_i^{\pi_i} T_i \rangle \, c^i_{\lambda} \\ & + \sum_{\nu\nu'} \int dr' r'^2 \int dr r^2 \frac{\gamma^{*f}_{\nu'}(r')}{r'} \langle \Phi^f_{\nu' r'} || \hat{\mathcal{A}}_{\nu'} \mathcal{M}^E_1 \hat{\mathcal{A}}_{\nu} || \Phi^i_{\nu r} \rangle \, \frac{\gamma^i_{\nu}(r)}{r} \end{aligned}$$

Photo-disassociation of ^{11}Be

Bound to bound	NCSM	NCSMC-phenom	Expt.
B(E1; $1/2^+ \rightarrow 1/2^-$) [e^2 fm^2]	0.0005	0.117	0.102(2)

NCSMC phenomenology



$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix}\begin{pmatrix} c \\ \gamma \end{pmatrix} = E \begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix}\begin{pmatrix} c \\ \gamma \end{pmatrix}$$

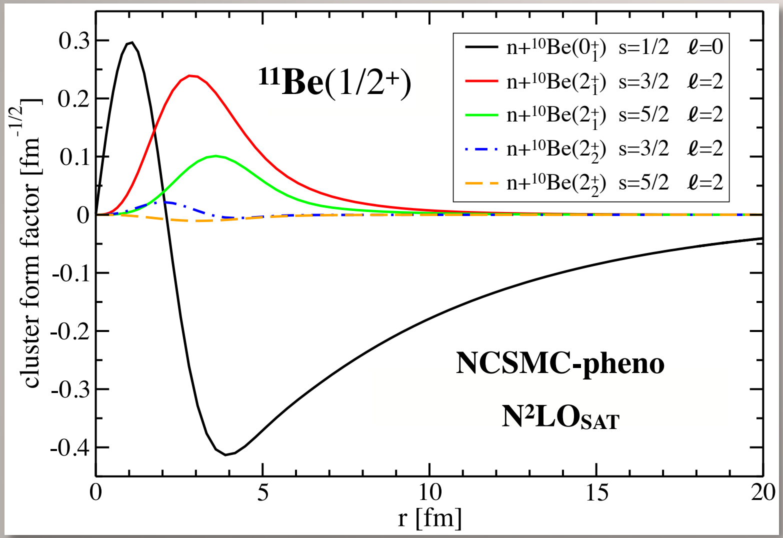
E_λ^{NCSM} energies treated as adjustable parameters

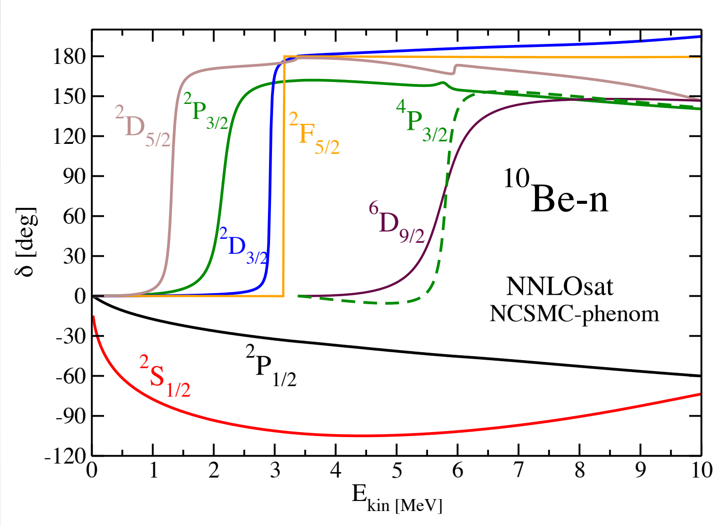
Cluster excitation energies set to experimental values

Photo-disassociation of ^{11}Be

Bound to bound	NCSM	NCSMC-phenom	Expt.
B(E1; $1/2^+ \rightarrow 1/2^-$) [e^2 fm^2]	0.0005	0.117	0.102(2)

Halo structure

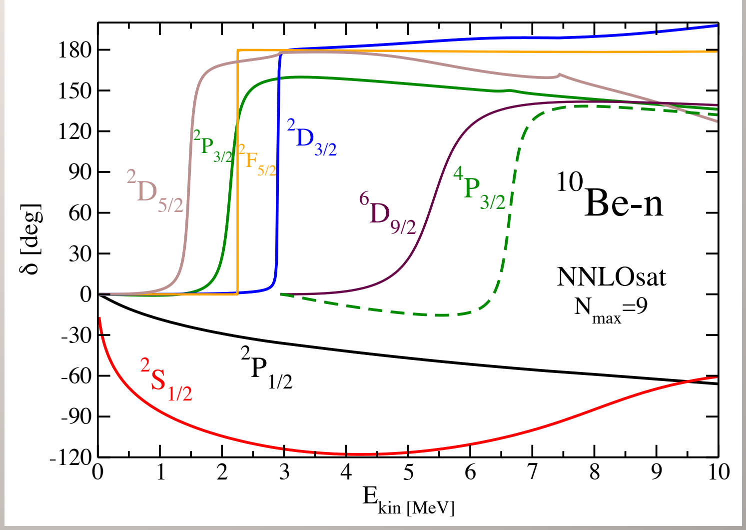




cluster form factor

$$= r \left\langle \Phi_{\nu r}^{J^\pi T} \middle| \hat{A}_\nu \middle| \psi^{J^\pi T} \right\rangle$$

$$\left| \Phi_{\nu r}^{J^\pi T} \right\rangle = \left[\left(\left| {}^{10}\mathrm{Be}\ \alpha_1 I_1^{\pi_1} T_1 \right\rangle \left| n \tfrac{1}{2}^+ \tfrac{1}{2} \right\rangle \right)^{(sT)} Y_\ell(\hat{r}_{10,1}) \right]^{(J^\pi T)} \frac{\delta(r - r_{10,1})}{r r_{10,1}}$$

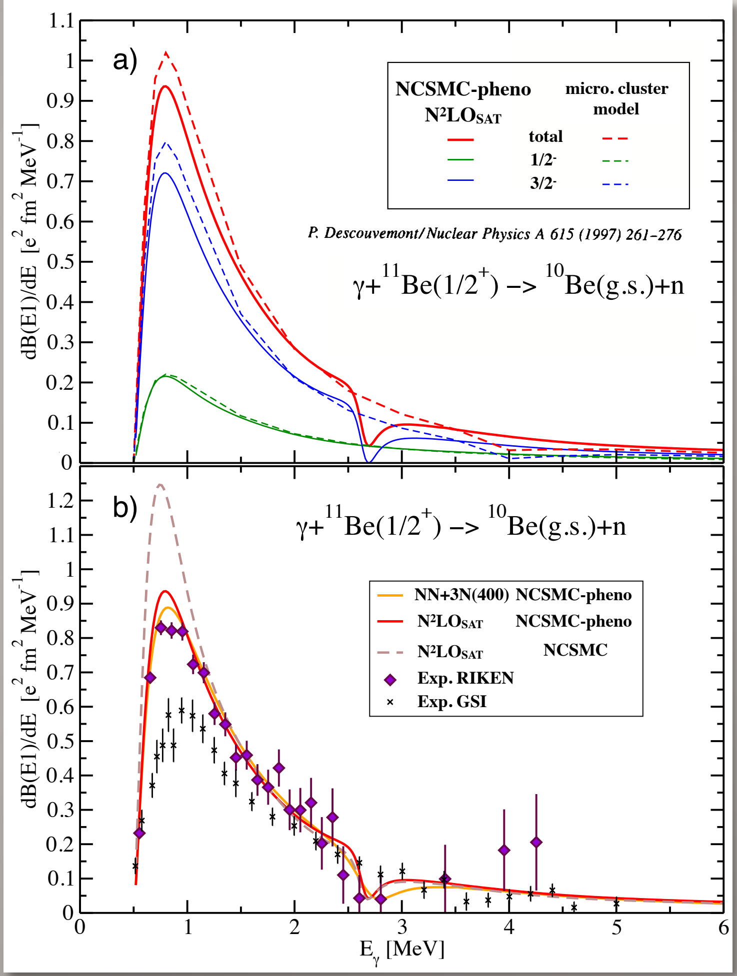


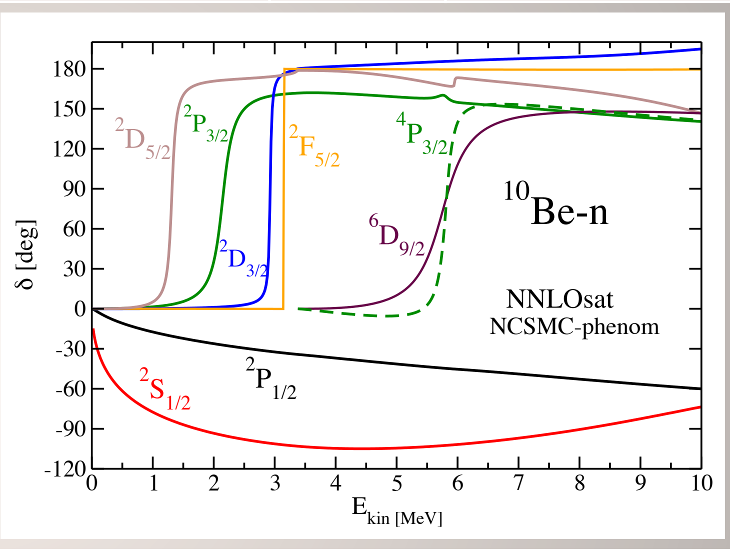
A. Calci, P. Navratil, R. Roth, J. Dohet-Eraly, S. Quaglioni, G. Hupin, arXiv: 1608.03318

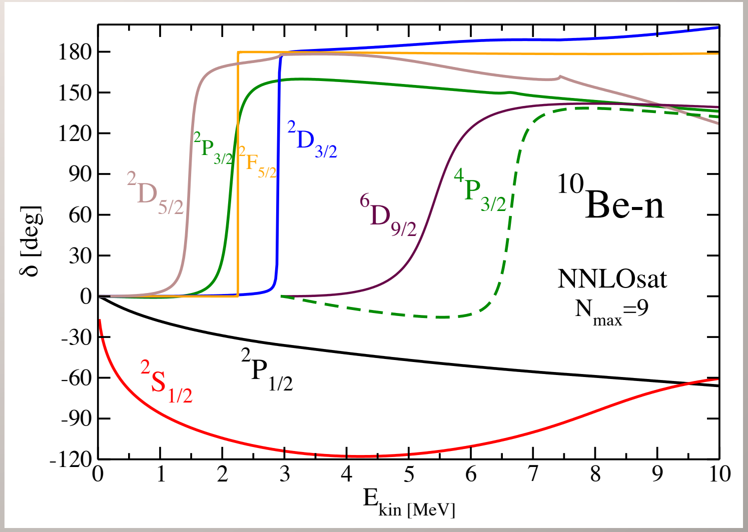
Photo-disassociation of ^{11}Be

Bound to continuum

Bound to bound	NCSM	NCSMC-phenom	Expt.
B(E1; $1/2^+ \rightarrow 1/2^-$) [e^2 fm^2]	0.0005	0.117	0.102(2)







A. Calci, P. Navratil, R. Roth, J. Dohet-Eraly, S. Quaglioni, G. Hupin, arXiv: 1608.03318

Next: p+^{11}C scattering and ^{11}C(p,γ)^{12}N capture

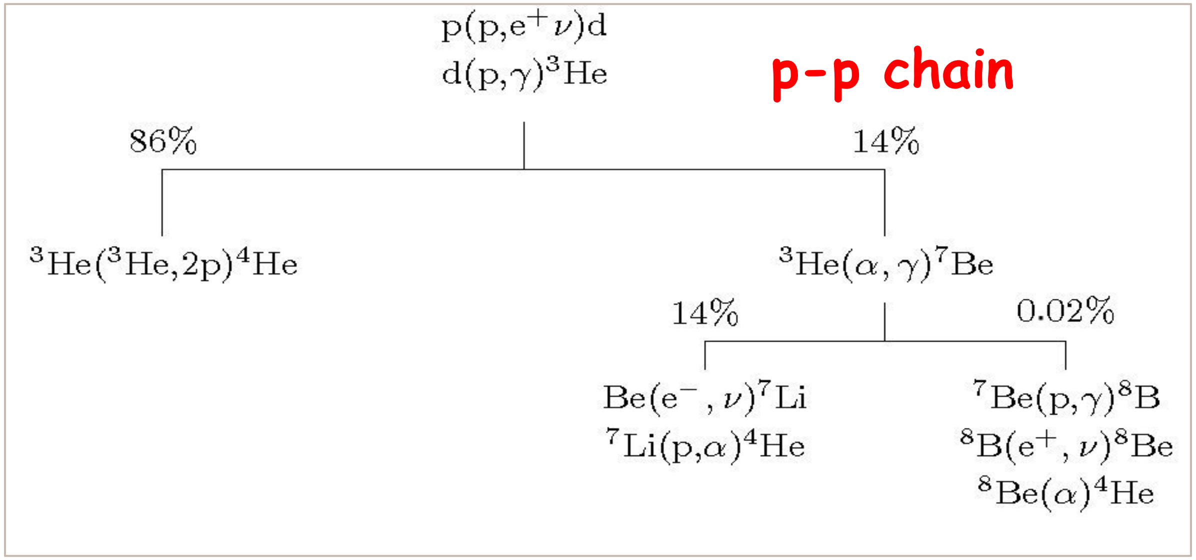
- Measurement of ^{11}C(p,p) resonance scattering planned at TRIUMF
    - TUDA facility
    - ^{11}C beam of sufficient intensity produced

- NCSMC calculations of ^{11}C(p,p) with chiral NN+3N under way

- Obtained wave functions will be used to calculate ^{11}C(p,γ)^{12}N capture relevant for astrophysics

Next: p+^{11}C scattering and ^{11}C(p,γ)^{12}N capture

- ^{11}C(p,γ)^{12}N capture relevant in hot *p-p* chain: Link between pp chain and the CNO cycle - bypass of slow triple alpha capture ^{4}He(αα,γ)^{12}C



$p(p,e^+\nu)d$
$d(p,\gamma)^3He$

p-p chain

86%

14%

$^3He(^3He,2p)^4He$

$^3He(\alpha,\gamma)^7Be$

14%

0.02%

$Be(e^-,\nu)^7Li$
$^7Li(p,\alpha)^4He$

$^7Be(p,\gamma)^8B$
$^8B(e^+,\nu)^8Be$
$^8Be(\alpha)^4He$

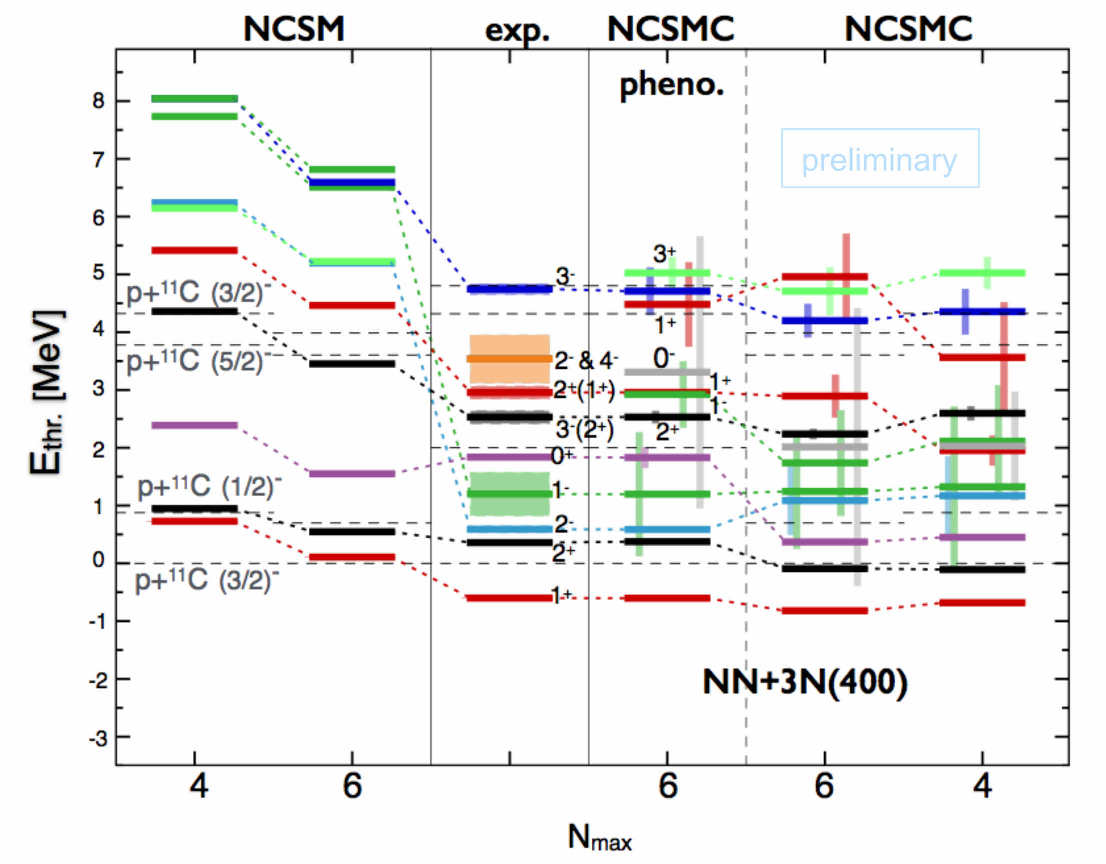
$$^3He(\alpha,\gamma)^7Be(\alpha,\gamma)^{11}C(p,\gamma)^{12}N(p,\gamma)^{13}O(\beta^+,\nu)^{13}N(p,\gamma)^{14}O$$

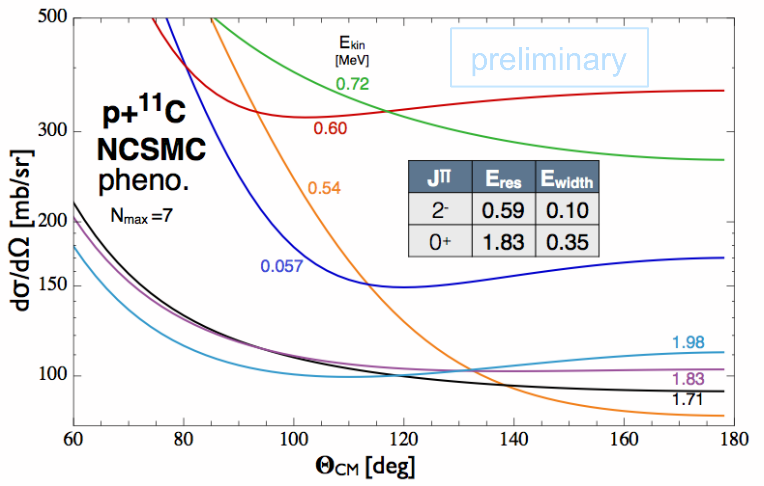
$$^3He(\alpha,\gamma)^7Be(\alpha,\gamma)^{11}C(p,\gamma)^{12}N(\beta^+,\nu)^{12}C(p,\gamma)^{13}N(p,\gamma)^{14}O$$

$$^{11}\mathrm{C}(\beta^+\ \nu)^{11}\mathrm{B}(p,\alpha)^8\mathrm{Be}(^4\mathrm{He},^4\mathrm{He})$$

Next: p+^{11}C scattering and ^{11}C(p,γ)^{12}N capture

- NCSMC calculations of ^{11}C(p,p) with chiral NN+3N under way



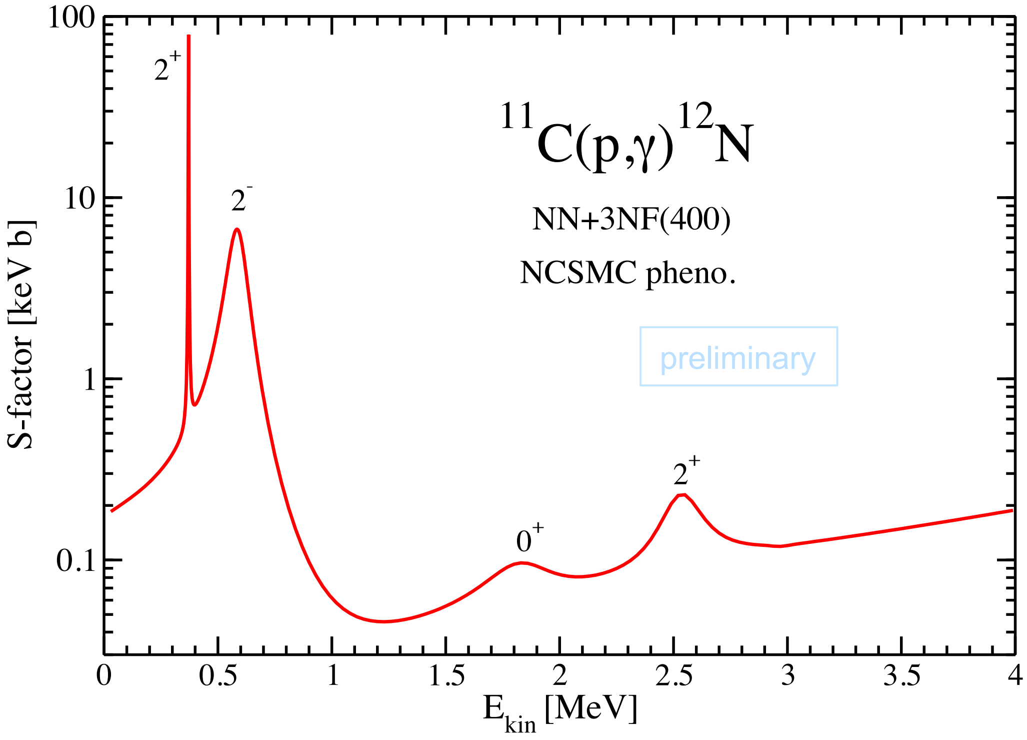


Jπ	E_{res}	E_{width}
2$^-$	0.59	0.10
0$^+$	1.83	0.35

NCSMC calculations to be validated by measured cross sections and applied to calculate the ^{11}C(p,γ)^{12}N capture

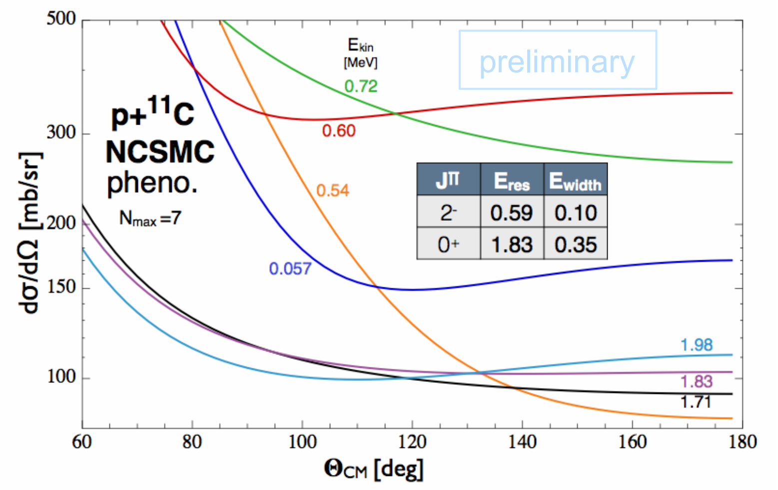
Next: p+^{11}C scattering and ^{11}C(p,γ)^{12}N capture

- NCSMC calculations of ^{11}C(p,p) with chiral NN+3N under way



$$S(E) = E\sigma(E)\exp[2\pi\eta(E)]$$

$$\eta(E) = Z_{A-a}Z_a e^2 / \hbar v_{A-a,a}$$



Jπ	E_{res}	E_{width}
2-	0.59	0.10
0+	1.83	0.35

Gamow factor

$$\psi_C(0) = \Gamma(1+i\eta)e^{-\eta\pi/2}$$

$$|\psi_C(0)|^2 \approx 2\pi\eta e^{-2\eta\pi} \quad \text{for} \quad \eta >> 1$$

…relevant for low-energy charged nuclear reactions - astrophysics

Solar *p-p* chain

$p(p,e^+\nu)d$

$d(p,\gamma)^3He$

p-p chain

86%

$^3He(^3He,2p)^4He$

14%

$^3He(\alpha,\gamma)^7Be$

14%

$^7Be(e^-,\nu)^7Li$

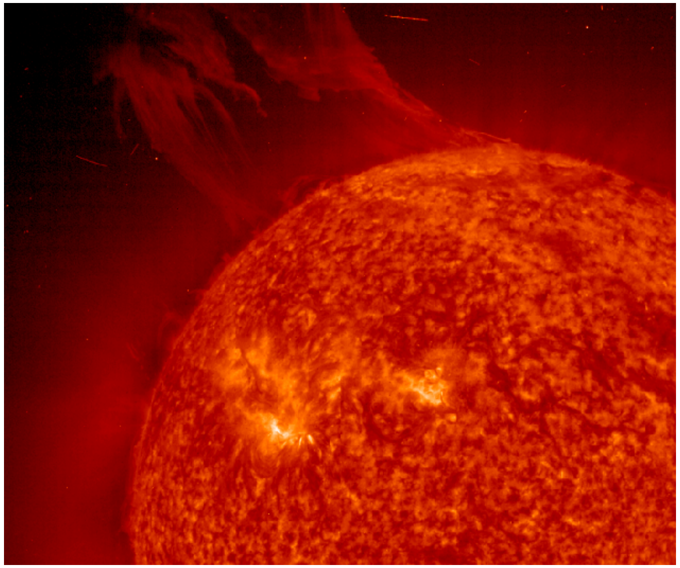
$^7Li(p,\alpha)^4He$

0.02%

$^7Be(p,\gamma)^8B$

$^8B(e^+,\nu)^8Be$

$^8Be(\alpha)^4He$



Solar neutrinos

$E_\nu < 15$ MeV

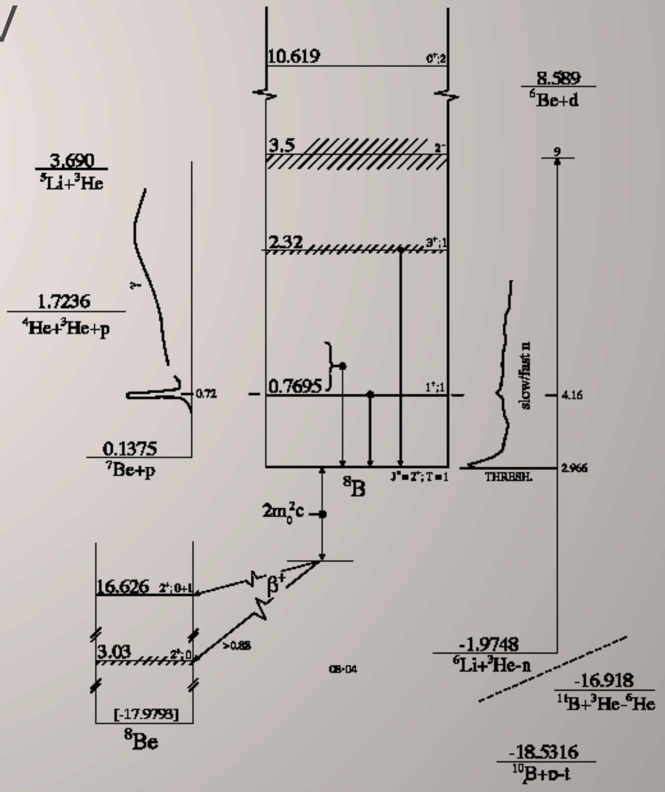
^{7}Be(p,γ)^{8}B S-factor

- S_{17} one of the main inputs for understanding the solar neutrino flux
  - Needs to be known with high precision
- Current evaluation has uncertainty ~ 10%
  - Theory needed for extrapolation to ~ 10 keV

$$S(E) = E\sigma(E)\exp[2\pi\eta(E)]$$

$$\eta(E) = Z_{A-a}Z_a e^2/\hbar v_{A-a,a}$$

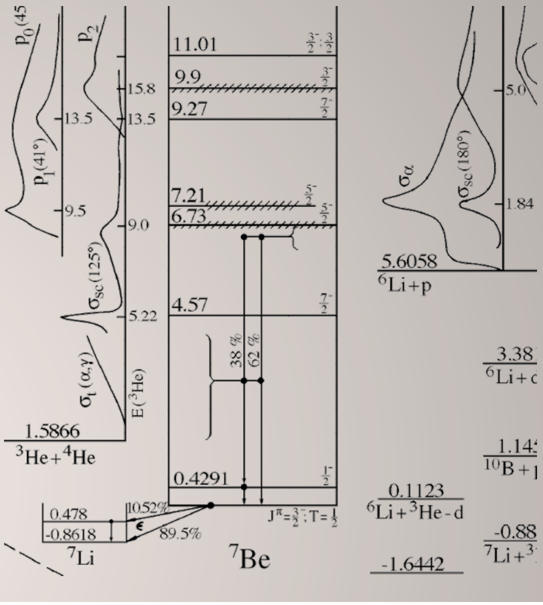
$$\boxed{\left\langle {}^8\mathrm{B}_{\text{g.s.}} \middle| E1 \middle| {}^7\mathrm{Be}_{\text{g.s.}} + \mathrm{p} \right\rangle}$$



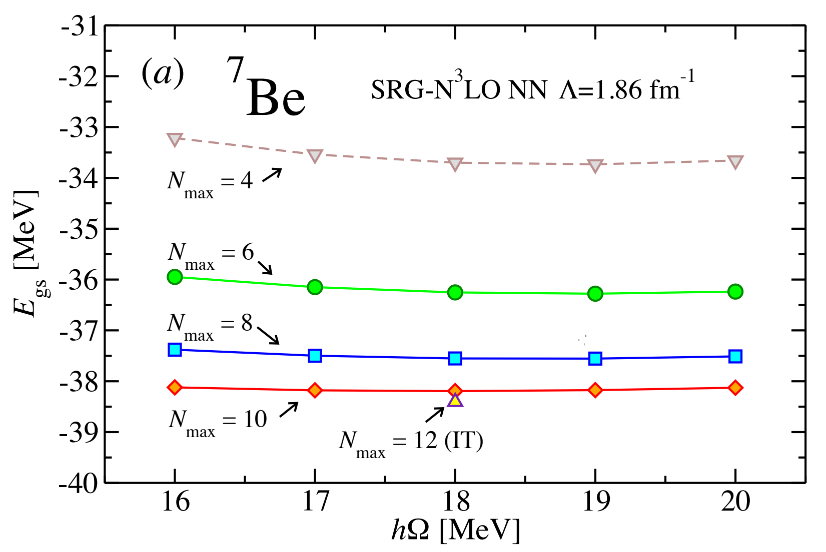
TRIUMF

^{7}Be(p,γ)^{8}B radiative capture: Input - *NN* interaction, ^{7}Be eigenstates

- Similarity-Renormalization-Group (SRG) evolved chiral N^{3}LO *NN* interaction
    - Accurate
    - Soft: Evolution parameter Λ
        - Study dependence on Λ



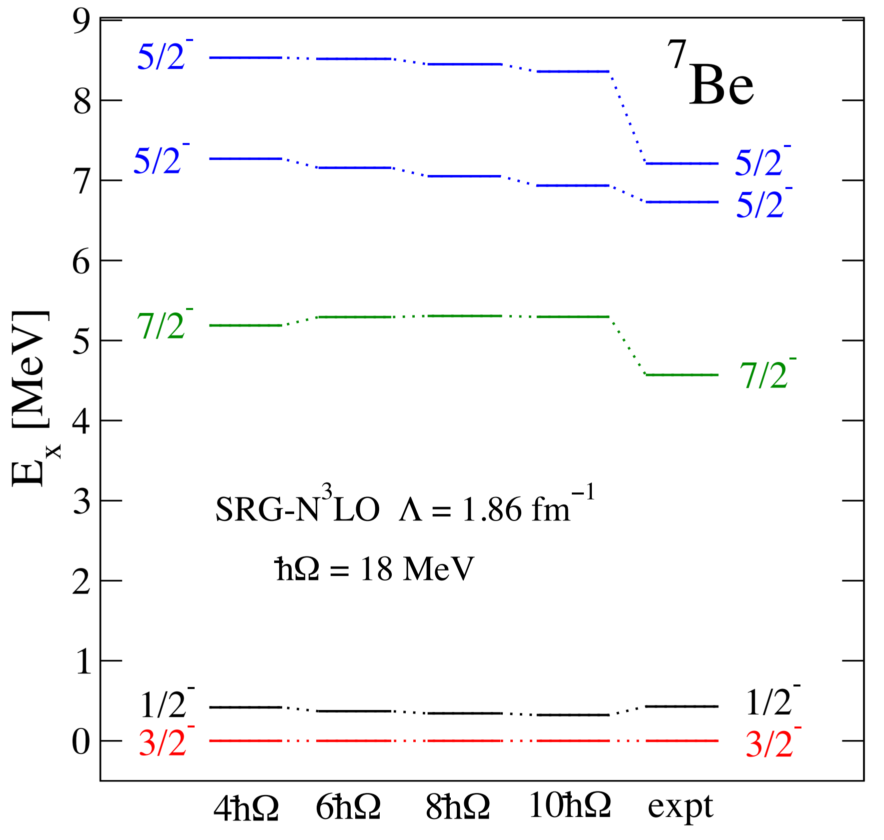
- ^{7}Be
    - NCSM up to N_{max}=10, Importance Truncated NCSM up to N_{max}=14
    - Variational calculation
        - optimal HO frequency from the ground-state minimum
        - For the selected NN potential with Λ=1.86 fm^{-1}: hΩ=18 MeV

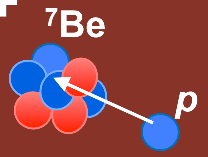


^{7}Be

Input: ^{7}Be eigenstates

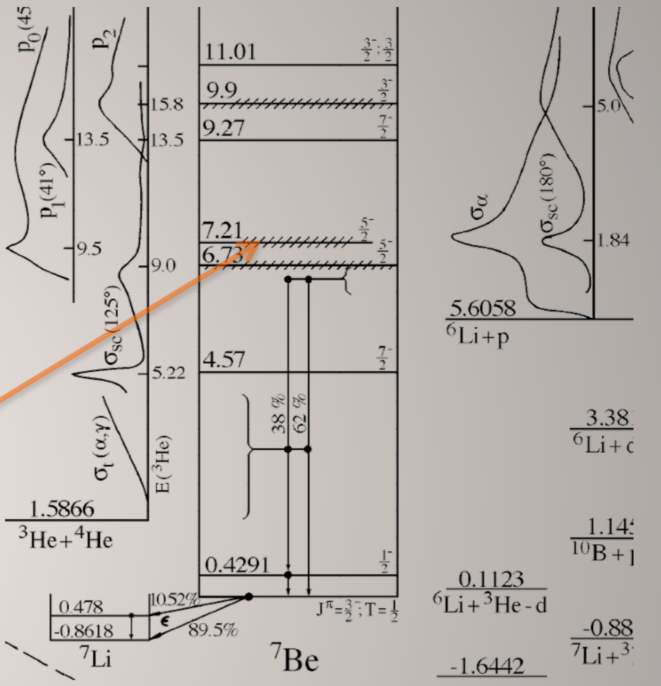
- Excited states at the optimal HO frequency, ħΩ=18 MeV

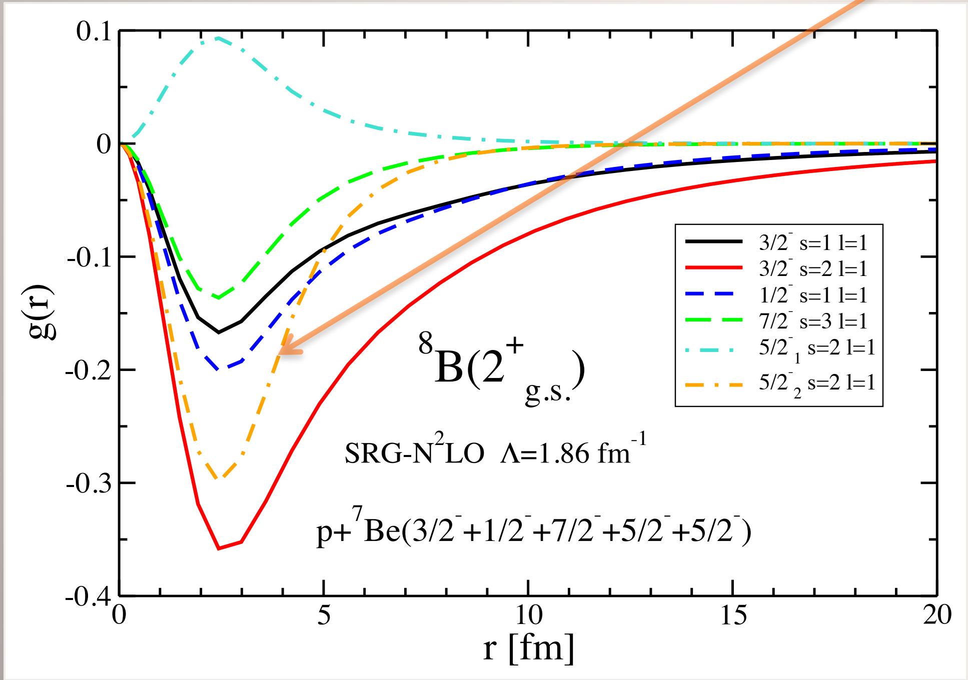




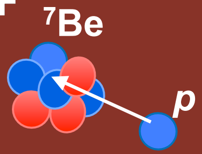
Structure of the ^{8}B ground state

- NCSM/RGM *p*-^{7}Be calculation
  - five lowest ^{7}Be states: $3/2^-$, $1/2^-$, $7/2^-$, $5/2^-_1$, $5/2^-_2$
  - Soft NN SRG-N^{3}LO with $\Lambda = 1.86\ \text{fm}^{-1}$
- ^{8}B 2^+ g.s. bound by 136 keV (Expt 137 keV)
  - Large *P*-wave $5/2^-_2$ component





$5/2^-_2$ state of ^{7}Be should be included in ^{7}Be$(p,\gamma)^8$B calculations



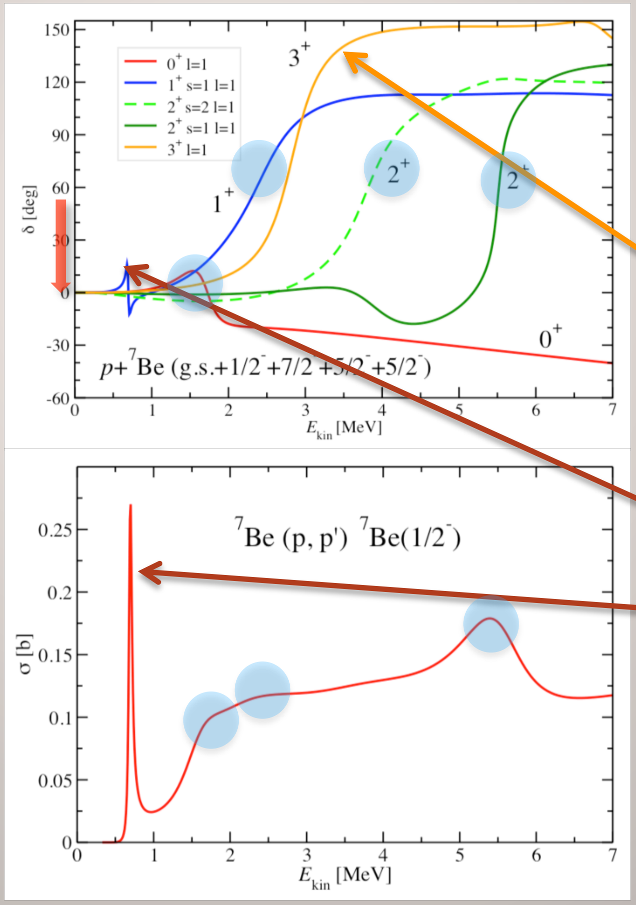
p-^{7}Be scattering

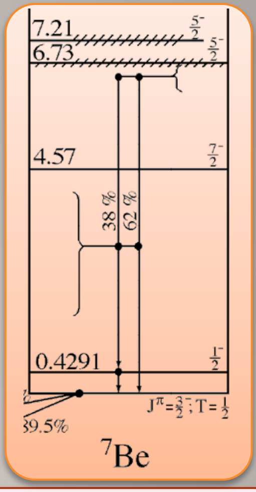
- NCSM/RGM calculation of p-^{7}Be scattering
  - ^{7}Be states $3/2^-$, $1/2^-$, $7/2^-$, $5/2^-_1$, $5/2^-_2$
  - Soft NN potential (SRG-N^{3}LO with $\Lambda = 1.86$ fm^{-1})

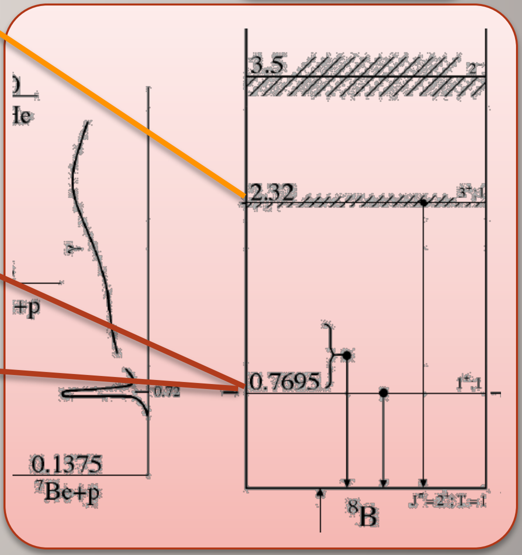
^{8}B 2^+ g.s. **bound** by 136 keV
(expt. bound by 137 keV)

New 0^+, 1^+, and two 2^+ resonances **predicted**

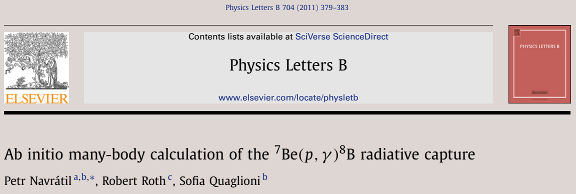
$s=1$ $l=1$ 2^+ clearly visible in (p,p') cross sections







PRC **82**, 034609 (2010)


Physics Letters B 704 (2011) 379–383

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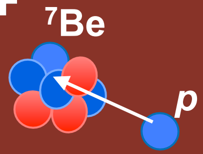
Ab initio many-body calculation of the ^{7}Be$(p,\gamma)^8$B radiative capture

Petr Navrátil [a,b,*], Robert Roth [c], Sofia Quaglioni [b]

TRIUMF



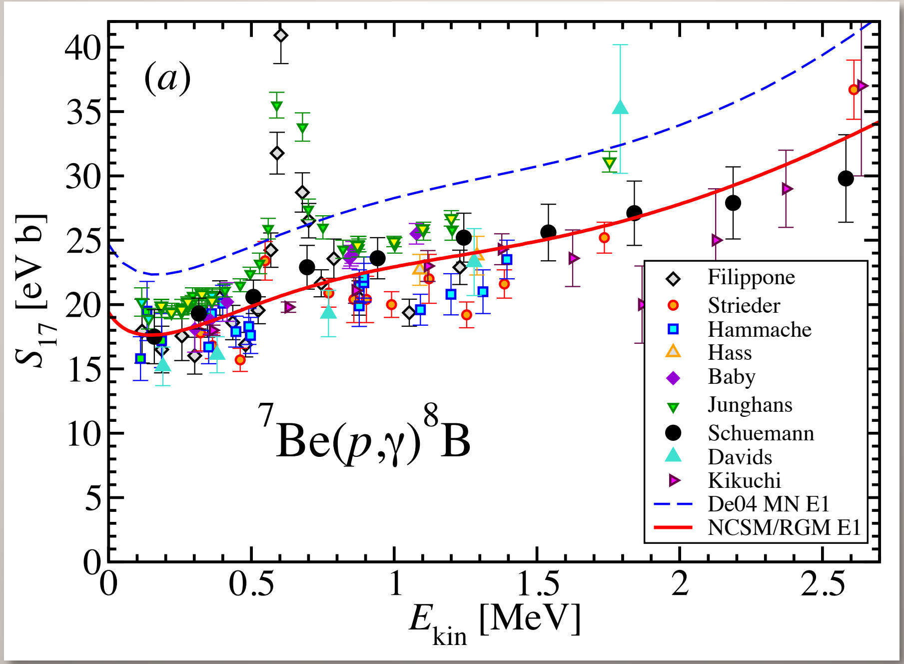
^{7}Be(p,γ)^{8}B radiative capture

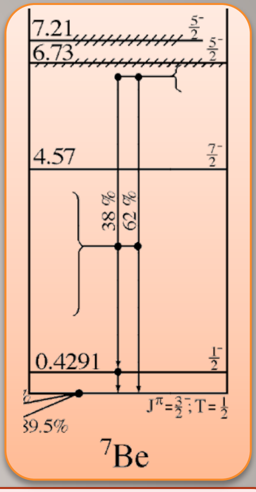
- NCSM/RGM calculation of ^{7}Be(p,γ)^{8}B radiative capture
  - ^{7}Be states $3/2^-$,$1/2^-$, $7/2^-$, $5/2^-_1$, $5/2^-_2$
  - Soft NN potential (SRG-N^{3}LO with Λ = 1.86 fm^{-1})

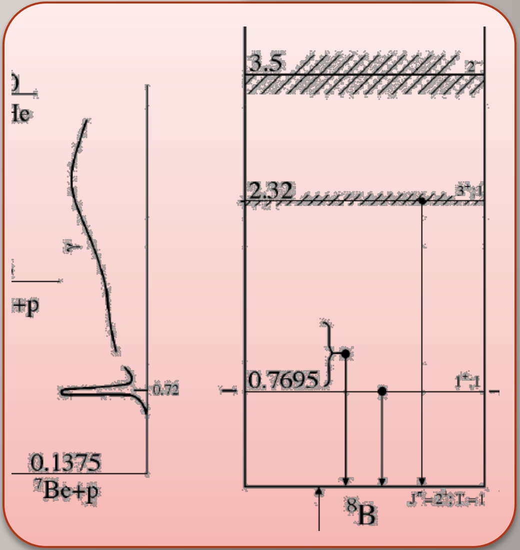
^{8}B 2^+ g.s. **bound** by 136 keV
(expt. 137 keV)

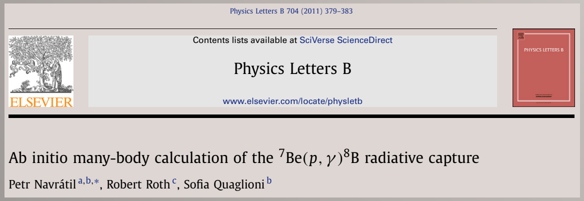
S(0) ~ 19.4(0.7) eV b

Data evaluation:
S(0)=20.8(2.1) eV b









Physics Letters B 704 (2011) 379–383

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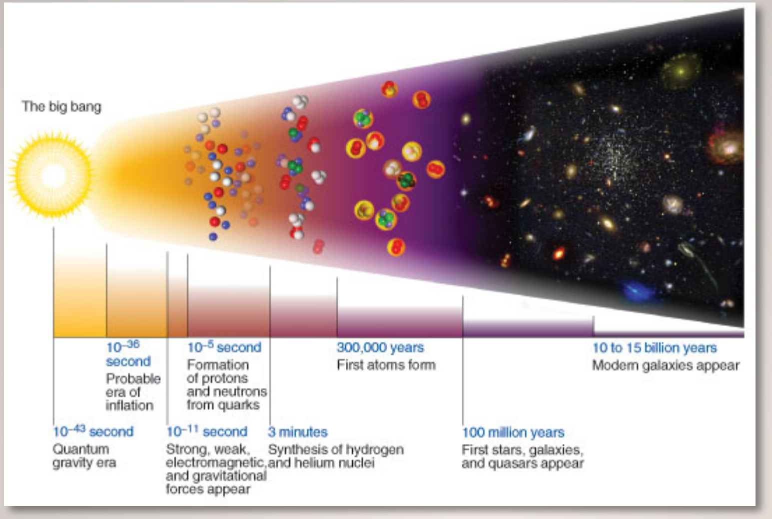
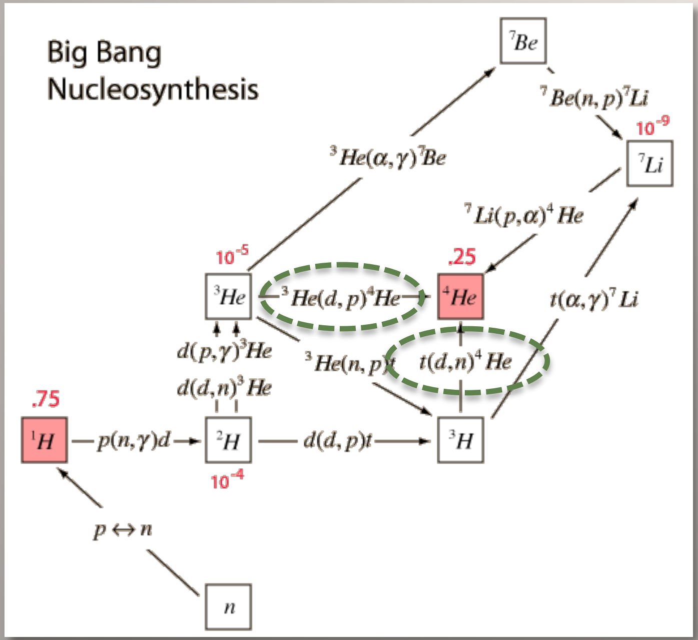
ELSEVIER

Ab initio many-body calculation of the ^{7}Be(p, γ)^{8}B radiative capture

Petr Navrátil[a,b,*], Robert Roth[c], Sofia Quaglioni[b]

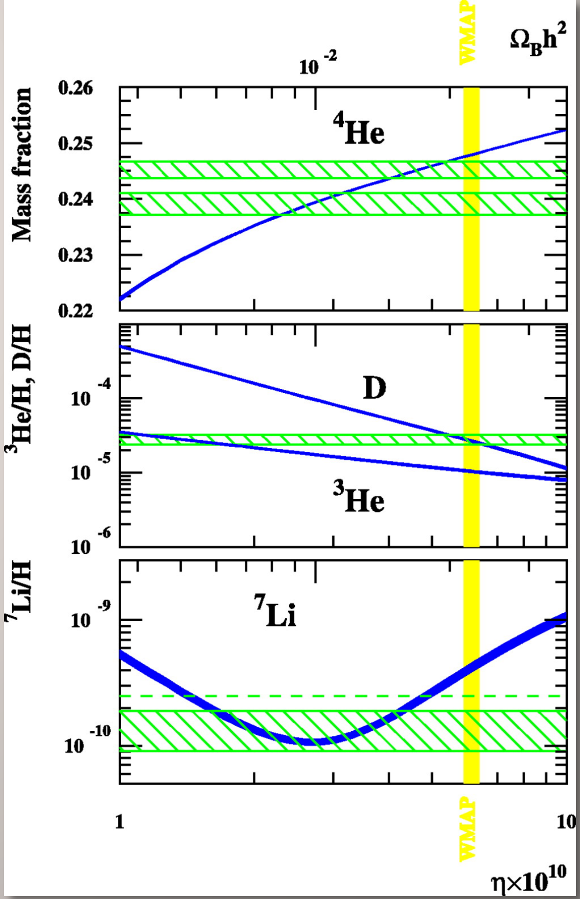
Big Bang nucleosythesis





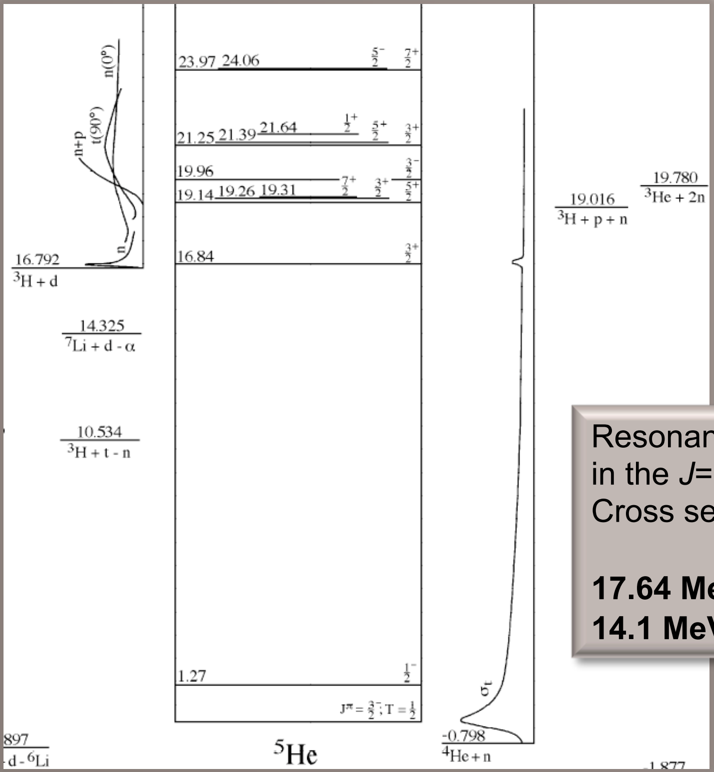
Key reactions

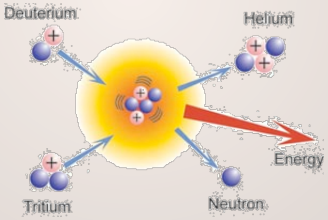
^{7}Li puzzle



Deuterium-Tritium fusion: a future energy source

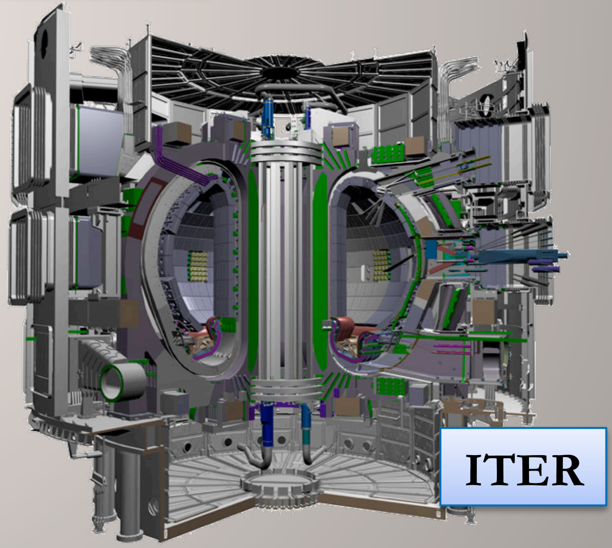
- The d+^{3}H→n+^{4}He reaction
  - The most promising for the production of fusion energy in the near future
  - Will be used to achieve inertial-confinement (laser-induced) fusion at NIF, and magnetic-confinement fusion at ITER
  - With its mirror reaction, ^{3}He(d,p)^{4}He, important for Big Bang nucleosynthesis



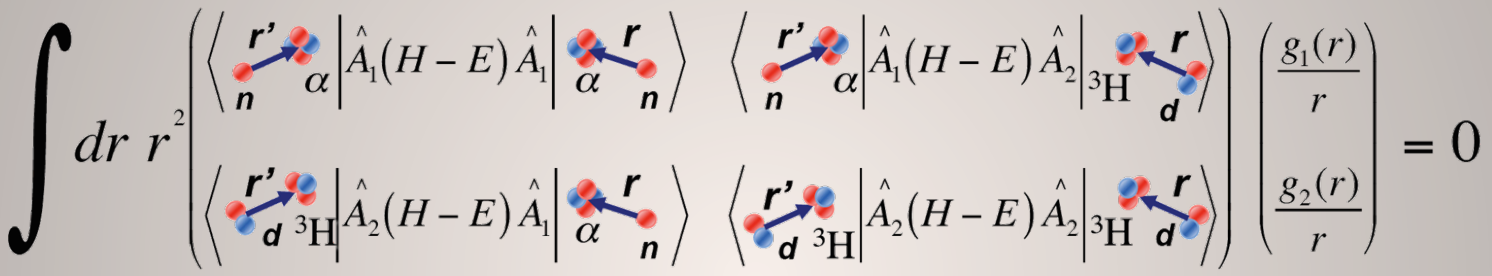


Resonance at E_{cm} =48 keV (E_d=105 keV) in the J=3/2$^+$ channel
Cross section at the peak: 4.88 b

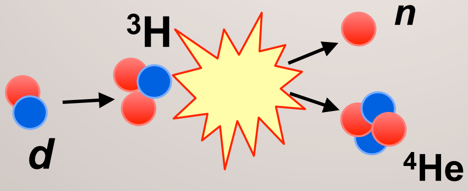
17.64 MeV energy released:
14.1 MeV neutron and 3.5 MeV alpha



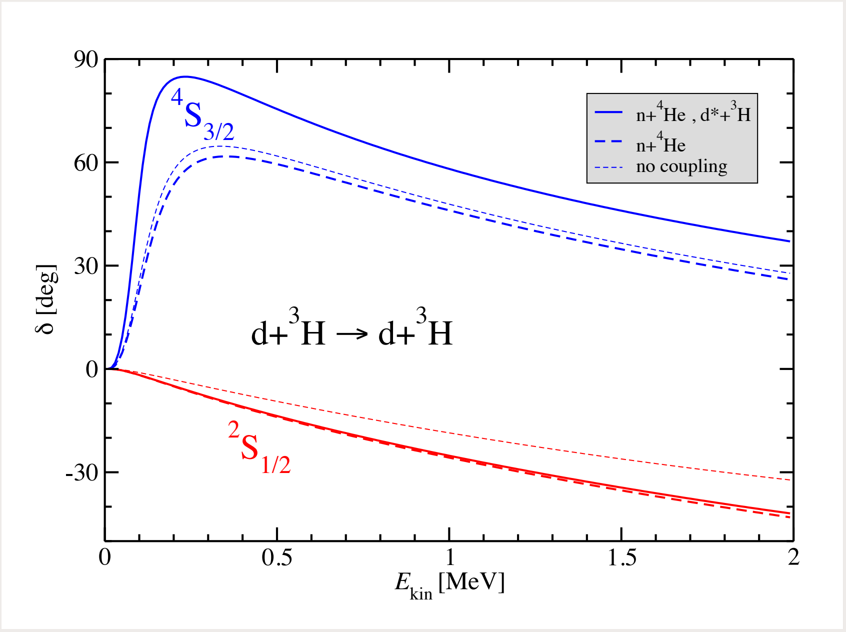
Ab initio calculation of the ^{3}H(*d*,*n*)^{4}He fusion

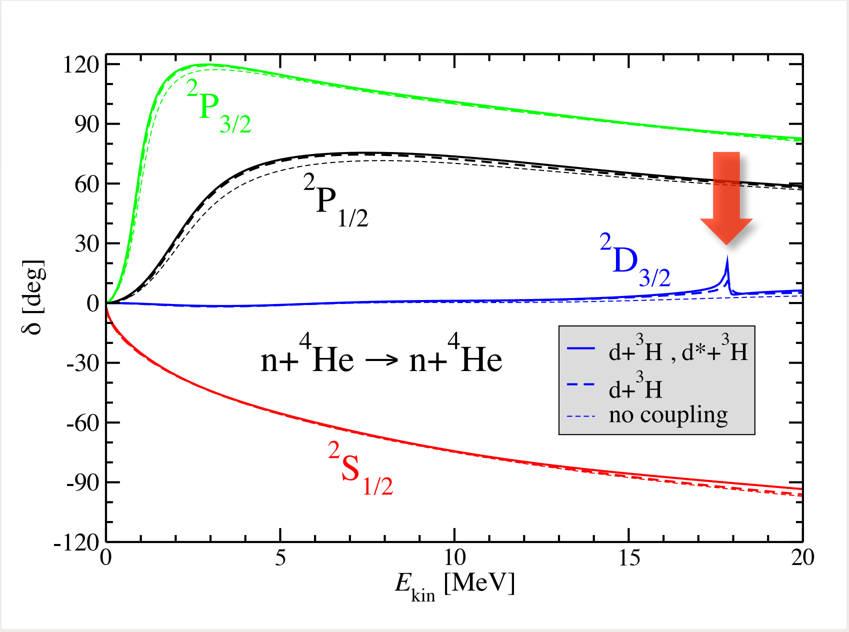


$$\int dr\, r^2 \begin{pmatrix} \left\langle \overset{\mathbf{r'}}{n\quad\alpha} \right| \hat{A}_1 (H-E) \hat{A}_1 \left| \overset{\mathbf{r}}{\alpha\quad n} \right\rangle & \left\langle \overset{\mathbf{r'}}{n\quad\alpha} \right| \hat{A}_1 (H-E) \hat{A}_2 \left| \overset{\mathbf{r}}{{}^3\mathrm{H}\quad d} \right\rangle \\ \left\langle \overset{\mathbf{r'}}{d\quad {}^3\mathrm{H}} \right| \hat{A}_2 (H-E) \hat{A}_1 \left| \overset{\mathbf{r}}{\alpha\quad n} \right\rangle & \left\langle \overset{\mathbf{r'}}{d\quad {}^3\mathrm{H}} \right| \hat{A}_2 (H-E) \hat{A}_2 \left| \overset{\mathbf{r}}{{}^3\mathrm{H}\quad d} \right\rangle \end{pmatrix} \begin{pmatrix} \dfrac{g_1(r)}{r} \\ \dfrac{g_2(r)}{r} \end{pmatrix} = 0$$



d+^{3}H and *n*+^{4}He elastic scattering: phase shifts





- *d*+^{3}H elastic phase shifts:
  - Resonance in the $^4S_{3/2}$ channel
  - Repulsive behavior in the $^2S_{1/2}$ channel ➔ Pauli principle

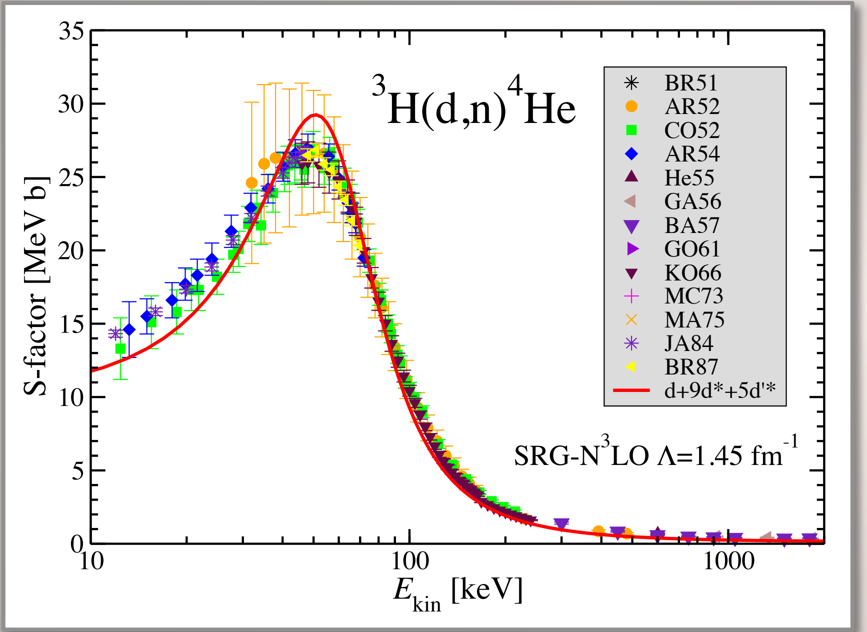
*d** deuteron pseudo state in $^3S_1$-$^3D_1$ channel:
deuteron polarization, virtual breakup

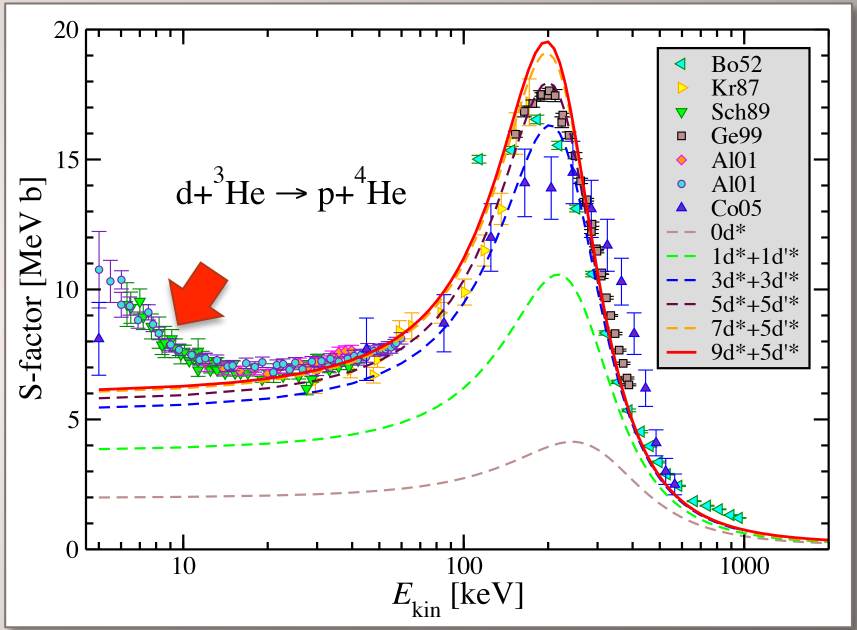
- *n*+^{4}He elastic phase shifts:
  - *d*+^{3}H channels produces slight increase of the *P* phase shifts
  - Appearance of resonance in the 3/2$^+$ *D*-wave, just above *d*-^{3}H threshold

The *d*-^{3}H fusion takes place through a transition of *d*+^{3}H is *S*-wave to *n*+^{4}He in *D*-wave:
Importance of the **tensor force**

^{3}H(*d*,*n*)^{4}He & ^{3}He(*d*,*p*)^{4}He fusion

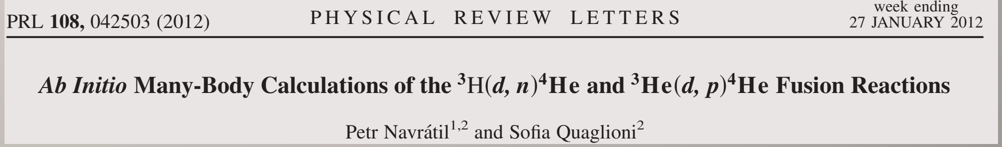
- NCSM/RGM with *SRG-N^{3}LO NN* potentials





Potential to address unresolved fusion research related questions:
^{3}H(d,n)^{4}He fusion with polarized deuterium and/or tritium,
^{3}H(d,n γ)^{4}He bremsstrahlung, electron screening at very low energies …

NCSMC calculations
with chiral NN+3N forces in progress…



PRL **108,** 042503 (2012) PHYSICAL REVIEW LETTERS week ending 27 JANUARY 2012

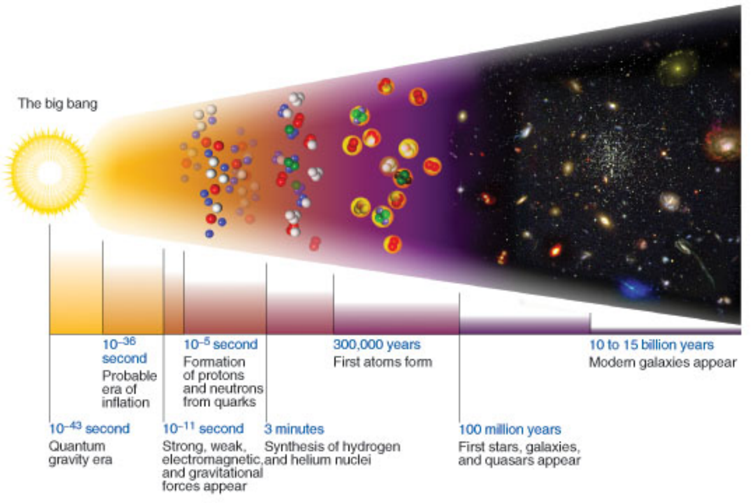
***Ab Initio* Many-Body Calculations of the ^{3}H(d, n)^{4}He and ^{3}He(d, p)^{4}He Fusion Reactions**

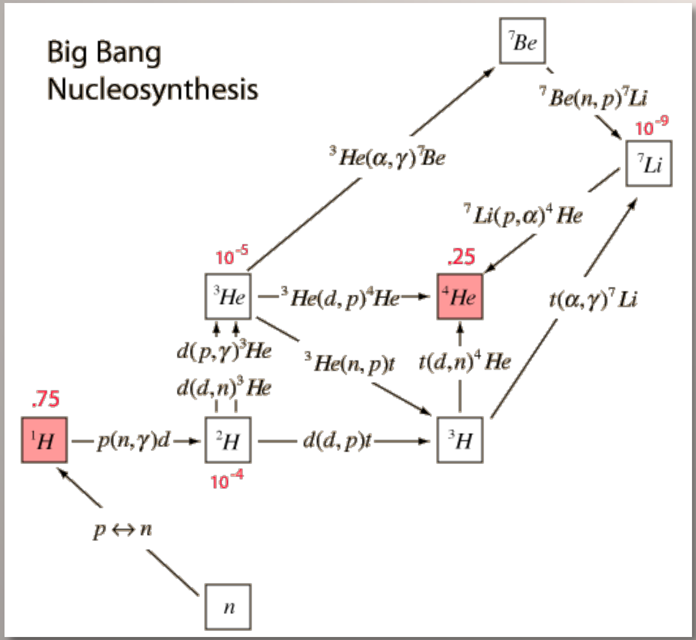
Petr Navrátil[1,2] and Sofia Quaglioni[2]

Big Bang nucleosythesis

^{6}Li puzzle

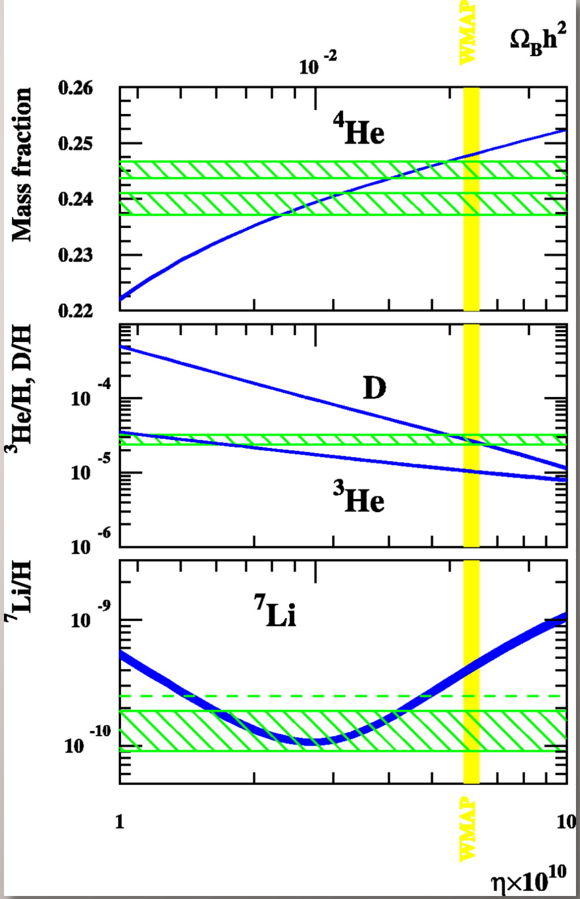
$^{2}\mathrm{H}(\alpha,\gamma)^{6}\mathrm{Li}$





Key reactions

^{7}Li puzzle

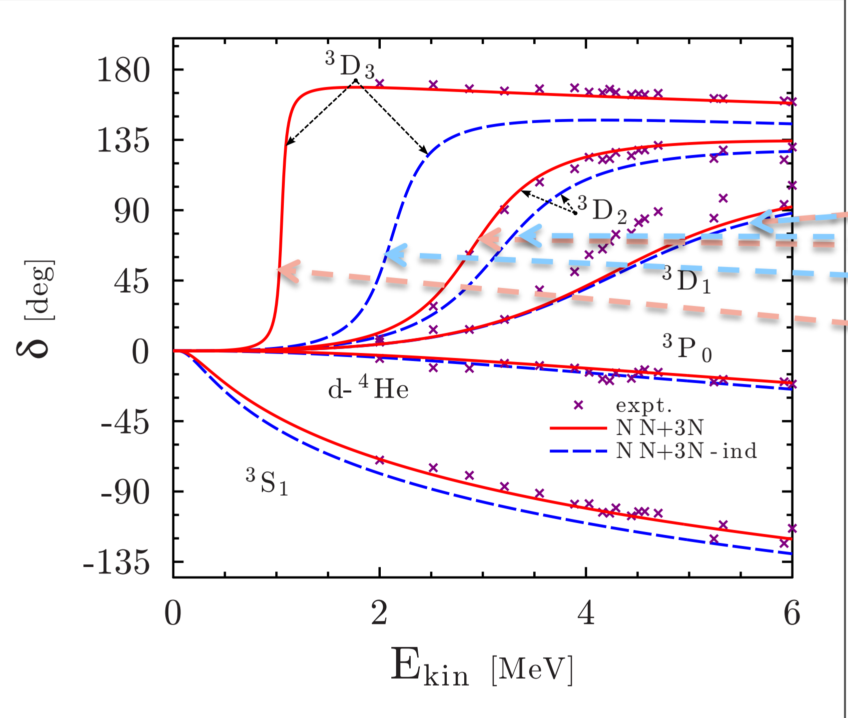


TRIUMF

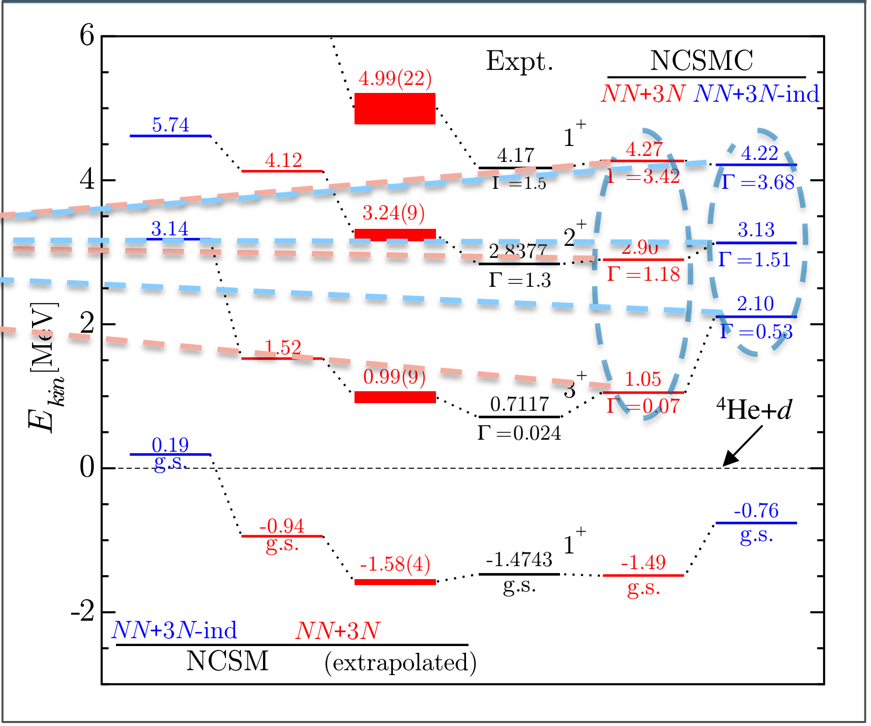
Unified description of ^{6}Li structure and d+^{4}He dynamics

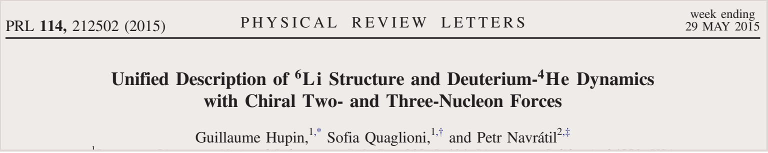
- Continuum and three-nucleon force effects on d+^{4}He and ^{6}Li

d+^{4}He Scattering Phase Shifts



^{6}Li vs. (^{4}He+d)+^{6}Li calculation



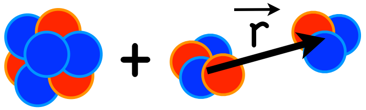


PRL **114,** 212502 (2015) PHYSICAL REVIEW LETTERS week ending 29 MAY 2015

Unified Description of ^{6}Li Structure and Deuterium-^{4}He Dynamics with Chiral Two- and Three-Nucleon Forces

Guillaume Hupin,[1,*] Sofia Quaglioni,[1,†] and Petr Navrátil[2,‡]

NCSMC



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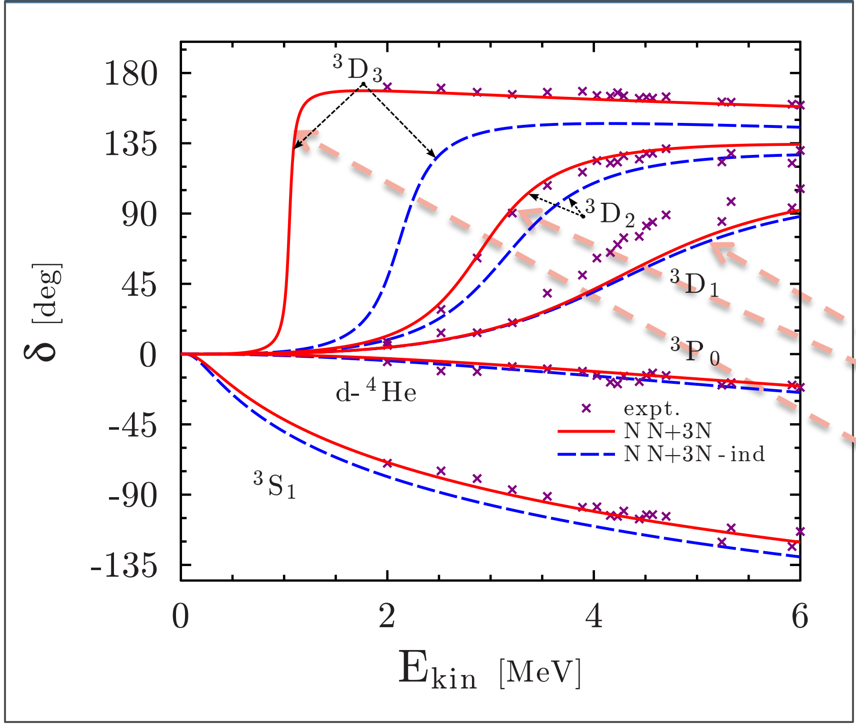

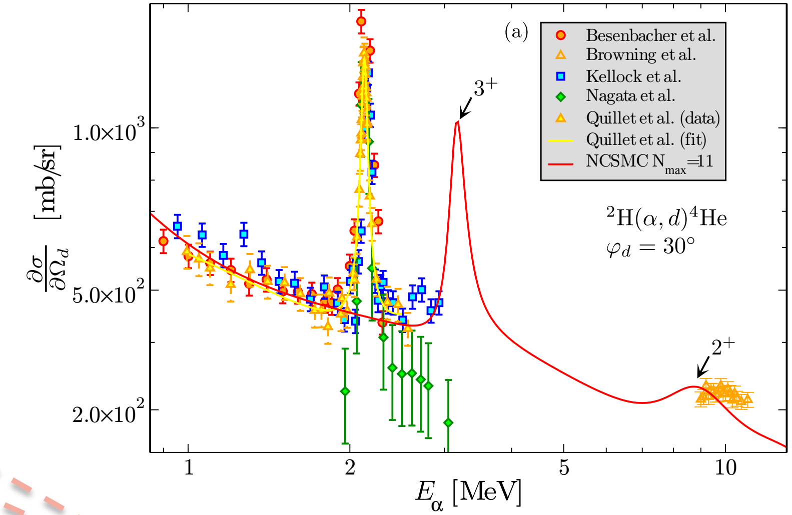

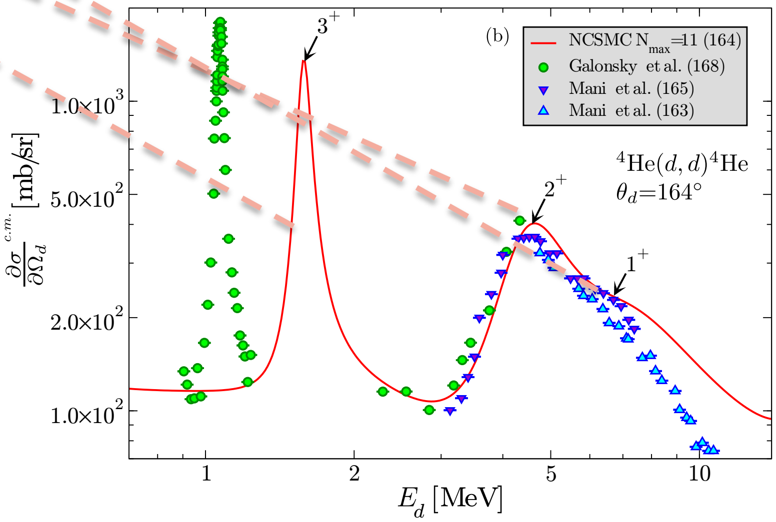

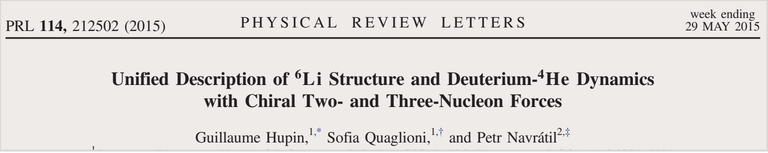
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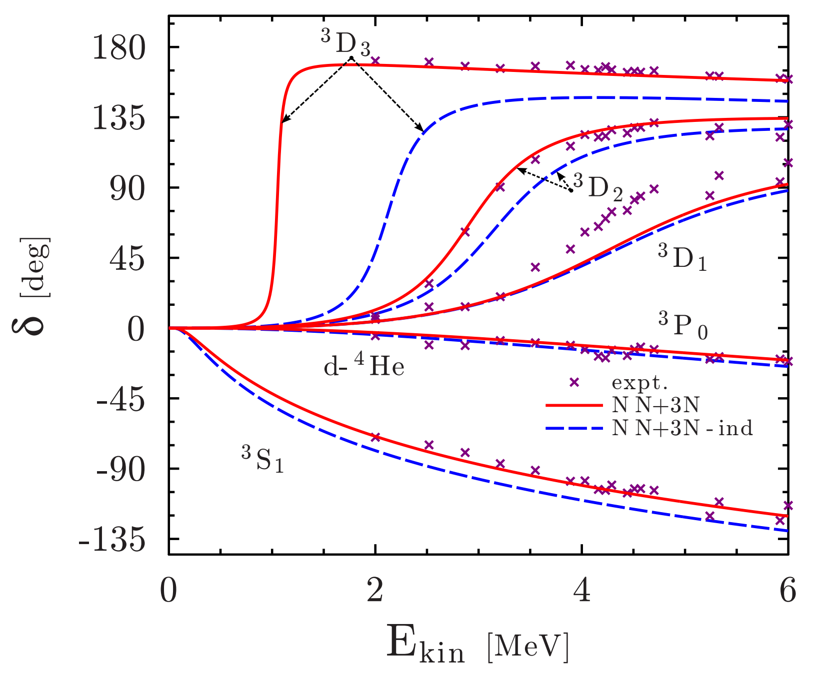

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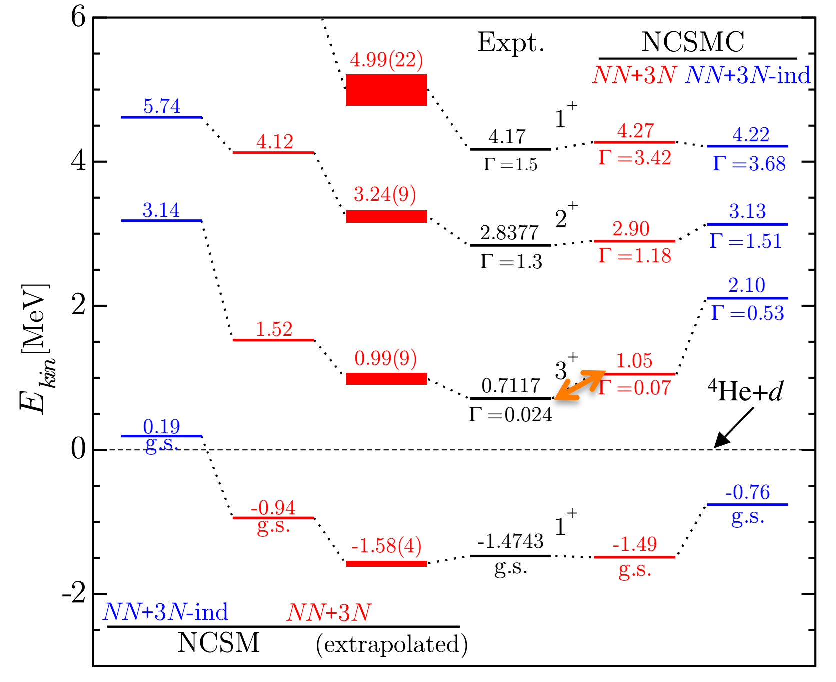

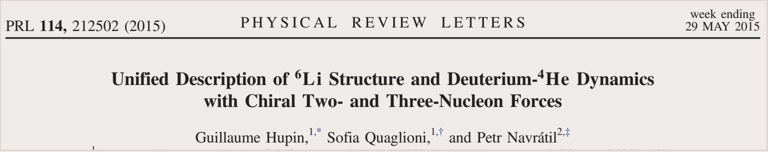

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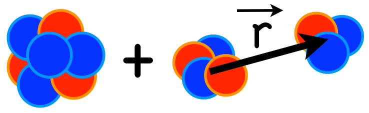

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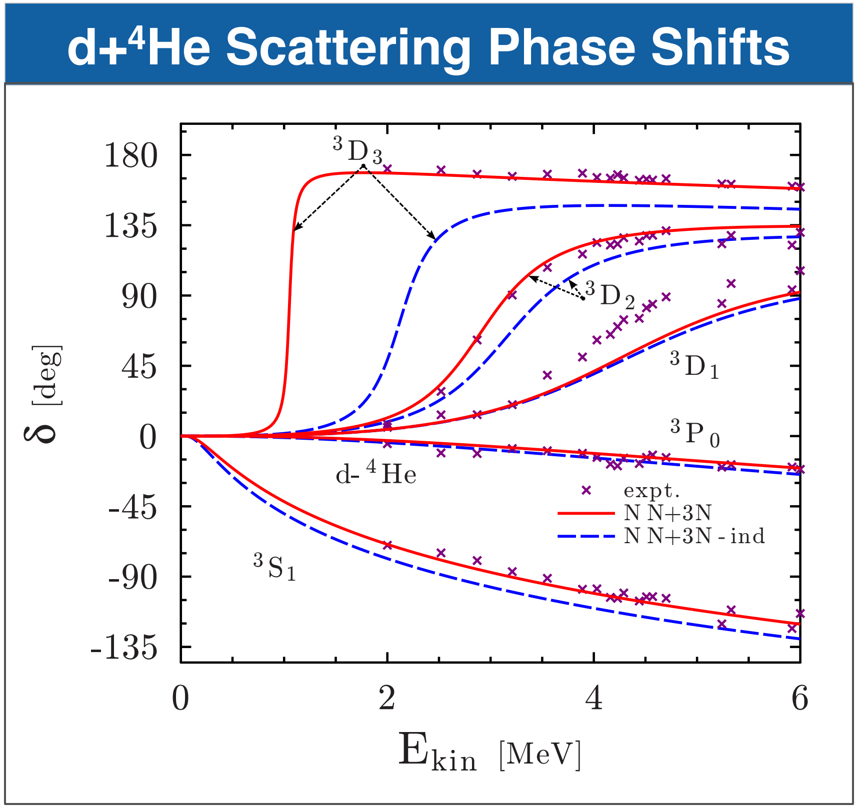
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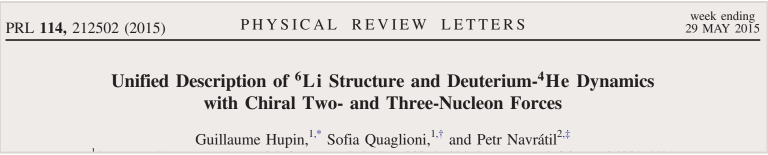
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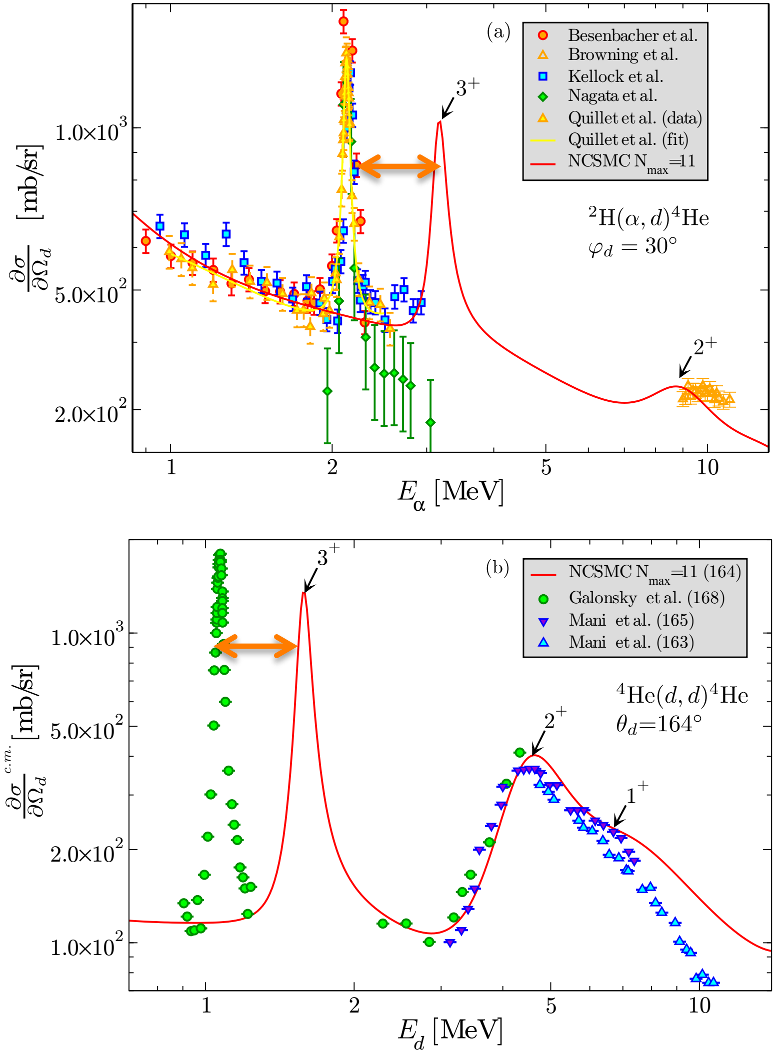

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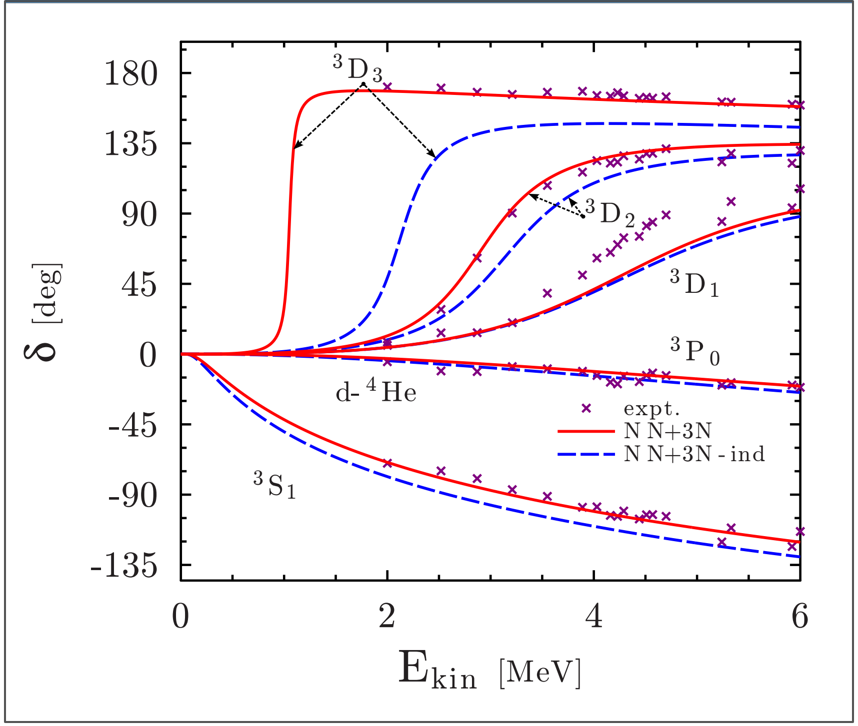

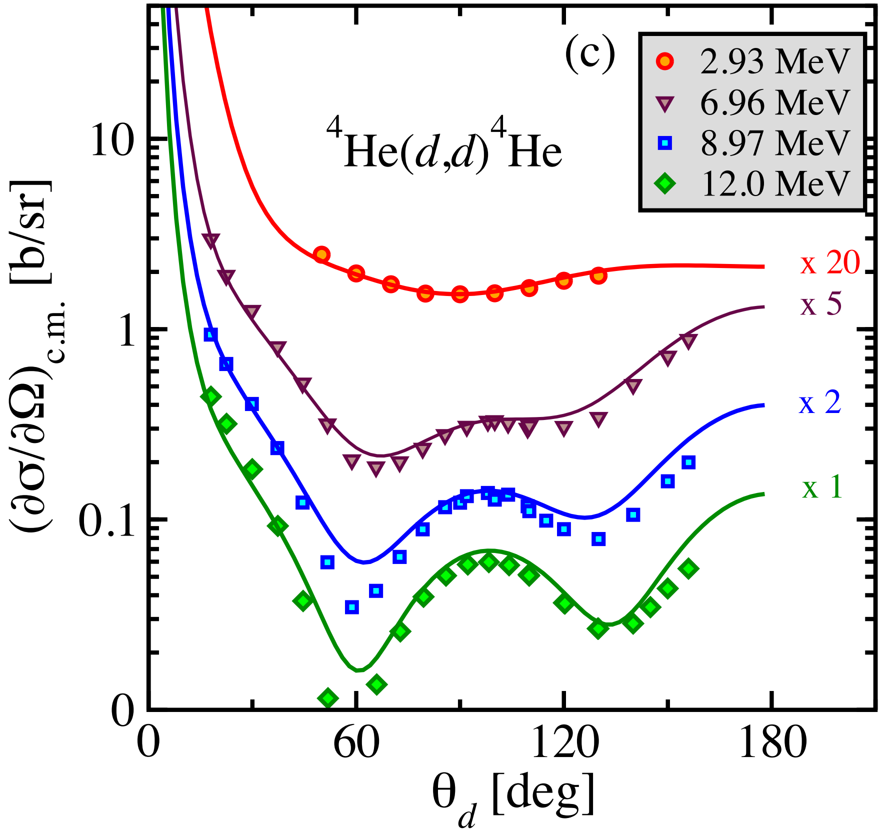

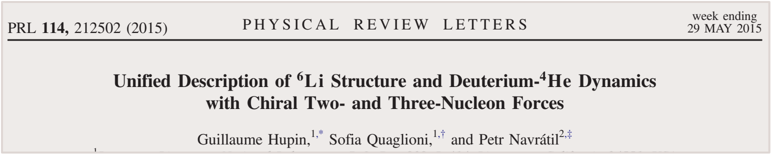

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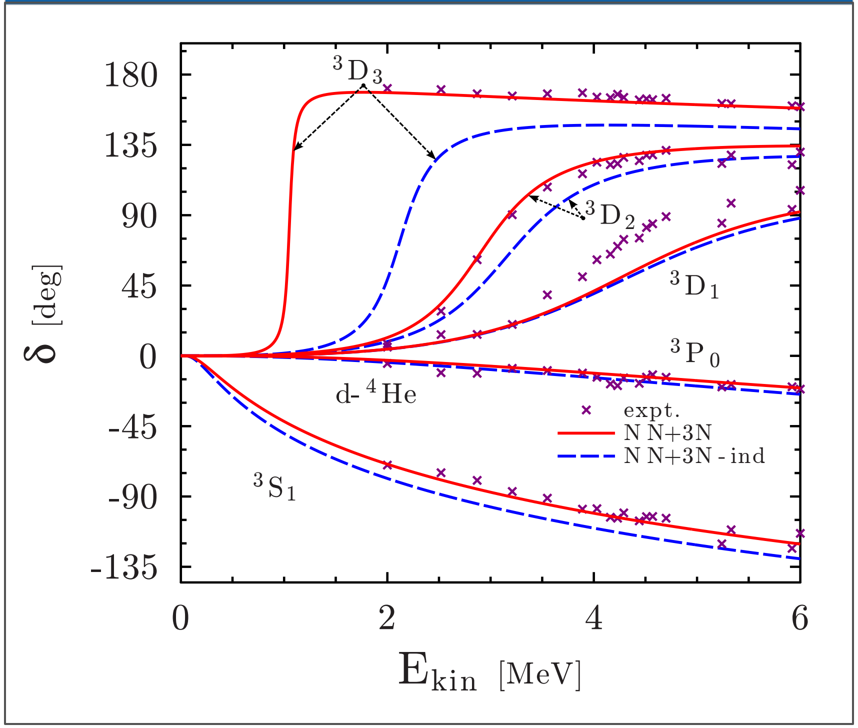
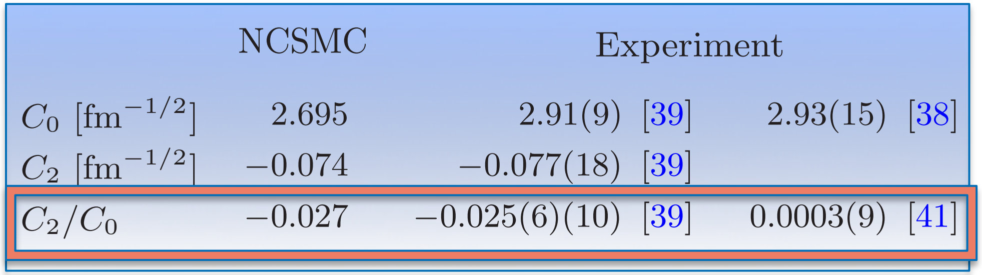


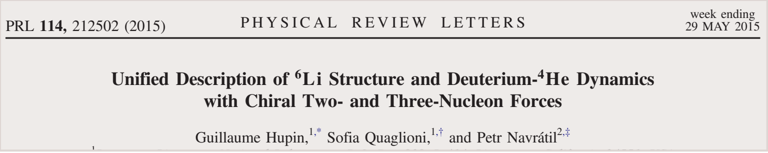


	NCSMC	Experiment			
C_0 [fm$^{-1/2}$]	2.695	2.91(9)	[39]	2.93(15)	[38]
C_2 [fm$^{-1/2}$]	-0.074	$-0.077(18)$	[39]		
C_2/C_0	-0.027	$-0.025(6)(10)$	[39]	0.0003(9)	[41]

[38] L. D. Blokhintsev, V. I. Kukulin, A. A. Sakharuk, D. A. Savin, and E. V. Kuznetsova, Phys. Rev. C **48**, 2390 (1993).

[39] E. A. George and L. D. Knutson, Phys. Rev. C **59**, 598 (1999).

[41] K. D. Veal, C. R. Brune, W. H. Geist, H. J. Karwowski, E. J. Ludwig, A. J. Mendez, E. E. Bartosz, P. D. Cathers, T. L. Drummer, K. W. Kemper, A. M. Eiró, F. D. Santos, B. Kozlowska, H. J. Maier, and I. J. Thompson, Phys. Rev. Lett. **81**, 1187 (1998).



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TRIUMF

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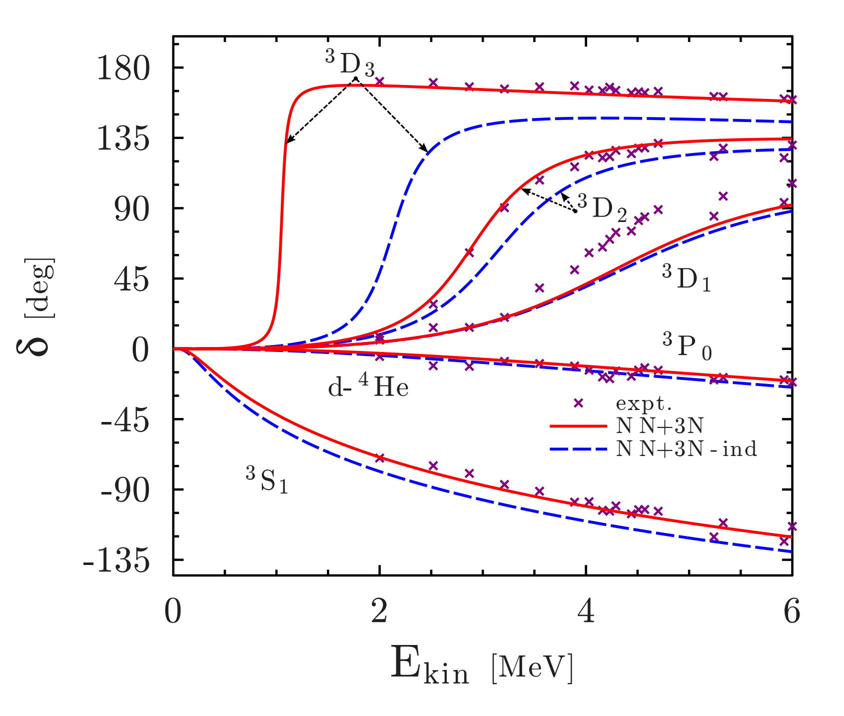

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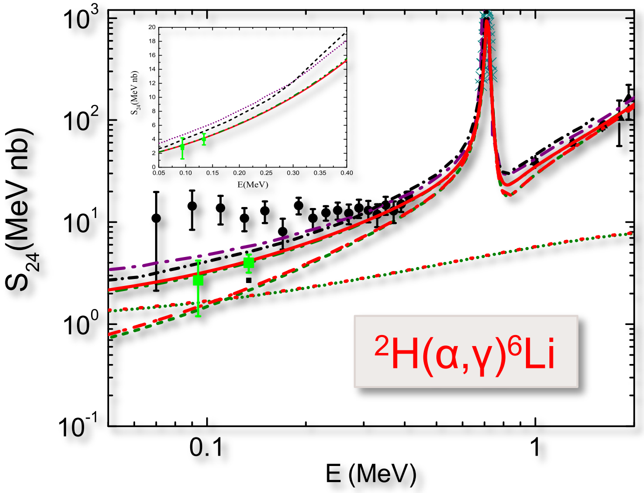
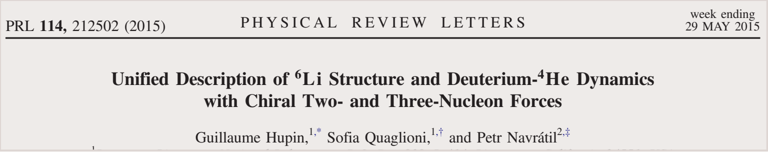
^{6}Li puzzle – too little ^{6}Li produced in BBN



^{2}H(α,γ)^{6}Li

A. M. Mukhamedzhanov *et al.*,1602.07395



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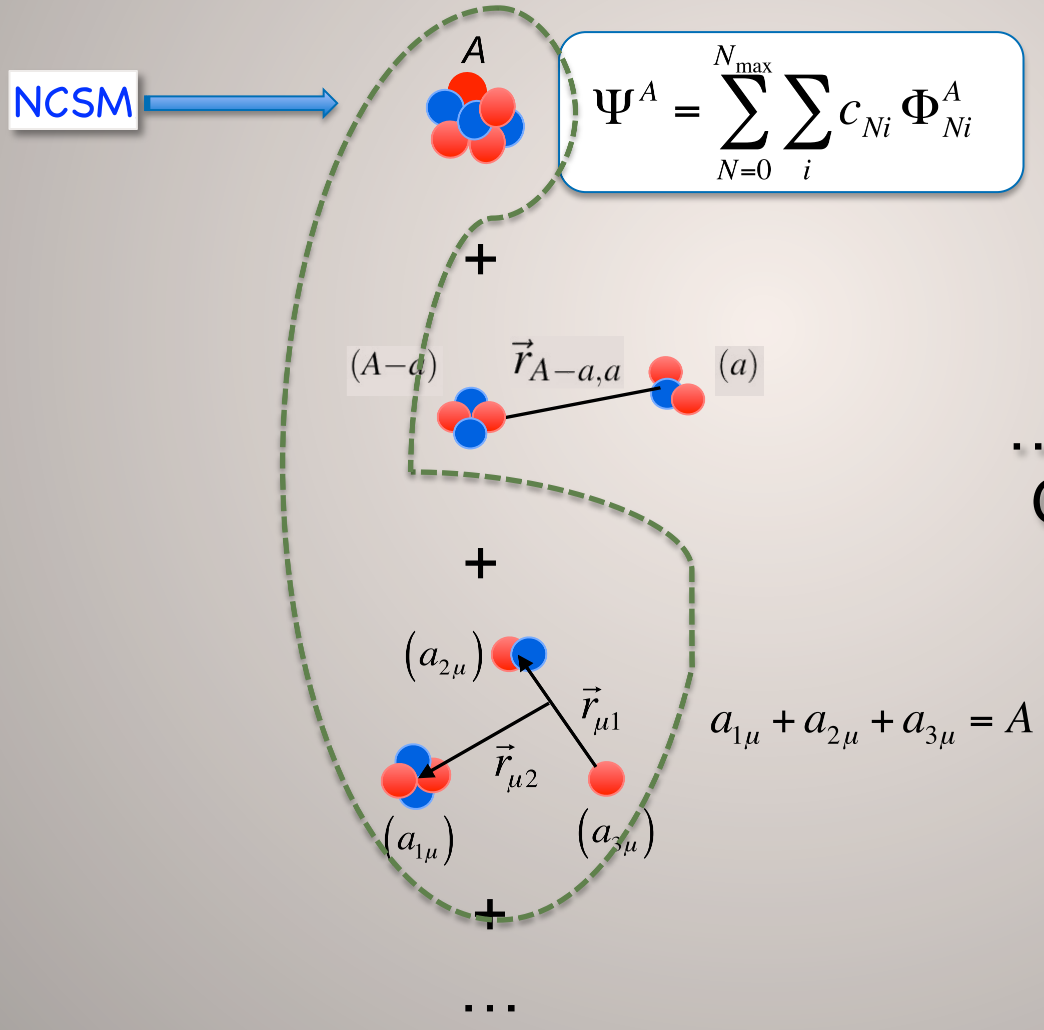
Guillaume Hupin,[1,*] Sofia Quaglioni,[1,†] and Petr Navrátil[2,‡]

TRIUMF

Extending no-core shell model beyond bound states

Include more many nucleon correlations…

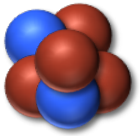


$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

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

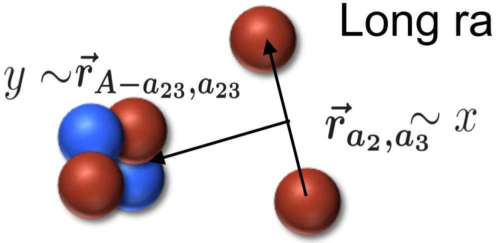
…using the Resonating Group Method (RGM) ideas

NCSMC for three-body clusters

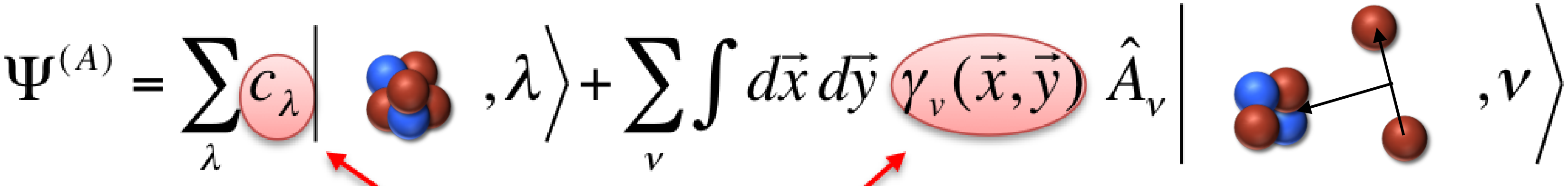


NCSM
Short range description

+



NCSM/RGM-3B
Long range description



$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \Big| \qquad ,\lambda \Big\rangle + \sum_{\nu} \int d\vec{x}\, d\vec{y}\; \gamma_{\nu}(\vec{x},\vec{y})\; \hat{A}_{\nu} \Big| \qquad ,\nu \Big\rangle$$

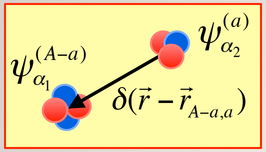
Unknowns

Three-body clusters in *ab initio* NCSM/RGM

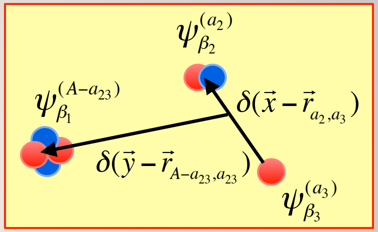
- Starts from:

$$\Psi^{(A)}_{RGM} = \sum_{\nu_2} \int g_{\nu_2}(\vec{r}\,)\hat{A}_{\nu_2} \underbrace{\left|\phi_{\nu_2 \vec{r}}\right\rangle}_{} d\vec{r} + \sum_{\nu_3} \iint G_{\nu_3}(\vec{x},\vec{y})\ \hat{A}_{\nu_3} \underbrace{\left|\Phi_{\nu_3 \vec{x}\vec{y}}\right\rangle}_{} d\vec{x}d\vec{y}$$

2-body channels

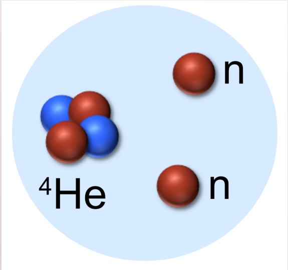


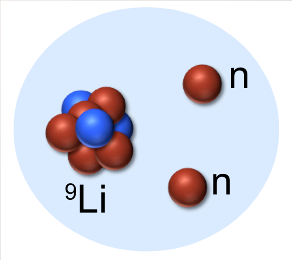
plus



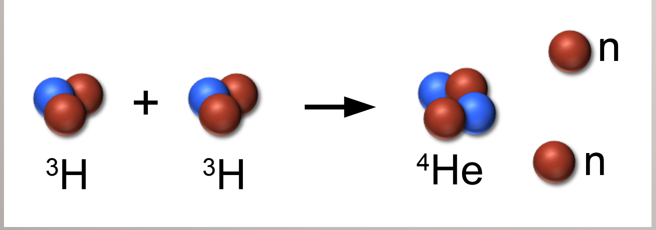
3-body channels

- Two-neutron halo nuclei





- Transfer reactions with three-body continuum final states



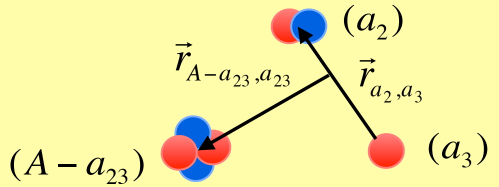
Three-cluster NCSM/RGM

- The starting point:

$$\Psi^{(A)}_{RGM} = \sum_{a_2 a_3 \nu} \int d\vec{x}\, d\vec{y}\; G_{\nu}^{(A-a_{23},a_2,a_3)}(x,y)$$

$$\times\, \hat{A}^{(A-a_{23},a_2,a_3)} \left| \Phi^{(A-a_{23},a_2,a_3)}_{\nu\vec{x}\vec{y}} \right\rangle$$

$$\rho^{5/2} \sum_{K} \chi^{(A-a_{23},a_2,a_3)}_{\nu K}(\rho)\, \phi_K^{\ell x \ell y}(\alpha)$$



$$\psi^{(A-a_{23})}_{\alpha_1}\psi^{(a_2)}_{\alpha_2}\psi^{(a_3)}_{\alpha_3} Y^{\ell x,\ell y}(\hat{x},\hat{y})$$

$$\times\, \delta\left(\vec{x} - \vec{r}_{a_2,a_3}\right)\delta\left(\vec{y} - \vec{r}_{A-a_{23},a_{23}}\right)$$

- Solves:

$$\sum_{a_2 a_3 \nu K} \int d\rho\; \rho^5 \left[H^{K',K}_{a'\nu',a\nu}(\rho',\rho) - E\, N^{K',K}_{a'\nu',a\nu}(\rho',\rho) \right] \rho^{-5/2} \chi^{(A-a_{23},a_2,a_3)}_{\nu K}(\rho) = 0$$

  - Where the hyperspherical coordinates are given by:

$$\rho = \sqrt{x^2 + y^2}, \quad \alpha = \arctan\left(\frac{y}{x}\right) \qquad \left(x = \rho\cos\alpha, \quad y = \rho\sin\alpha\right)$$

NCSMC for three-body clusters: ^{6}He ~ ^{4}He+n+n

C. Romero-Redondo, S. Quaglioni, P. Navratil, G. Hupin, arXiv: 1606.00066

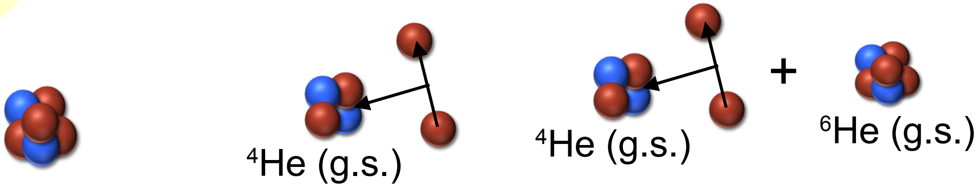
The **NCSM** 6-nucleon eigenstate compensates for the missing many-body correlations

λ=1.5 fm^{-1}

SRG N^{3}LO NN potential

Experimental value
-29.269 MeV

Energy of 0$^+$ g.s.



N_{max}	NCSM	NCSM/RGM	NCSMC (0^+_1)
4	-27.70	-27.14	-28.29
6	-27.98	-28.91	-30.02
8	-28.95	-28.61	-29.69
10	-29.45	-28.70	-29.86
12	-29.66	-28.70	-29.86
Extrapolation	-29.84(4)	---	---

NCSMC for three-body clusters: ^{6}He ~ ^{4}He+n+n

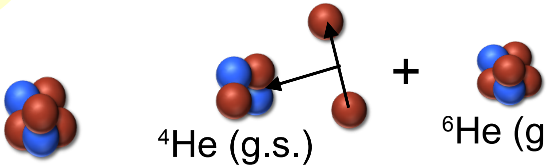
C. Romero-Redondo, S. Quaglioni, P. Navratil, G. Hupin, arXiv: 1606.00066

The **NCSM** 6-nucleon eigenstate compensates for the missing many-body correlations

λ= 2.0 fm^{-1}

SRG N^{3}LO NN potential

Experimental value
-29.269 MeV



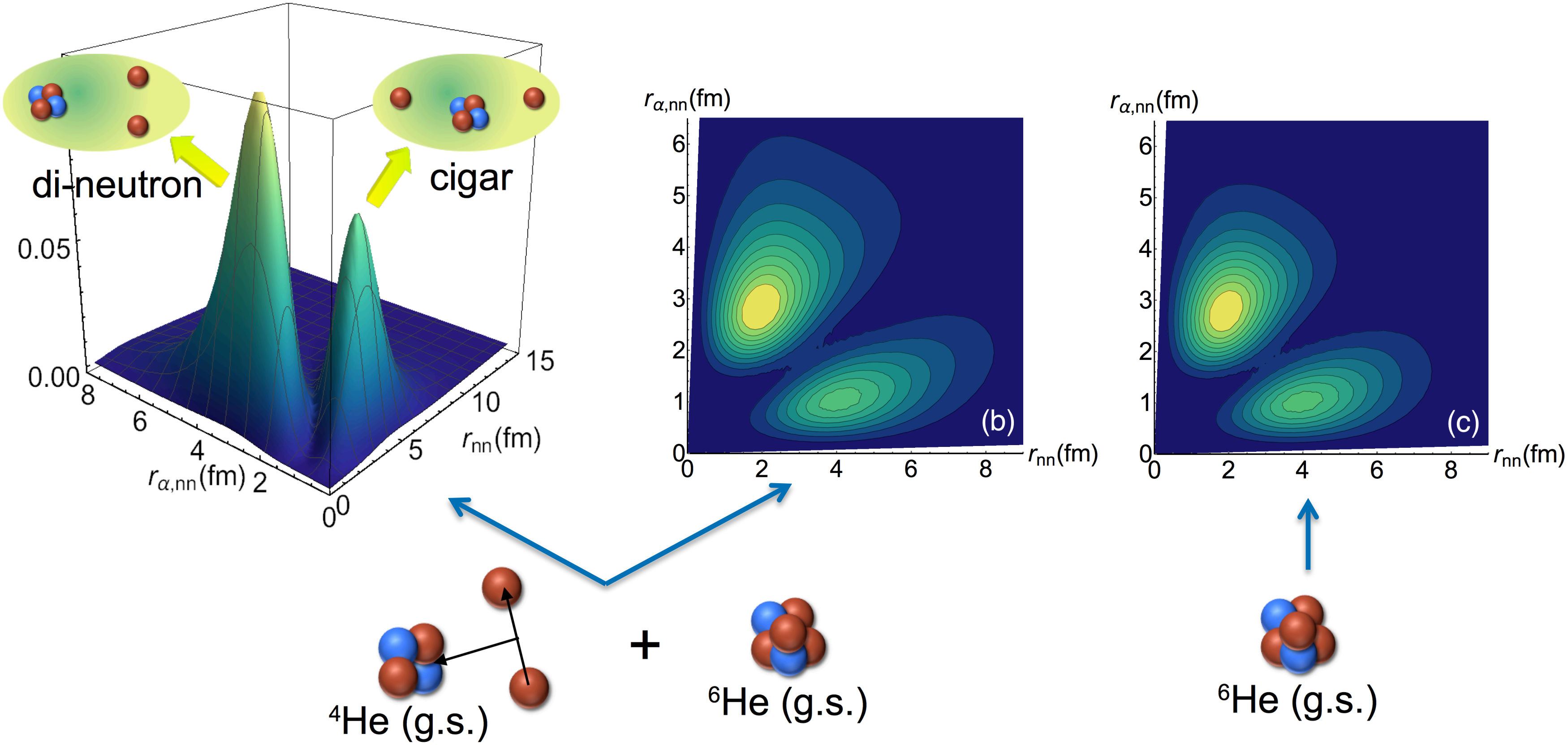
Energy of 0$^+$ g.s.

N$_{max}$	NCSM	NCSMC (0^+_1)
8	-26.44	-28.81
10	-27.70	-28.97
12	-28.37	-29.17
Extrapolation	-29.20(11)*	---

*D. Sääf, C. Forssén, PRC **89** 011303 (2014)

NCSMC for three-body clusters: ^{6}He ~ ^{4}He+n+n

C. Romero-Redondo, S. Quaglioni, P. Navratil, G. Hupin, arXiv: 1606.00066

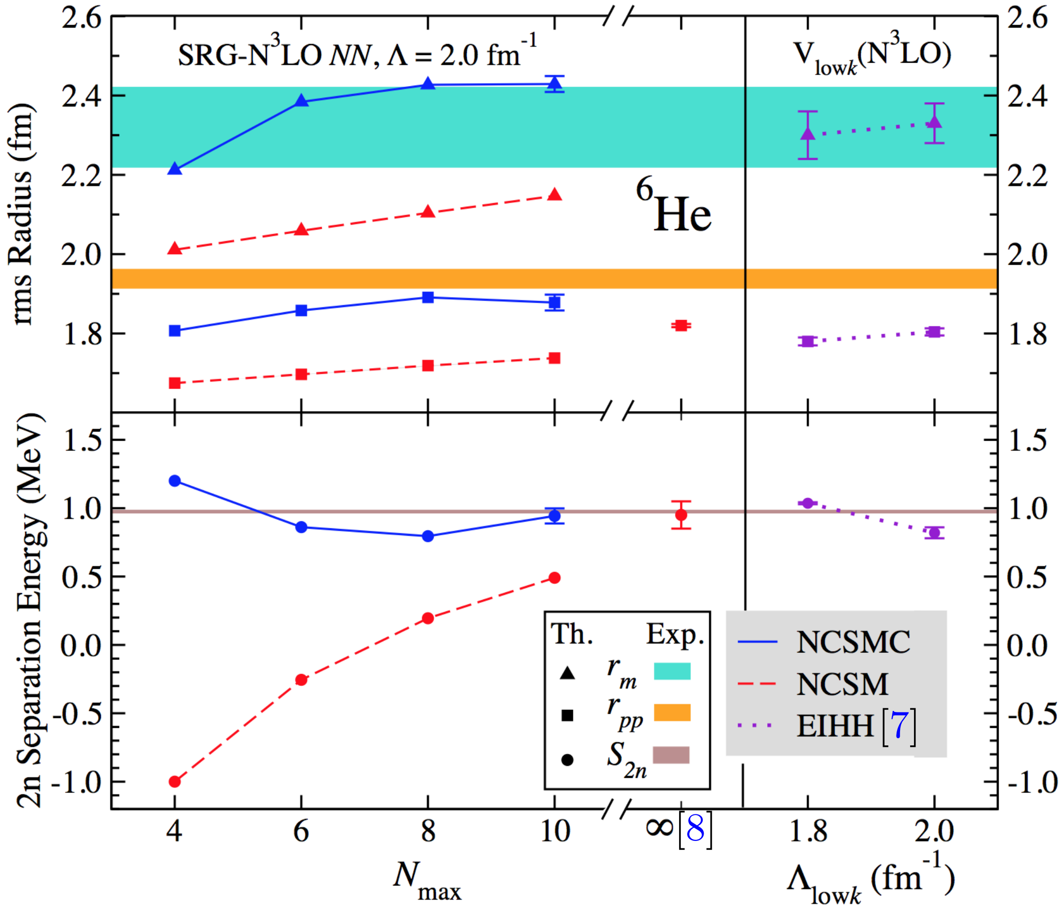


The probability distribution of the ^{6}He ground state presents
two peaks corresponding to the di-neutron and cigar configurations

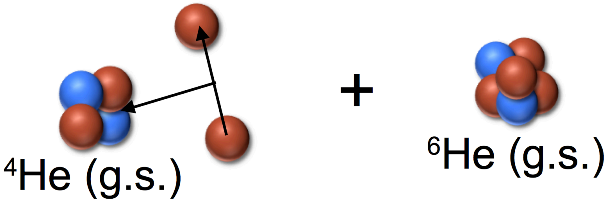
TRIUMF

NCSMC for three-body clusters: ^{6}He ~ ^{4}He+n+n

C. Romero-Redondo, S. Quaglioni, P. Navratil, G. Hupin, arXiv: 1606.00066

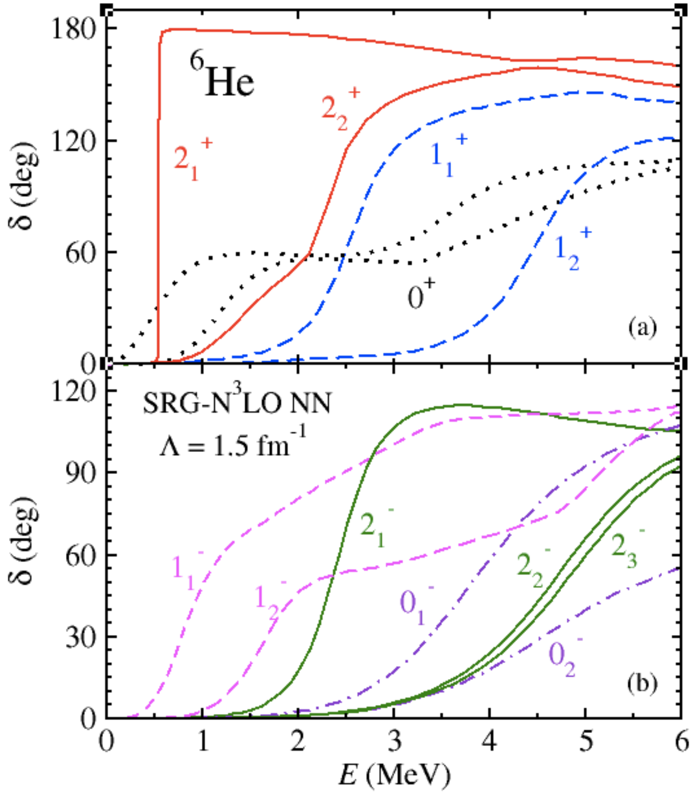


SRG N^{3}LO NN potential
with λ=2 fm^{-1}

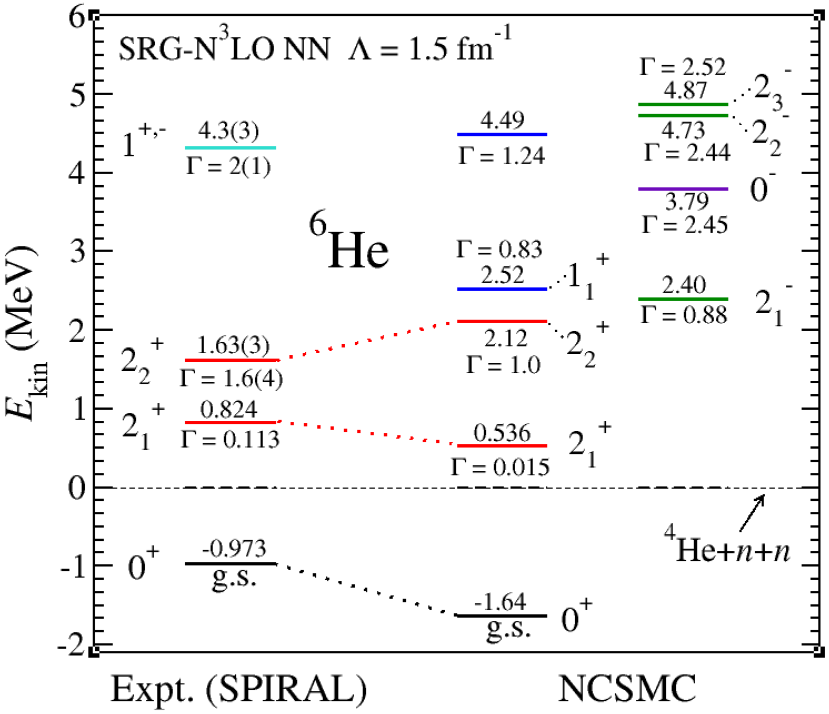


Separation energy, point proton and matter radius simultaneously consistent with experiment

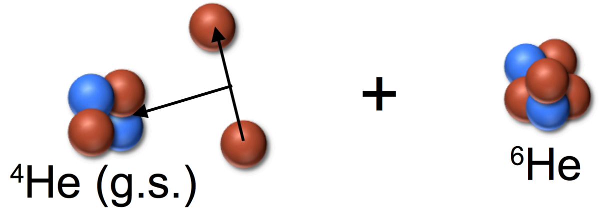
NCSMC for three-body clusters: ^{6}He ~ ^{4}He+n+n



C. Romero-Redondo, S. Quaglioni, P. Navratil, G. Hupin, arXiv: 1606.00066

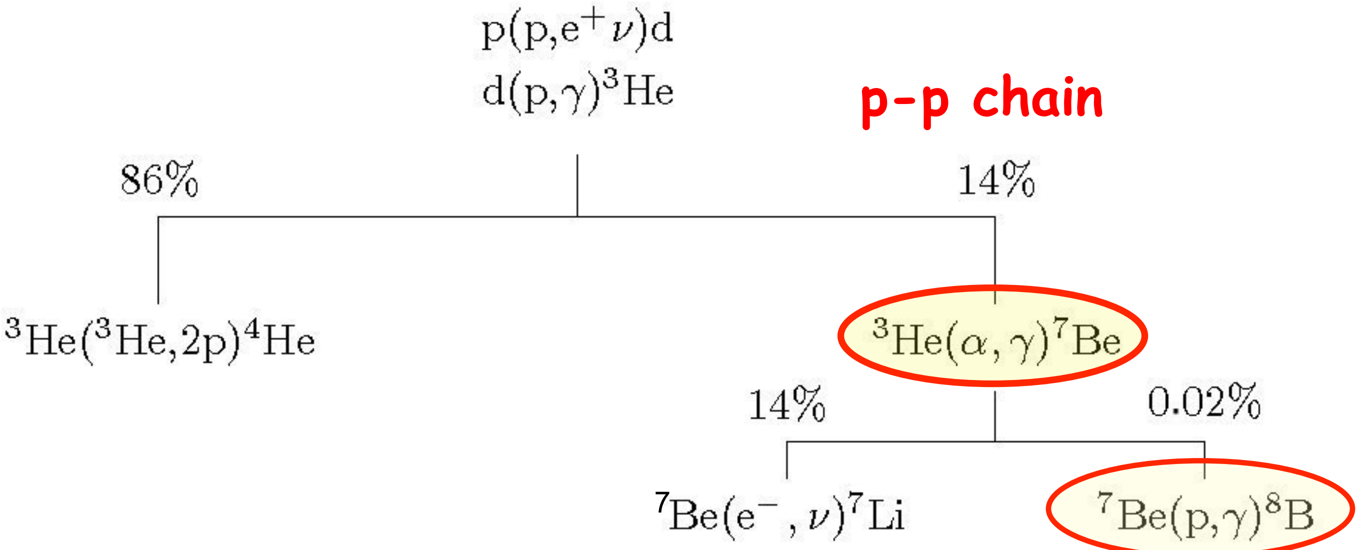


Prediction of lots of low-lying resonances.
Experimental picture incomplete



Ground-state and scattering state wave functions available.
Calculation of ^{4}He(nn,γ)^{6}He in progress…

Solar *p-p* chain



$p(p,e^+\nu)d$

$d(p,\gamma)^3He$

p-p chain

86%

14%

$^3He(^3He,2p)^4He$

$^3He(\alpha,\gamma)^7Be$

14%

0.02%

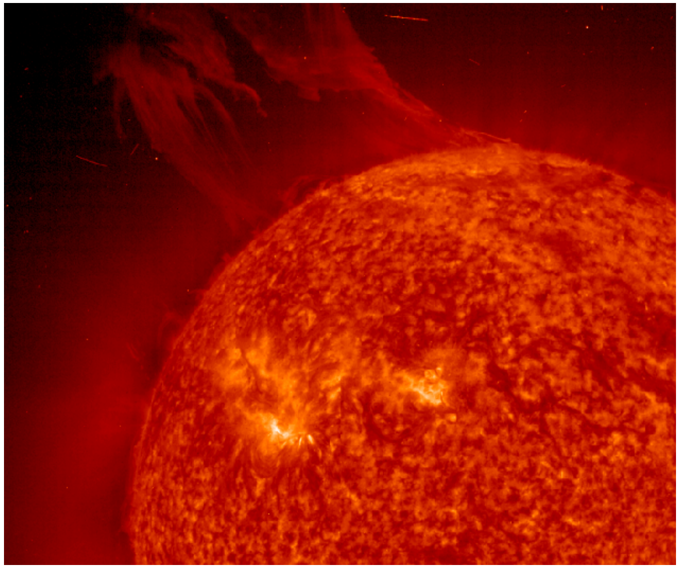
$^7Be(e^-,\nu)^7Li$

$^7Li(p,\alpha)^4He$

$^7Be(p,\gamma)^8B$

$^8B(e^+,\nu)^8Be$

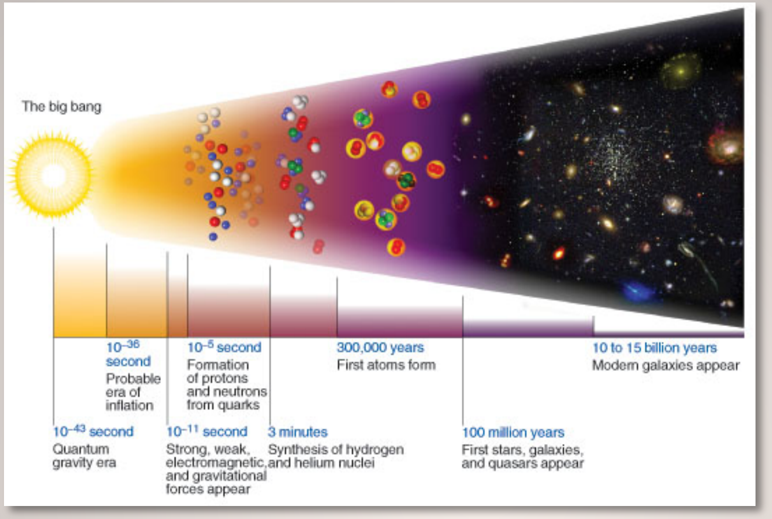
$^8Be(\alpha)^4He$

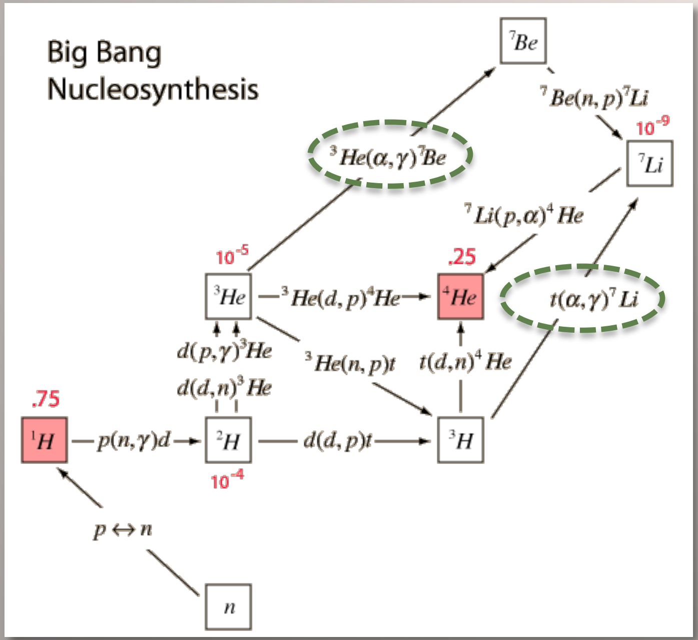


Solar neutrinos

E_ν < 15 MeV

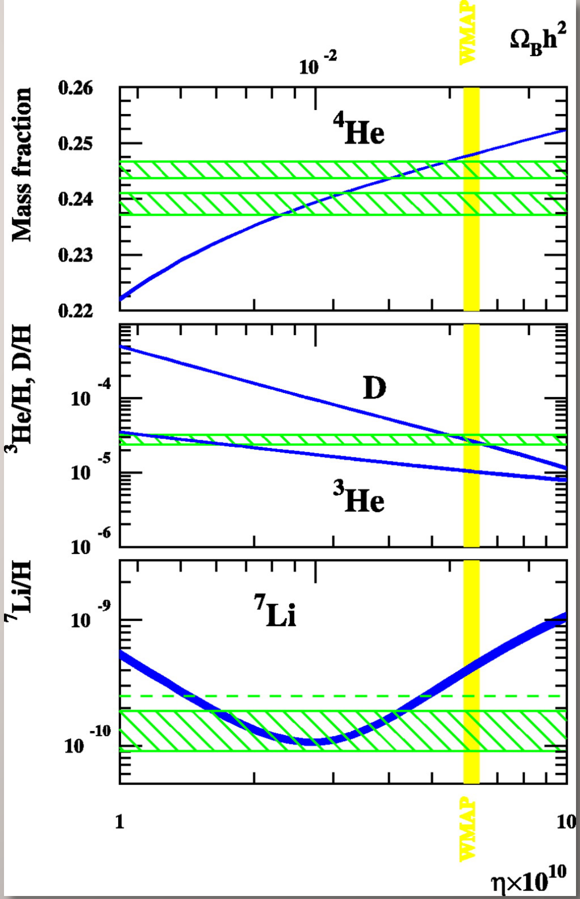
Big Bang nucleosythesis

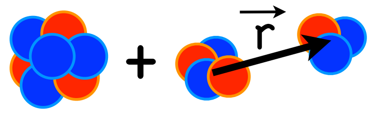




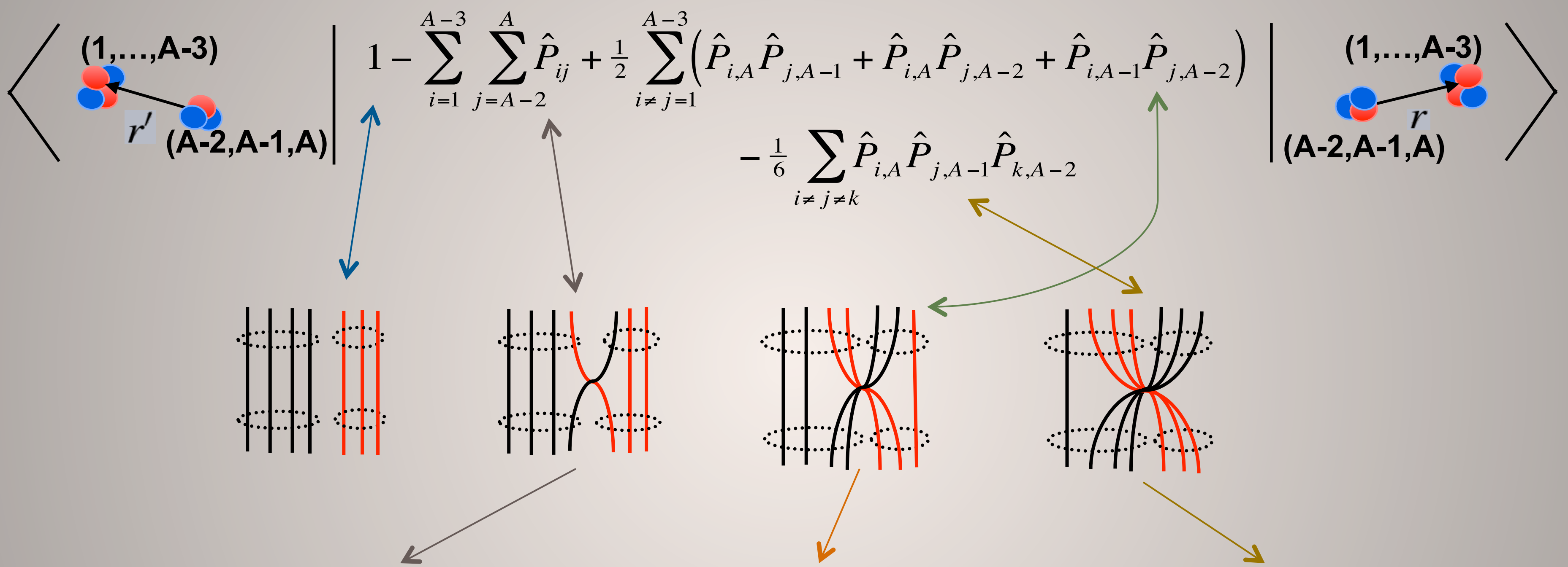
Key reactions

^{7}Li puzzle





^{3}He-^{4}He and ^{3}H-^{4}He scattering

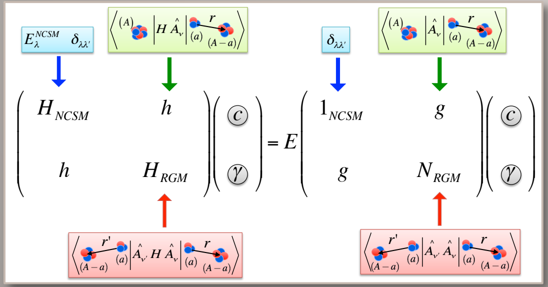


$$\left\langle \right| 1-\sum_{i=1}^{A-3}\sum_{j=A-2}^{A}\hat{P}_{ij}+\tfrac{1}{2}\sum_{i\neq j=1}^{A-3}\left(\hat{P}_{i,A}\hat{P}_{j,A-1}+\hat{P}_{i,A}\hat{P}_{j,A-2}+\hat{P}_{i,A-1}\hat{P}_{j,A-2}\right) -\tfrac{1}{6}\sum_{i\neq j\neq k}\hat{P}_{i,A}\hat{P}_{j,A-1}\hat{P}_{k,A-2} \left| \right\rangle$$

$${}_{\mathrm{SD}}\left\langle \psi^{(A-3)}_{\mu_1}\right| a^+ a \left| \psi^{(A-3)}_{\nu_1}\right\rangle_{\mathrm{SD}}$$

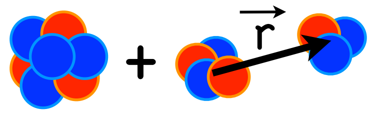
$${}_{\mathrm{SD}}\left\langle \psi^{(A-3)}_{\mu_1}\right| a^+ a^+\, a\, a \left| \psi^{(A-3)}_{\nu_1}\right\rangle_{\mathrm{SD}}$$

$${}_{\mathrm{SD}}\left\langle \psi^{(A-3)}_{\mu_1}\right| a^+ a^+ a^+ a\, a\, a \left| \psi^{(A-3)}_{\nu_1}\right\rangle_{\mathrm{SD}}$$



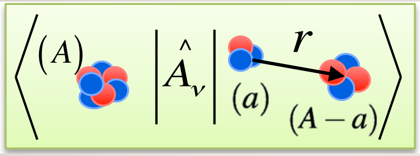
$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix}\begin{pmatrix} c \\ \chi \end{pmatrix} = E \begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix}\begin{pmatrix} c \\ \chi \end{pmatrix}$$

For *A*=7 use completeness



^{3}He-^{4}He and ^{3}H-^{4}He scattering

NCSMC coupling kernels:

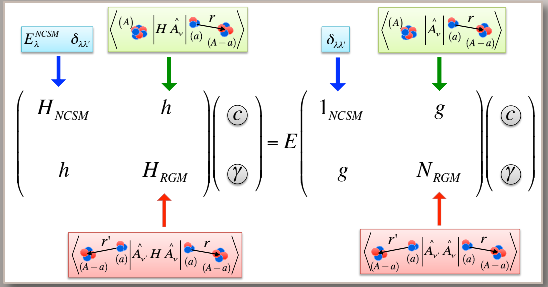


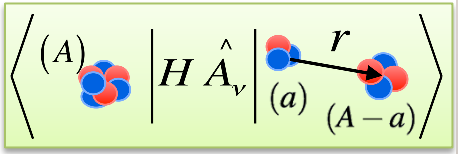
$$g \propto {}_{SD}\left\langle A \lambda J^\pi M T M_T \middle| \mathcal{A}\left[\left| A-3 \alpha_1 I_1 T_1 \right\rangle_{SD} ((\varphi_a(A)\varphi_b(A-1))^{(I_{ab}t_2)} \varphi_c(A-2))^{(I_{abc}t_3)} \right]^{(J^\pi T)}_{MM_T} \right. =$$

$$\sum \tfrac{1}{\sqrt{6}} (I_1 M_1 I_{abc} M_{abc} \mid JM)(T_1 M_{T_1} t_3 m_{t3} \mid T M_T)(I_{ab} M_{ab} j_c m_c \mid I_{abc} M_{abc})$$

$$\times \; (t_2 m_{t2} 1/2 m_{tc} \mid t_3 m_{t3})(j_a m_a j_b m_b \mid j_c m_c)(1/2 m_{ta} 1/2 m_{tb} \mid t_2 m_{t2})$$

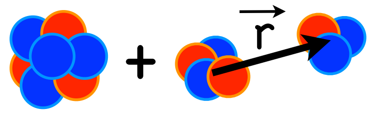
$$\times \; {}_{SD}\left\langle A \lambda J^\pi M T M_T \middle| a_a^+ a_b^+ a_c^+ \middle| A-3 \alpha_1 I_1 M_1 T_1 M_{T_1} \right\rangle_{SD}$$



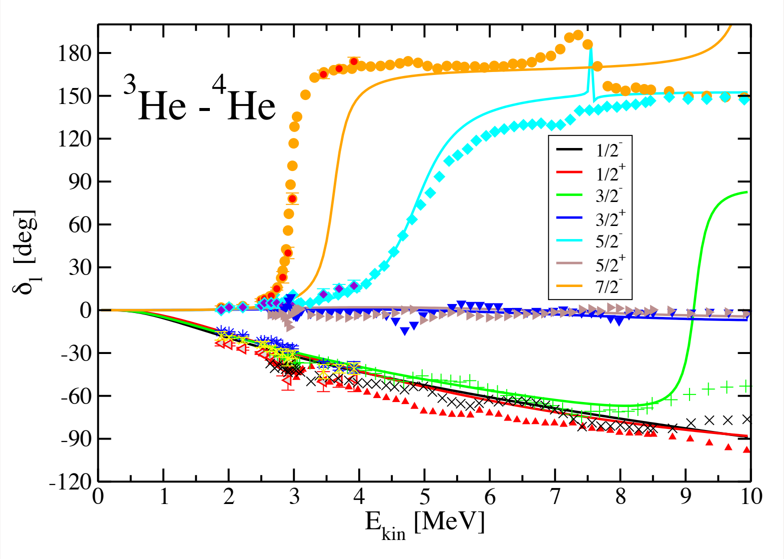


… a bit more complicated

TRIUMF



^{3}He-^{4}He and ^{3}H-^{4}He scattering



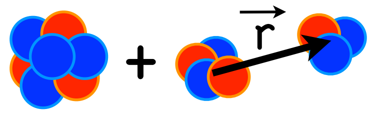
	^{7}Be		^{7}Li	
	NCSMC	Expt.	NCSMC	Expt.
$E_{3/2^-}$ [MeV]	-1.52	-1.586	-2.43	-2.467
$E_{1/2^-}$ [MeV]	-1.26	-1.157	-2.15	-1.989
r_{ch} [fm]	2.62	2.647(17)	2.42	2.390(30)
Q [e fm^2]	-6.14		-3.72	-4.00(3)
μ [μ_N]	-1.16	-1.3995(5)	+3.02	+3.256

J. Dohet-Eraly, P.N., S. Quaglioni, W. Horiuchi, G. Hupin, F. Raimondi, PLB **757**, 430 (2016)

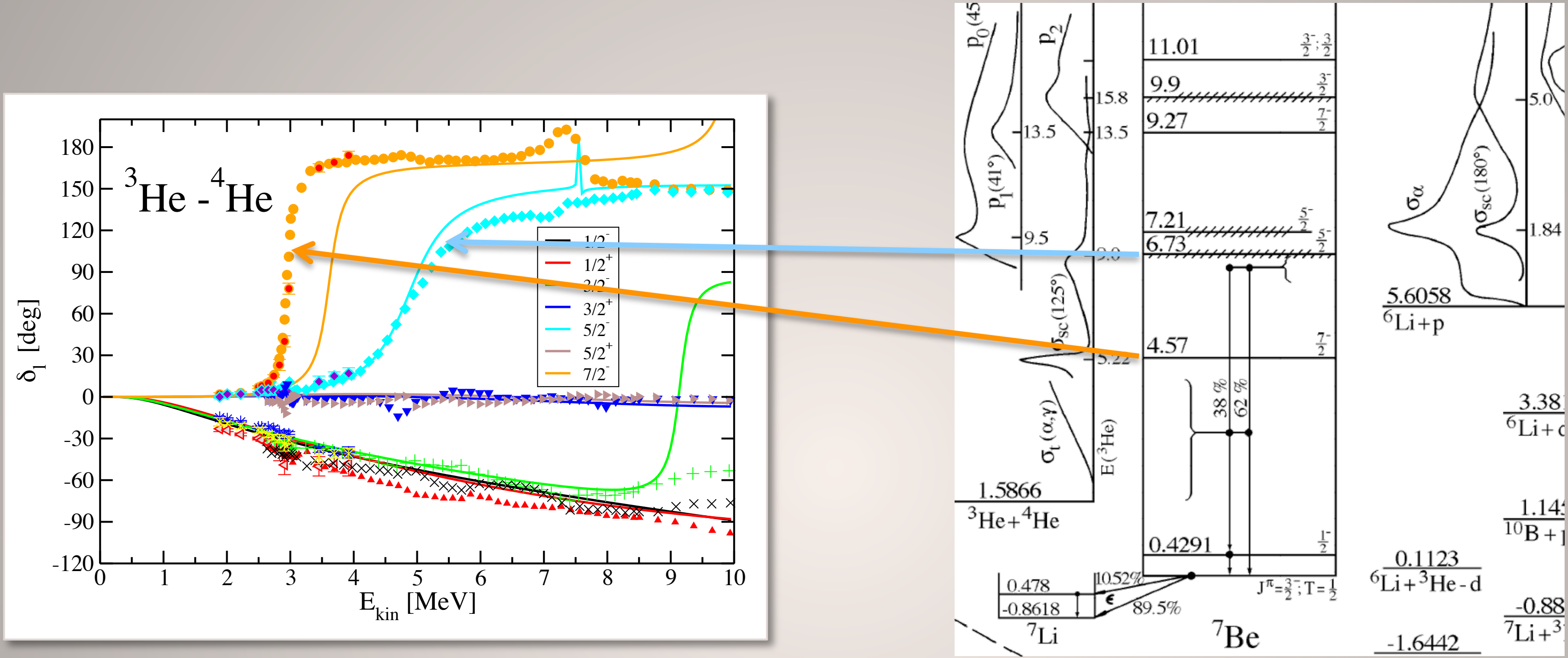
NCSMC calculations with chiral SRG-N^{3}LO *NN* potential (λ=2.15 fm^{-1})

^{3}He, ^{3}H, ^{4}He ground state, 8(π-) + 6(π+) eigenstates of ^{7}Be and ^{7}Li

Preliminary: N_{max}=12, hΩ=20 MeV



^{3}He-^{4}He and ^{3}H-^{4}He scattering



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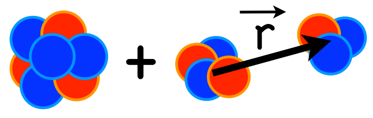
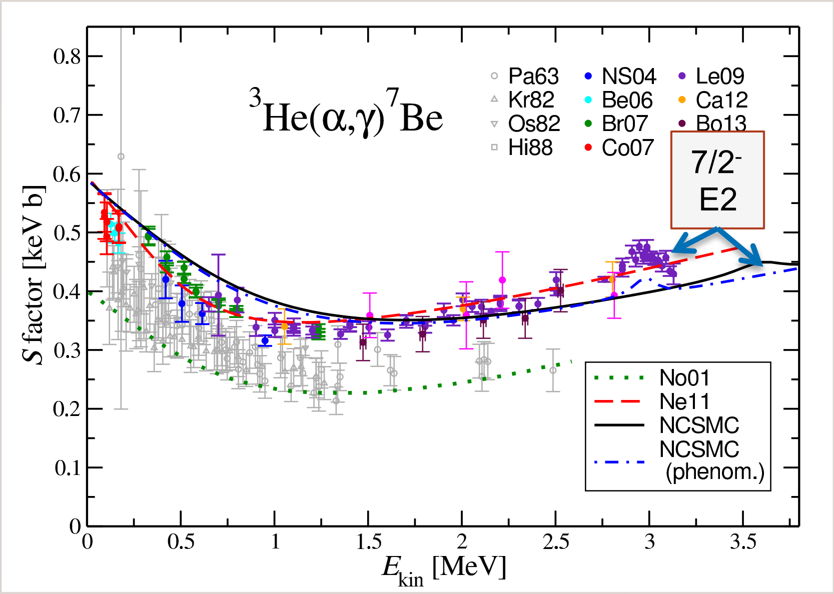
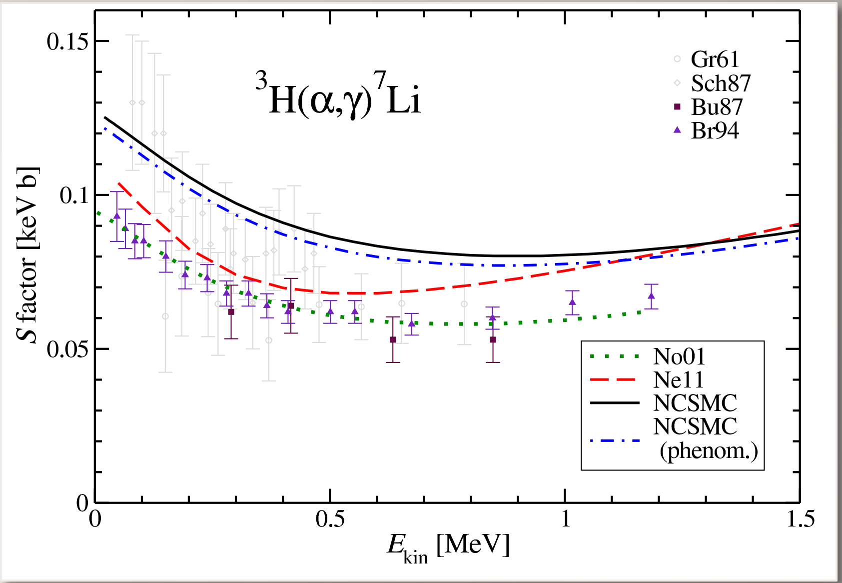


^{3}He-^{4}He and ^{3}H-^{4}He capture

E1 radiative capture with small E2 contribution at 7/2$^-$ resonance





J. Dohet-Eraly, P.N., S. Quaglioni, W. Horiuchi, G. Hupin, F. Raimondi, PLB **757**, 430 (2016)

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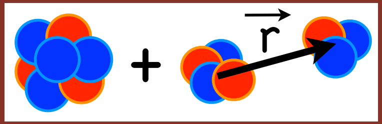
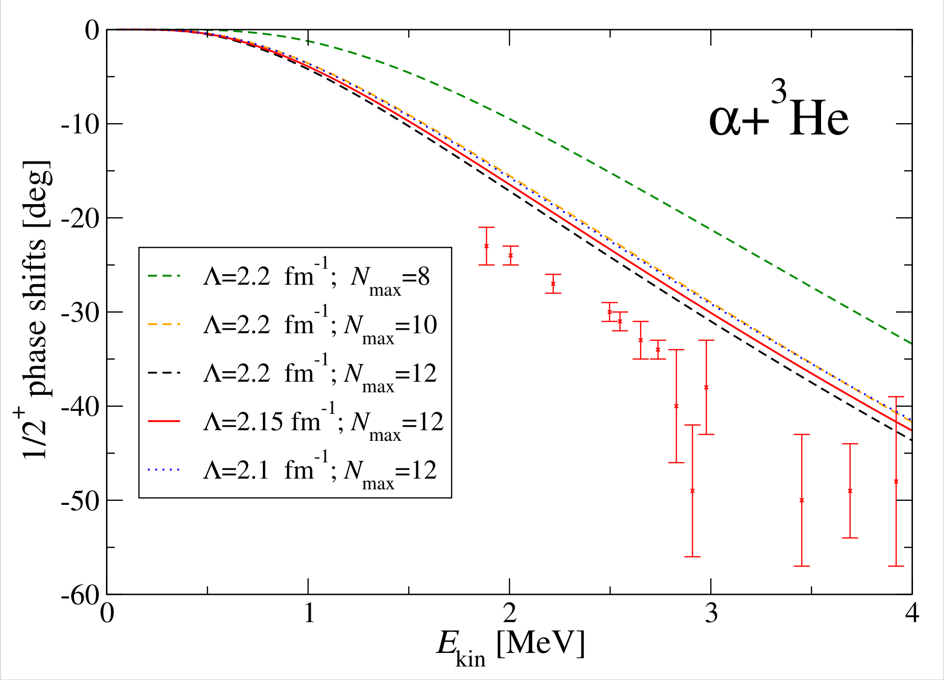
^{3}He, ^{3}H, ^{4}He ground state, 8(π-) + 6(π+) eigenstates of ^{7}Be and ^{7}Li

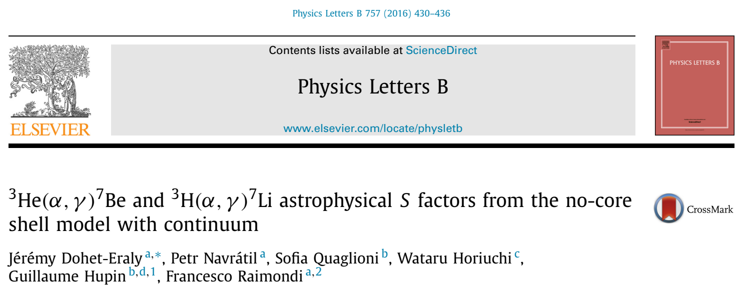
Preliminary: N_{max}=12, hΩ=20 MeV

Theoretical calculations suggest that the most recent and precise ^{7}Be and ^{7}Li data are inconsistent



^{3}He-^{4}He S-wave phase shifts





Physics Letters B 757 (2016) 430–436

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^{3}He(α,γ)^{7}Be and ^{3}H(α,γ)^{7}Li astrophysical S factors from the no-core shell model with continuum

Jérémy Dohet-Eraly[a,*], Petr Navrátil[a], Sofia Quaglioni[b], Wataru Horiuchi[c], Guillaume Hupin[b,d,1], Francesco Raimondi[a,2]

J. Dohet-Eraly, P.N., S. Quaglioni, W. Horiuchi, G. Hupin, F. Raimondi, PLB **757**, 430 (2016)

NCSMC calculations with chiral SRG-N^{3}LO *NN* potential (λ=2.15 fm^{-1})

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Preliminary: N_{max}=12, hΩ=20 MeV

NCSMC calculations with chiral NN+3N forces in preparation

Conclusions and Outlook

Ab initio calculations of nuclear structure and reactions with predictive power becoming feasible beyond the latest nuclei.

Ab initio structure calculations can even reach (selected) medium & medium-heavy mass nuclei

These calculations make the connection between the low-energy QCD, many-body systems, and **nuclear astrophysics**.

Thank you!

NCSMC and NCSM/RGM collaborators

Sofia Quaglioni (LLNL)

Jeremy Dohet-Eraly, Angelo Calci (TRIUMF)

Guillaume Hupin (CEA/DAM)

Carolina Romero-Redondo (LLNL)

Francesco Raimondi (Surrey)

Wataru Horiuchi (Hokkaido)

Robert Roth (TU Darmstadt)

Literature

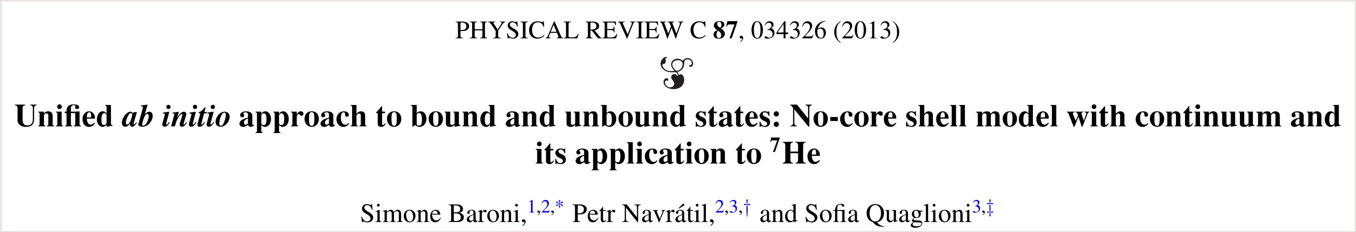
IOP Publishing | Royal Swedish Academy of Sciences Physica Scripta

Phys. Scr. **91** (2016) 053002 (38pp) doi:10.1088/0031-8949/91/5/053002

Invited Comment

Unified *ab initio* approaches to nuclear structure and reactions

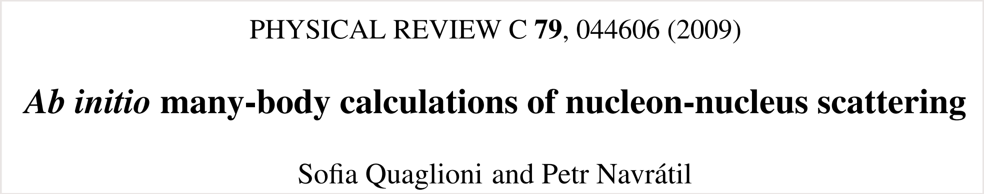
Petr Navrátil[1], **Sofia Quaglioni**[2], **Guillaume Hupin**[3,4], **Carolina Romero-Redondo**[2] and **Angelo Calci**[1]



PHYSICAL REVIEW C **87**, 034326 (2013)

Unified *ab initio* approach to bound and unbound states: No-core shell model with continuum and its application to ^{7}He

Simone Baroni,[1,2,*] Petr Navrátil,[2,3,†] and Sofia Quaglioni[3,‡]



PHYSICAL REVIEW C **79**, 044606 (2009)

Ab initio many-body calculations of nucleon-nucleus scattering

Sofia Quaglioni and Petr Navrátil