Nuclear Structure from First Principles: Ab Initio No-Core Shell Model for Light Nuclei



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Nuclear structure from first principles



Do we really know how nuclei are put together?

- Nuclear physics is a mature field, but there are still many unanswered questions about nuclei
- Atomic nuclei make up the vast majority of matter that we can see. How did they get there?
 - One of the key questions in science
 - Nucleosynthesis
 - Structure plays an important role
- The nuclear many-body problem is one of the hardest problems in all of physics!
 - Because nucleon-nucleon interaction is complicated
- A canonical nuclear structure problem: What are the properties of a system that consists of
 - ► A point-like nucleons
 - Nonrelativistic
 - Interact by inter-nucleon interactions that describe exactly (*or* as accurately as possible) two-nucleon system or two-and three-nucleon system





Why nuclear structure from first principles right now?



- 1993: New Nijmegen database of nucleon-nucleon data
 - Partial wave analysis of all NN scattering data below 350 MeV
 - Resulted in construction of high quality NN potentials that fit the data with $\chi^2/N \approx 1$
 - →Nijmegen I,II, Argonne V18, Reid 93, CD-Bonn
- These potentials difficult to use in few- and many-body calculations
 - Short range repulsive core
- However: Increase of computing power makes such calculations feasible & stimulates development of new methods

Terascale Simulation Facility





- What does the two-nucleon interaction predict for *A*-nucleon system?
- Do we need higher-body forces (three-nucleon...)?

Accurate inter-nucleon interactions plus working many-body methods allow us to predict properties of light nuclei even in a situation where no experimental data exist as well as interpret known experimental data

What are the forces in nuclei?



- Start with the simplest case: Two nucleons
 - The deuteron
 - binding energy: 2.224 MeV
 - quadrupole moment: 0.282 fm²
 - NN-scattering
 - For example: Scattering lengths and ranges for spin singlet S-wave pp, nn, and analog pn channels

$$a_{pp} = -17.3 \pm 0.4 \text{ fm}$$
 $a_{nn} = -189 \pm 0.4 \text{ fm}$ $a_{pn} = -23.74 \pm 0.02 \text{ fm}$
 $r_{pp} = 2.85 \pm 0.04 \text{ fm}$ $r_{nn} = 2.75 \pm 0.11 \text{ fm}$ $r_{pn} = 2.77 \pm 0.05 \text{ fm}$

→ Unbound!

- → Note that $V_{pp} \neq V_{nn} \neq V_{pn}$: Charge independence breaking (CIB), charge symmetry breaking (CSB)
- From these we infer the form of the nucleon-nucleon interaction
 - The starting point is the Yukawa hypothesis of meson exchange
 - Pion, rho, omega, two pion (sigma), etc.
- Features: short range, attractive in its intermediate range, repulsive core, tensor force, spinorbit force
- Two-nucleon channels: spin *s*, relative orbital momentum *l*, total angular momentum *j* $/l \cdot s / \le j \le l + s$, isospin *t*, parity = $(-1)^l$, antisymmetry: $(-1)^{l+s+t} = -1$
 - Coupled channels: s=1, l=j-1, j+1- ${}^{3}S_{1}-{}^{3}D_{1}$... deuteron, ${}^{3}P_{2}-{}^{3}F_{2}$, ${}^{3}D_{3}-{}^{3}G_{3}$...
 - Uncoupled channels: s=0, l=j or s=1, l=j or s=1, l=1, j=0
 - $-{}^{1}S_{0}, {}^{3}P_{0}, {}^{1}P_{1}, {}^{3}P_{1}, {}^{1}D_{2}, {}^{3}D_{2} \dots$
 - ► *s*, *j*, parity, *t* conserved

NN potentials

Designed to reproduce the deuteron and NN-scattering

- Argonne potentials (AV18, AV8')
 - R.B. Wiringa, V.G.J. Stoks, R. Schiavilla, PRC **51**, 38 (1995)
 - Electromagnetic + one pion exchange + intermediate- and short-range, local, in coordinates
- Bonn potential (CD-Bonn 2000)
 - R. Machleidt, PRC 63, 024001 (2001)
 - Based on meson-exchange
 - Nonlocal, in momentum space

• Effective field theory

- C. Ordóñez, L. Ray, U. van Kolck, PRC 53, 2086 (1996);
 E. Epelbaoum, W. Glöckle, Ulf-G. Meißner, NP A637, 107 (1998)
- D. R. Entem and R. Machleidt, PRC 68, 041001(R) (2003)
 - N³LO fourth order of perturbation theory
- Based on Chiral Lagrangians
- Expansion in momentum relative to a cutoff parameter (~ 1 GeV)
- Generally has a soft core, nonlocal, in momentum space
- Phenomenolgical nonlocal potential in coordinate space
 - INOY = Inside nonlocal, outside Yukawa
 - P. Doleschall *et al.*, PRC **67**, 064005 (2003)
 - Fits both two-nucleon and three-nucleon properties





A>2 systems and off-shell components of NN interactions

- Pion exchange is an integral part of NN interactions
 - Elastic scattering in momentum space

$$V_{local}^{\pi NN}(\mathbf{q}=\mathbf{k'}-\mathbf{k}) = -\frac{g_{\pi}^2}{4M^2} \frac{(\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q})}{\mathbf{q}^2 + m_{\pi}^2}$$



• Or, through a Fourier transform, coordinate space ($\mu = m_{\pi}c/\hbar$)

$$V_{\pi} = \frac{g_{\pi}^{2}}{4M^{2}} \frac{1}{3} m_{\pi} \left[\sigma_{1} \cdot \sigma_{2} + \left(1 + \frac{3}{\mu r} + \frac{3}{(\mu r)^{2}} \right) \left(3\sigma_{1} \cdot \hat{\mathbf{r}} \sigma_{2} \cdot \hat{\mathbf{r}} - \sigma_{1} \cdot \sigma_{2} \right) \right] \frac{e^{-\mu r}}{\mu r}$$
Tensor operator

• Off-shell $(|\mathbf{k}| \neq |\mathbf{k'}|)$ component present, e.g. in the Bonn or EFT potentials

$$V^{\pi NN}(\mathbf{k}',\mathbf{k}) = -\frac{g_{\pi}^2}{4M^2} \frac{(E'+M)(E+M)}{(\mathbf{k}'-\mathbf{k})^2 + m_{\pi}^2} \left(\frac{\sigma_1 \cdot \mathbf{k}'}{E'+M} - \frac{\sigma_1 \cdot \mathbf{k}}{E+M}\right) \times \left(\frac{\sigma_2 \cdot \mathbf{k}'}{E'+M} - \frac{\sigma_2 \cdot \mathbf{k}}{E+M}\right)$$

- Nonlocal
 - Depends on the energies *E* and *E*' of the initial and final state
 - Or, through a Fourier transform, on relative positions r and r' in initial and final state
- Plays a role in many-body (A>2) applications and provides more binding



Methods for solving few-nucleon (A=3,4) systems with realistic inter-nucleon interactions



Nonrelativistic point-like nucleons interacting by realistic two- and three-nucleon forces

- A=3,4 many exact methods • Faddeev equations for A=3 - Jacobi coordinates - Faddeev amplitude $\Phi_3(\vec{r}, \vec{y})$ $\Psi = \Phi_1 + \Phi_2 + \Phi_3$ $\left[T + V(\vec{r})(1 + \tau_+ + \tau_-)\right]\Phi_3 = E\Phi_3$ $\vec{r} = \frac{1}{\sqrt{2}}[\vec{r_1} - \vec{r_2}]$ $\vec{y} = \sqrt{\frac{2}{3}}[\frac{1}{2}(\vec{r_1} + \vec{r_2}) - \vec{r_3}]$ 2
 - 2001: A=4 benchmark paper: 7 different approaches obtained the same ⁴He bound state properties using the Argonne V8' nucleon-nucleon potential
 - Faddeev-Yakubovsky equations
 - CRCGV = coupled-rearrangement-channel Gaussian-basis variational method
 - SVM = stochastic variational method
 - GFMC = Green's function Monte Carlo method
 - HH variational = hyperspherical harmonic variational method
 - EIHH = effective interaction hyperspherical harmonic method
 - NCSM = no-core shell model

Methods for solving A>4 systems with realistic inter-nucleon interactions

Nonrelativistic point-like nucleons interacting by realistic two- and three-nucleon forces

- A>4 few methods applicable when realistic two- and three-nucleon forces used
 - Green's Function Monte Carlo (GFMC)

- Results published up to A=10, ¹²C calculations under way
- Coupled-Cluster Method (CCM), Unitary Model Operator Approach (UMOA)
 - Applicable mostly to closed shell nuclei
 - → ¹O results by Mihaila and Heisenberg, D. Dean and M. Hjort-Jensen (CCM) $|\Psi_0\rangle = e^{s^+} |\Phi_0\rangle$; $S^+ = \sum S_n^+$
 - →K. Suzuki and R. Okamoto (UMOA)
- Effective Interaction Hyperspherical Harmonic Method (EIHH)
 - N. Barnea, W. Leidemann, G. Orlandini
 - Converged results for A=6,7 with semi-realistic forces, first results for ⁶Li with AV8'
 - Now in principle capable of using realistic three-body forces
- ► Ab Initio No-Core Shell Model (NCSM)
 - Very simple, when just the two-body effective interaction considered
 - It works
 - Much more complicated when three-body interaction included
 - D.-C. Zheng, B. R. Barrett and J. P. Vary, 1993, G-matrix
 - P. N. and B. R. Barrett, 1996
 - →unitary transformation based effective interaction
 - \rightarrow convergence to exact solution
 - P. N. and W. E. Ormand, 2003
 - \rightarrow Three-body interaction included in *p*-shell nuclei calculations



 $\Psi_0 = \lim_{\tau \to \infty} e^{-(H - E_0)\tau} \Psi_T$



Goal: Solution of nuclear structure problem for light nuclei

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

- Many-body Schroedinger equation
 - A-nucleon wave function
- Hamiltonian

$$H = \sum_{i=1}^{A} \frac{\vec{p}_{i}^{2}}{2m} + \sum_{i < j}^{A} V_{NN}(\vec{r}_{i} - \vec{r}_{j}) \quad \left(+ \sum_{i < j < k}^{A} V_{ijk}^{3b} \right)$$

- Realistic nucleon-nucleon potentials
 - Coordinate space Argonne V18, AV8', (three-body Tucson-Melbourne)
 - Momentum space CD-Bonn, Chiral
- Modification by center-of-mass harmonic oscillator (HO) potential (Lipkin 1958)

$$\frac{1}{2}Am\Omega^{2}\vec{R}^{2} = \sum_{i=1}^{A} \frac{1}{2}m\Omega^{2}\vec{r_{i}}^{2} - \sum_{i< j}^{A} \frac{m\Omega^{2}}{2A}(\vec{r_{i}} - \vec{r_{j}})^{2} \qquad \qquad \vec{R} = \frac{1}{A}\sum_{i=1}^{A}\vec{r_{i}}$$

- No influence on the internal motion (in infinite space)
- Introduces mean field for sub-clusters
- Convenient to work in the HO basis

$$H^{\Omega} = \sum_{i=1}^{A} \left[\frac{\vec{p}_{i}^{2}}{2m} + \frac{1}{2} m \Omega^{2} \vec{r}_{i}^{2} \right] + \sum_{i< j}^{A} \left[V_{NN}(\vec{r}_{i} - \vec{r}_{j}) - \frac{m \Omega^{2}}{2A} (\vec{r}_{i} - \vec{r}_{j})^{2} \right] \left(+ \sum_{i< j< k}^{A} V_{ijk}^{3b} \right)$$

Origin of the shell model



• Goeppert-Mayer and Haxel, Jensen, and Suess proposed the independent-particle shell model to explain the magic numbers





M.G. Mayer and J.H.D. Jensen, *Elementary Theory of Nuclear* Shell Structure, p. 58, Wiley, New York, 1955

Coordinates, basis and model space

Bound states or narrow resonances: square-integrable A-nucleon basis

- NN (and three-nucleon) interaction depends on relative coordinates
 - Translationally invariant system
 - We should use Jacobi (relative) coordinates
- However:

• We use (a finite) harmonic-oscillator basis

- Bad asymptotics
 - Large basis, renormalization
- The only basis that allows a switch from Jacobi coordinates to Cartesian coordinates without violating translational invariance
 - Use of powerful second quantization shell model techniques
 - − Choice of whatever is more efficient
 →A>4 Cartesian coordinate Slater determinant basis
- And complete N_{\max} $\hbar \Omega$ model space
 - Translational invariance even when Cartesian coordinate Slater determinant basis used
 - →True only for harmonic oscillator basis

$$\varphi_{nlm}\left(\vec{\mathbf{r}}\right) = R_{nl}\left(r\right)Y_{lm}\left(\hat{\mathbf{r}}\right)$$
$$\varphi_{nljj_{z}}\left(\vec{\mathbf{r}},\sigma,\tau\right) = R_{nl}\left(r\right)\left[Y_{l}\left(\hat{\mathbf{r}}\right)\otimes\chi_{\frac{1}{2}}^{S}\left(\sigma\right)\right]_{j_{z}}^{(j)}\chi_{\frac{1}{2}m_{t}}^{T}\left(\tau\right)$$
$$\left[Y_{l}\left(\hat{\mathbf{r}}\right)\otimes\chi_{\frac{1}{2}}^{S}\left(\sigma\right)\right]_{j_{z}}^{(j)} = \sum_{ms_{z}}\left(lm\frac{1}{2}s_{z} \mid jj_{z}\right)Y_{lm}\left(\hat{\mathbf{r}}\right)\chi_{\frac{1}{2}s_{z}}^{S}$$





Translationally-invariant HO basis



Jacobi coordinates

Larger model space

 \odot

- Remove COM degrees of freedom
- HO basis depending on Jacobi coordinates coupled to J and T

Two-, three- and higher-body interaction

- Flexible basis rearangements, different clustering
- Limitations
 - Complicated antisymmetrization

– Profitable for few-nucleon systems A=3-4

Antisymmetrization of translationally-invariant HO basis





Antisymmetrizer for A=3



• Basis
$$|nlsjt, \text{NLJ}, JT\rangle$$

 $\langle \vec{r}, \sigma_1, \sigma_2, \tau_1, \tau_2 | nlsjt \rangle = R_{nl}(r) \Big[Y_l(\hat{r}) \otimes \Big[\chi_{\frac{1}{2}}^S(\sigma_1) \otimes \chi_{\frac{1}{2}}^S(\sigma_2) \Big]^{(s)} \Big]^{(j)} \Big[\chi_{\frac{1}{2}}^T(\tau_1) \otimes \chi_{\frac{1}{2}}^T(\tau_2) \Big]^{(t)}$
 $\langle \vec{y}, \sigma_3, \tau_3 | \text{NLJ} \rangle = R_{\text{NL}}(y) \Big[Y_L(\hat{y}) \otimes \chi_{\frac{1}{2}}^S(\sigma_3) \Big]^{(J)} \chi_{\frac{1}{2}}^T(\tau_3)$

- No antisymmetrization except for $1 \leftrightarrow 2$: $(-1)^{l+s+t} = -1$
- $\langle X \rangle = 1/3 \langle 1 \tau_{13} \tau_{23} \rangle$
 - Eigenspace corresponding to eigenvalue $1 \rightarrow physical$ eigenstates
 - Eigenspace corresponding to eigenvalue $0 \rightarrow spurious$ eigenstates

$$\begin{split} & \left\langle n_{1}l_{1}s_{1}t_{1}j_{1},\mathsf{N}_{1}\mathsf{L}_{1}\mathsf{J}_{1},JT \left| \tau_{+} + \tau_{-} \right| n_{2}l_{2}s_{2}t_{2}j_{2},\mathsf{N}_{2}\mathsf{L}_{2}\mathsf{J}_{2},JT \right\rangle = -\delta_{N_{1},N_{2}}\hat{t}_{1}\hat{t}_{2} \begin{cases} \frac{1}{2} & \frac{1}{2} & t_{1} \\ \frac{1}{2} & T & t_{2} \end{cases} \right. \\ & \left. \times \sum_{LS} \hat{L}^{2}\hat{S}^{2}\hat{s}_{1}\hat{s}_{2}\hat{j}_{1}\hat{j}_{2}\hat{\mathsf{J}}_{1}\hat{\mathsf{J}}_{2}(-1)^{L} \begin{cases} l_{1} & s_{1} & j_{1} \\ \mathsf{L}_{1} & \frac{1}{2} & \mathsf{J}_{1} \\ L & S & J \end{cases} \begin{cases} l_{2} & s_{2} & j_{2} \\ \mathsf{L}_{2} & \frac{1}{2} & \mathsf{J}_{2} \\ L & S & J \end{cases} \begin{cases} \frac{1}{2} & \frac{1}{2} & s_{1} \\ \frac{1}{2} & S & s_{2} \end{cases} \\ & \left. \times \left[(-1)^{s_{1}+s_{2}+t_{1}+t_{2}-\mathsf{L}_{1}-l_{1}} \langle \mathsf{N}_{1}\mathsf{L}_{1}n_{1}l_{1}L \right| n_{2}l_{2}\mathsf{N}_{2}\mathsf{L}_{2}L \rangle_{d=3} + \left\langle n_{1}l_{1}\mathsf{N}_{1}\mathsf{L}_{1}L \right| \mathsf{N}_{2}\mathsf{L}_{2}n_{2}l_{2}L \rangle_{d=3} \end{cases} \\ & \left. - \left\langle \tau_{13} \right\rangle = \left\langle \tau_{23} \right\rangle \end{split}$$

Slater-determinant HO basis



Single-particle coordinates

- Complete N_{\max} h Ω space
 - Total separation of center-of-mass and internal motion
 - Physical eigenstates contain $0\hbar\Omega$ center-of-mass wave function \otimes
 - Eigenstates that contain higher than $0\hbar\Omega$ CM components spurious
 - Shifted to higher energy by Lawson projection term
- Application of powerful second quantization techniques 😊 😊

• Limits

- Huge dimensions
- ► Three- and higher-body interactions not easy to implement 🛛 😕

Slater determinant basis and second quantization

- Second quantization is one of the most useful representations in many-body theory
- Creation and annhilation operators
 - Denote $|0\rangle$ as the state with no particles (the vacuum)
 - a_i^+ creates a particle in state *i*;
 - a_i annhilates a particle in state i;
 - Anticommutation relations:

$$a_i^+ |0\rangle = |i\rangle, \quad a_i^+ |i\rangle = 0$$

 $a_i^- |i\rangle = |0\rangle, \quad a_i^- |0\rangle = 0$

$$\{a_i^+, a_j^+\} = \{a_i, a_j\}$$

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

• Many-body Slater determinant

$$\phi_{i}(\mathbf{r}) = \left\langle \vec{r}, \sigma, \tau \middle| i \equiv nljmm_{t} \right\rangle = R_{nl}(r) \left[Y_{l}(\hat{r}) \otimes \chi_{\frac{1}{2}}^{S}(\sigma) \right]_{m}^{(j)} \chi_{\frac{1}{2}m_{t}}^{T}(\tau)$$

$$\Phi = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_i(\mathbf{r}_1) & \phi_i(\mathbf{r}_2) & \dots & \phi_i(\mathbf{r}_A) \\ \phi_j(\mathbf{r}_1) & \phi_j(\mathbf{r}_2) & \dots & \phi_j(\mathbf{r}_A) \\ \vdots & \ddots & \vdots \\ \phi_l(\mathbf{r}_1) & \phi_l(\mathbf{r}_2) & \dots & \phi_l(\mathbf{r}_A) \end{vmatrix} = a_l^+ \dots a_j^+ a_i^+ | 0 \rangle$$

Building the shell-model basis states



- Need to construct the many-body basis states to calculate matrix elements of *H*
- Choose states with definite parity, J_z and T_z and let the Hamiltonian do the rest
 - A very useful approach is a bit-representation known as the M-scheme



A single integer represents a complicated Slater Determinant

Lanczos algorithm for large matrix diagonalization

• Setup Hamiltonian matrix $\langle j|H|i\rangle$ and diagonalize

- Lanczos algorithm
 - Bring matrix to tri-diagonal form

$$\hat{H}\mathbf{v}_{1} = \boldsymbol{\alpha}_{1}\mathbf{v}_{1} + \boldsymbol{\beta}_{1}\mathbf{v}_{2}$$
$$\hat{H}\mathbf{v}_{2} = \boldsymbol{\beta}_{1}\mathbf{v}_{1} + \boldsymbol{\alpha}_{2}\mathbf{v}_{2} + \boldsymbol{\beta}_{2}\mathbf{v}_{3}$$
$$\hat{H}\mathbf{v}_{3} = \boldsymbol{\beta}_{2}\mathbf{v}_{2} + \boldsymbol{\alpha}_{3}\mathbf{v}_{3} + \boldsymbol{\beta}_{3}\mathbf{v}_{4}$$
$$\hat{H}\mathbf{v}_{4} = \boldsymbol{\beta}_{3}\mathbf{v}_{3} + \boldsymbol{\alpha}_{4}\mathbf{v}_{4} + \boldsymbol{\beta}_{4}\mathbf{v}_{5}$$



- nth iteration computes 2nth moment
 - But you can't find eigenvalues with calculated moments
- Eigenvalues converge to extreme (largest and smallest) values
- \sim 100-200 iterations needed for 10 eigenvalues (even for 10⁸ states)



Slater Det vs. Jacobi-coordinate HO basis



Transformations possible \rightarrow choose the more efficient

	Slater Det	Jacobi coordinates
Effective interaction $(V_{2eff}, V_{3eff}, V_{3b}, V_{4eff})$	-	exact
A=3	$\sim\!22$ ት Ω	60 ት $oldsymbol{\Omega}$
A=4	$\sim\!\!22$ ћ Ω	18 ћ $\Omega~{ m V}_{ m 2eff}$, 16 ћ $\Omega~{ m V}_{ m 3eff}$
A=5	~ 16 ћ Ω	8九 Ω V _{3eff}
A=6,7	~16 $\hbar\Omega$ $V_{ m 2eff}$, 6 $\hbar\Omega$ $V_{ m 3eff}$	4ክ Ω V_{3eff}
A=8	10 ħ Ω $\mathrm{V}_{\mathrm{2eff}}$, 4ħ Ω $\mathrm{V}_{\mathrm{3eff}}$	0 h Ω $V_{ m 2eff}$
A=9,10	$10\hbar\Omega~V_{ m 2eff}$, $4\hbar\Omega~V_{ m 3eff}$	-
A=11-16	$8\hbar\Omega~V_{2eff}$, $4\hbar\Omega~V_{3eff}$	-
Limitations	dimension $\sim 7 \times 10^8$ V _{3eff} , V _{4eff} complicated	antisymmetrization

Model space, truncated basis and effective interaction

Strategy: Define Hamiltonian, basis, calculate matrix elements and diagonalize. But:

- Finite harmonic-oscillator Jacobi coordinate or Cartesian coordinate Slater determinant basis
 - Complete N_{\max} h Ω model space

Nucleon-nucleon interaction

150

100

50

-50

-100

OTENTIAL (MeV)



NN Repulsive core in V_{NN} cannot be accomodated in a truncated HO basis

Need for the effective interaction



• Choice of X $X = \exp(-\omega)$; $\omega = Q\omega P \Rightarrow \omega^2 = 0 \Rightarrow X = 1 - \omega$; $X^{-1} = 1 + \omega$ • Decoupling condition QXHX⁻¹P=0

 $QXHX^{-1}P = Q\exp(-\omega)H\exp(\omega)P = QHP - Q\omega PHP + QHQ\omega P - Q\omega PHQ\omega P = 0$



- Schroedinger equation
 - Full space $H |\Psi_k\rangle = E_k |\Psi_k\rangle; \quad k = 1, \dots, M_p, \dots \infty$
 - Model space $H_{eff} P |\Psi_k\rangle = E_k P |\Psi_k\rangle; \quad k = 1, ... d_P$ $H_{eff} = PHP + PHQ\omega P$
- Formal solution for ω

$$Q|\Psi_{k}\rangle = Q\omega P|\Psi_{k}\rangle; \quad k = 1, \dots d_{P}$$

$$\left\langle \alpha_{Q} \left| \omega \right| \alpha_{P} \right\rangle = \sum_{k=1}^{d_{P}} \left\langle \alpha_{Q} \left| \Psi_{k} \right\rangle \left\langle \widetilde{\Psi}_{k} \left| \alpha_{P} \right\rangle; \quad \sum_{k=1}^{d_{P}} \left\langle \alpha_{P'} \left| \Psi_{k} \right\rangle \left\langle \widetilde{\Psi}_{k} \left| \alpha_{P} \right\rangle = \delta_{PP'}$$

- Two iterative solutions $\leftrightarrow Q\omega_n PHQ\omega_{n-1}P \quad OP \quad Q\omega_{n-1}PHQ\omega_n P$
 - Convergence to states with largest P-space overlap Krenciglowa-Kuo
 - Convergence to states closest to energy ε ($\pm \varepsilon H_0$) Suzuki-Lee



H hermitian $\rightarrow H_{\text{eff}}$ quasi-hermitian

• Metric operator and hermitian effective Hamiltonian

$$T = P + \omega^{+} \omega$$

$$TH_{eff} = H_{eff}^{+} T$$

$$\overline{H}_{eff} = (P + \omega^{+} \omega)^{-1/2} (P + \omega^{+} \omega) H_{eff} (P + \omega^{+} \omega)^{-1/2} = (P + \omega^{+} \omega)^{-1/2} (P + \omega^{+}) H(P + \omega) (P + \omega^{+} \omega)^{-1/2}$$

$$= (P + \omega^{+} \omega)^{1/2} (PHP + PH\omega P) (P + \omega^{+} \omega)^{-1/2}$$

• Corresponding effective general operator

$$\overline{O}_{eff} = (P + \omega^+ \omega)^{-1/2} (P + \omega^+) O(P + \omega) (P + \omega^+ \omega)^{-1/2}$$

Okubo transformation

Alternatively - Suzuki and Okamoto - unitary decoupling transformation

$$\overline{H}_{eff} = P \exp[-\arctan h(\omega^+ - \omega)]H \exp[\arctan h(\omega^+ - \omega)]P$$

 $\overline{O}_{eff} = P \exp[-\arctan h(\omega^{+} - \omega)]O \exp[\arctan h(\omega^{+} - \omega)]P$

Hermitization not unique

Additional P-space unitary transformation possible





H:
$$E_1, E_2, E_3, \dots, E_{dP}, \dots, E_{\infty}$$

H. $E_1, E_2, E_3, \dots, E_{dP}$
 $Dimension of P$
 $QXHX^{-1}P = 0$
 $H_{eff} = PXHX^{-1}P$
 $Unitary X = exp[- arctan h(\omega^+ - \omega)]$

- Properties of \mathbb{H}_{eff} for *A*- nucleon system
 - A-body operator
 - Even if H two- (three-) body

$$\blacktriangleright \text{ For } \mathbf{P} \Rightarrow \mathbf{1} \quad \mathbb{H}_{\text{eff}} \Rightarrow \mathbb{H}$$

- *n*-body cluster approximation, $2 \le n \le A$
 - $\mathbb{H}^{(n)}_{eff}$ *n*-body operator
 - Two ways of convergence:
 - ► For $\mathbf{P} \Rightarrow 1$ $\mathbb{H}^{(n)}_{\text{eff}} \Rightarrow \mathbb{H}$
 - ► For $n \Rightarrow A$ and fixed P $\mathbb{H}^{(n)}_{eff} \Rightarrow \mathbb{H}_{eff}$

Effective interaction calculation in the NCSM



Ρ

n-body approximation

- Full space Hamiltonian
- Goal: effective Hamiltonian P, Q, P + Q=1

$$H^{\Omega} = \sum_{i=1}^{A} h_i + \sum_{i < j}^{A} V_{ij} + \sum_{i < j < k}^{A} V_{ijk}$$
$$PH^{\Omega}_{eff} P = P\left[\sum_{i=1}^{A} h_i + \left(\sum_{i < j}^{A} V_{ij} + \sum_{i < j < k}^{A} V_{ijk}\right)_{eff}\right] P$$

What is the best *n*-body effective interaction?

- For *A*=*n* reproduces exactly the full space results for a subset of eigenstates in the $P_n \subset P$ subspace
 - \triangleright *n*=2, two-body effective interaction approximation

$$h_{1} + h_{2} + V_{12} \rightarrow X_{2} \rightarrow P_{2} \Big[h_{1} + h_{2} + V_{2eff,12} \Big] P_{2} \rightarrow P \Big[\sum_{i=1}^{n} h_{i} + \sum_{i < j}^{n} V_{2eff,ij} \Big] P$$

$$\bullet n=3, \text{ three-body effective interaction approximation}$$

$$h_{1} + h_{2} + h_{3} + V_{12} + V_{13} + V_{23} + V_{123} \rightarrow X_{3} \rightarrow P_{3} \Big[h_{1} + h_{2} + h_{3} + V_{3eff,123}^{2b+3b} \Big] P_{3} \rightarrow P \Big[\sum_{i=1}^{n} h_{i} + \frac{1}{A-2} \sum_{i < j < k}^{n} V_{3eff,ijk}^{2b} + \sum_{i < j < k}^{n} V_{3eff,ijk}^{3b} + \sum_{i$$



$$\begin{split} H^{\Omega} &= \sum_{i=1}^{A} h_{i} + \sum_{i < j}^{A} V_{ij} + \sum_{i < j < k}^{A} V_{ijk} \\ H^{\Omega} &= \sum_{i=1}^{A} \left[\frac{\vec{p}_{i}^{2}}{2m} + \frac{1}{2} m \Omega^{2} \vec{r}_{i}^{2} \right] + \sum_{i < j}^{A} \left[V_{NN}(\vec{r}_{i} - \vec{r}_{j}) - \frac{m \Omega^{2}}{2A} (\vec{r}_{i} - \vec{r}_{j})^{2} \right] + \sum_{i < j < k}^{A} V_{ijk}^{3b} \end{split}$$



$$h_{1} + h_{2} + V_{12}$$

$$H^{\Omega} = \frac{\vec{p}_{1}^{2}}{2m} + \frac{1}{2}m\Omega^{2}\vec{r}_{1}^{2} + \frac{\vec{p}_{2}^{2}}{2m} + \frac{1}{2}m\Omega^{2}\vec{r}_{2}^{2} + V_{NN}(\vec{r}_{1} - \vec{r}_{2}) - \frac{m\Omega^{2}}{2A}(\vec{r}_{1} - \vec{r}_{2})^{2}$$

$$Q_2 X_2 [h_1 + h_2 + V_{12}] X_2^{-1} P_2 = 0$$

 $P_2 X_2 [h_1 + h_2 + V_{12}] X_2^{-1} P_2 = P_2 [h_1 + h_2 + V_{2eff,12}] P_2$





$$P\left[\sum_{i$$



Test of convergence



³H with the CD-Bonn NN potential

Dependence on the basis size (N_{max}) and the HO frequency $(\hbar \Omega)$



Convergence for different cluster approximations



Many-body effective interaction code



manyeff

• Jacobi-coordinate HO basis

- Antisymmetrization for any A (in practice up to A=6)
 - Starts with $A=3\rightarrow A=4\rightarrow \dots \rightarrow A$
- Basis transformations for different sets of Jacobi coordinates
- Calculates effective interaction by the Lee-Suzuki method
 - Two-nucleon solutions $\rightarrow V_{2\text{eff}}$
 - Three-nucleon solutions $\rightarrow V_{3\text{eff}}$
 - ► V_{4eff} generalization possible

• Solves A-nucleon system using the effective interactions

- A=3 up to $60\hbar\Omega$, A=4 up $18\hbar\Omega$
 - Sufficient for convergence
- ▶ *A*=5 up to 8ħΩ

• Fortran90

- OpenMP parallelization
- NN-potential codes as subroutines
- Eispack routines used for diagonalization of matrices
 - dimensions a few thousand

Now includes Tucson-Melbourne *NNN*-interaction

Yet another test of convergence



⁴He with the CD-Bonn 2000 NN interaction

Dependence of the $0^+ 0$ ground state and the $0^+ 0$ excited state energies on the basis size (N_{max}) and the HO frequency ($\hbar\Omega$)



Shell model codes



- NCSM two-body effective interaction code
 - Two-nucleon solutions in all NN channels
 - LS two-body effective interaction (in relative coordinates)
 - Transformation to single-particle basis \Rightarrow input to shell model codes
- M-scheme shell model codes with Lanczos diagonalization
 - Many-fermion dynamics (MFD) shell model code
 - James P. Vary (ISU), D.-C. Zheng, P. N.
 - In 1st Lanczos iteration calculates non-zero matrix elements and stores them on disk
 - In subsequent Lanczos iterations matrix elements read from the disk
 - Three-body interaction capability
 - Antoine (no-core version)
 - Etienne Caurier (Strasbourg)
 - Non-zero matrix elements calculated on the fly no disk storage
 - Sofisticated basis ordering and matrix elements enumeration
 - Exploits the fact that the shell model problem consists of proton and neutron subsystems
 - Reaches huges dimensions: 10⁹
 - Redstick
 - W. E. Ormand
 - Similar algorithm as Antoine
 - Three-body interaction capability
- Wave function processing
 - Specialized transition density code
 - Reads wave functions obtained by the MFD or Antoine

⁶Li with a realistic NN potential







⁶Li with accurate NN potential at fourth order of chiral-perturbation theory (N³LO)



⁶Li quadrupole moment




p-shell nuclei with realistic NN forces





⁹Be - negative- & positive-parity states



- Levels of both parity at low excitation enegy
- Experimental spin and parity assignments uncertain
- Existence of second low-lying 1/2⁻, 3/2⁻, 5/2⁻ states
- Cluster calculations (Koike) suggest the 11.28 MeV state to be 9/2⁻ rather than experimentally assigned 7/2⁺





Nuclear structure of exotic nuclei



⁸Be



Intruder states relevant to the R-matrix analysis



Intruder T=0 states in ⁸Be



- Required in R-matrix fits of $\alpha + \alpha$ scattering (Barker)
- Disputed in shell model calculations (Zamick)
- NCSM up to $10\hbar\Omega$ basis space (10^8 dimensions)
 - Fast decrease of intruder state excitation energy
 - ► 0⁺ 0 state below 18 MeV and below 0⁺ 1 state
 - Likely a two- α cluster l=0 state
 - <u>Configuration</u>
 - $0\hbar\Omega$ $2\hbar\Omega$ $4\hbar\Omega$ $6\hbar\Omega$ $8\hbar\Omega$ $10\hbar\Omega$
 - 0⁺ 0(intruder) 9% 41% 21% 16% 8% 5%
 - $0\hbar\Omega$ $2\hbar\Omega$ $4\hbar\Omega$ $6\hbar\Omega$ $8\hbar\Omega$ $10\hbar\Omega$
 - $-0^{+}0$ (gr. st.) 55% 19% 12% 7% 4% 3%
 - Relation to R-matrix analysis
 - Wave function overlap of ⁸Be and ⁴He
 - → Possible even using the Slater determinant basis

Intruder states in ¹⁰Be







NCSM description of ¹²C





¹⁰B binding energy



Comparison with the Green's Function Monte Carlo for AV8'



Problems in complex *p*-shell nuclei with realistic NN interactions

E [MeV]



¹¹B negative & positive-parity states



Why we need a three-nucleon interaction

^{Sea} High Quality

• Realistic two-nucleon potentials highly accurate

- Coordinate space potentials
 - Local: AV18, AV8', Nijmegen II
 - Nonlocal: Nijmegen I
- Momentum space nonlocal potentials
 - Boson-exchange potentials: CD-Bonn
 - Effective field theory potentials: N³LO
- Exact few-body calculations with these potentials show that ³H, ³He, ⁴He underbound by 5-10%
- Problems in A=3 scattering: p+d, n+d A_y puzzle
- Nuclear structure calculations with realistic two-nucleon potentials in the p-shell
 - ► GFMC, NCSM, CCM
 - Underbinding
 - Level spacing not quite right
 - Ordering of lowest states not correct for some nuclei

Regardless of which realistic two-nucleon potential used problems remain Need to include a three-nucleon interaction

What is a three-body interaction?

Two-pion exchange among three-nucleons

- Not a sequence of two two-body interactions
- Virtual Δ excitation
 - Fujita-Miazawa term

- Detailed form, spin, isospin dependence and parameters not well known
- Several three-body interactions used in few-body calculations:
 - Urbana IX: Argonne group
 - Illinois II: Argonne group, three-pion loops
 - ► Tucson-Melbourne': S. Coon *et al.*, two-pion exchange only
- Effective field theory (S. Weinberg)
 - Nucleon and pion degrees of freedom (low energies)
 - Chiral symmetry of QCD
 - Systematic expansion: Predicts three-nucleon interaction,TM' is a leading term





 (Ξ)



NCSM: Matrix element in Jacobi-coordinate HO three-nucleon basis

• Three-nucleon interaction depends on two sets of Jacobi coordinates (or momenta) $W = W_1 + W_2 + W_3$ $W_1 = \sum c_i^{k_1 k_2 K} \left[f_{3i}^{(k_1)}(\vec{x}_3) f_{2i}^{(k_2)}(\vec{x}_2) \right]^{(K)} \cdot S_i^{(K)}(\sigma_1, \sigma_2, \sigma_3) T_i^{(0)}(\tau_1, \tau_2, \tau_3)$ $\vec{x}_3 = \vec{r}_1 - \vec{r}_2 \quad ; \quad \vec{y}_3 = \frac{1}{2}(\vec{r}_1 + \vec{r}_2) - \vec{r}_3$ $\vec{x}_2 = \vec{r}_3 - \vec{r}_1 \quad ; \quad \vec{y}_2 = \frac{1}{2}(\vec{r}_3 + \vec{r}_1) - \vec{r}_2$

• Basis depends on a single set of Jacobi coordinates

 $\vec{x}_3; \vec{y}_3$

• Two tricks

• Using antisymmetry, apply permutation operators on initial state

 $- \quad \vec{x}_3 ; \vec{y}_3 \rightarrow \quad \vec{x}_2 ; \vec{y}_2$

• Insert complete set of coordinate HO states depending on \vec{x}_3 ; \vec{y}_3 between $f_{3i}^{(k_1)}(\vec{x}_3)f_{2i}^{(k_2)}(\vec{x}_2)$ and for the bra HO functions use Moshinsky transformations to \vec{x}_2 ; \vec{y}_2

Realistic three-nucleon interaction in the NCSM



The lowest possible approximation $n=3 \leftrightarrow$ three-body effective interaction

- Calculations performed in four steps
 - ▶ 1) Three-nucleon solutions for all relevant $n=3 J^{\pi}T$ channels with and without V^{3b}

$$H^{\Omega} = \sum_{i=1}^{3} \left[\frac{\vec{p}_{i}^{2}}{2m} + \frac{1}{2} m \Omega^{2} \vec{r}_{i}^{2} \right] + \sum_{i< j}^{3} \left[V_{NN} (\vec{r}_{i} - \vec{r}_{j}) - \frac{m \Omega^{2}}{2A} (\vec{r}_{i} - \vec{r}_{j})^{2} \right] + V_{123}^{3b}$$

- 2) Three-body effective interaction by unitary transformation method
 X₃
- 3) Effective interaction in Jacobi coordinate HO basis, *p*-shell nuclei calculations more efficient in Cartezian coordinate Slater determinant basis
 - \rightarrow transformation must be performed
- 4) A-nucleon calculation performed by a shell model code with a three-body capability – MFD, REDSTICK

$$h_{1} + h_{2} + h_{3} + V_{12} + V_{13} + V_{23} + V_{123} \rightarrow X_{3} \rightarrow P_{3} \Big[h_{1} + h_{2} + h_{3} + V_{3eff,123}^{2b+3b} \Big] P_{3} \rightarrow P \Big[\sum_{i=1}^{A} h_{i} + \frac{1}{A-2} \sum_{i < j < k}^{A} V_{3eff,ijk}^{2b} + \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} \Big] P_{3} \rightarrow P_{3} \Big[h_{1} + h_{2} + h_{3} + V_{3eff,123}^{2b+3b} \Big] P_{3} \rightarrow P \Big[\sum_{i=1}^{A} h_{i} + \frac{1}{A-2} \sum_{i < j < k}^{A} V_{3eff,ijk}^{2b} + \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} \Big] P_{3} \rightarrow P \Big[\sum_{i=1}^{A} h_{i} + \frac{1}{A-2} \sum_{i < j < k}^{A} V_{3eff,ijk}^{2b} + \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} \Big] P_{3} \rightarrow P \Big[\sum_{i=1}^{A} h_{i} + \frac{1}{A-2} \sum_{i < j < k}^{A} V_{3eff,ijk}^{2b} + \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} \Big] P_{3} \rightarrow P \Big[\sum_{i=1}^{A} h_{i} + \frac{1}{A-2} \sum_{i < j < k}^{A} V_{3eff,ijk}^{2b} + \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} \Big] P_{3} \rightarrow P \Big[\sum_{i=1}^{A} h_{i} + \frac{1}{A-2} \sum_{i < j < k}^{A} V_{3eff,ijk}^{2b} + \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} \Big] P_{3} \rightarrow P \Big[\sum_{i=1}^{A} h_{i} + \frac{1}{A-2} \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} + \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} \Big] P_{3} \rightarrow P \Big[\sum_{i=1}^{A} h_{i} + \frac{1}{A-2} \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} + \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} \Big] P_{3} \rightarrow P \Big[\sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} + \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} \Big] P_{3} \rightarrow P \Big[\sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} + \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} \Big] P_{3} \rightarrow P \Big[\sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} + \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} \Big] P_{3} \rightarrow P \Big[\sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} + \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} + \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} \Big] P_{3} \rightarrow P \Big[\sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} + \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} + \sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} \Big] P_{3} \rightarrow P \Big[\sum_{i < j < k}^{A} V_{3eff,ijk}^{3b} + \sum_{i < j < k$$

$n=3, V_{3eff}$: I. Exact Solutions



- Finding exact solutions $H^{(n=3)} = h_1 + h_2 + h_3 + V_{12} + V_{13} + V_{23} + V_{123}$ - For A>3 three nucleons bound in a HO well $H^{(n=3)} |k\rangle = E_k |k\rangle$
 - All $J^{\pi}T n=3$ channels:
 - $-J=1/2...N_{max}+3/2; T=1/2,3/2; \pi=+,-$
 - ► Number of needed exact eigenstates \leftrightarrow dimension of the model space (defined by N_{max}) in each $J^{\pi}T n=3$ channel
 - Faster convergence achieved by with $N_{3max} \approx 30-40 >> N_{max}$ $V_{ij} \rightarrow V_{2eff,ij}$
 - Separate contribution of the three-body interaction Calculations with and without V_{123}
 - Antisymmetrized Jacobi coordinate HO basis

$$\vec{r} = \frac{1}{\sqrt{2}} [\vec{r}_1 - \vec{r}_2]$$

$$\vec{y} = \sqrt{\frac{2}{3}} [\frac{1}{2} (\vec{r}_1 + \vec{r}_2) - \vec{r}_3]$$

$$\vec{y} = \sqrt{\frac{2}{3}} [\frac{1}{2} (\vec{r}_1 + \vec{r}_2) - \vec{r}_3]$$

$$\mathscr{A}\left(\varphi_{nlsjt}(\vec{r})\varphi_{\mathcal{N}}\left(\vec{y}\right)\right)^{(J^{\pi}T)}$$

 $2n+l+2\mathcal{N}+\mathscr{L} \leq N_{3\max}$



$n=3, V_{3eff}$: II. Lee-Suzuki method



• Model space
$$P_3$$
: $2n + l + 2\mathcal{N} + \mathscr{D} \leq N_{\max}$
 $Q_3 e^{-\omega} H^{(n=3)} e^{\omega} P_3 = 0$; $\omega = Q_3 \omega P_3$
 $H^{(n=3)} |k\rangle = E_k |k\rangle$
 $\langle \alpha_Q |\omega| \alpha_P \rangle = \sum_{k \in K} \langle \alpha_Q |k\rangle \langle \widetilde{k} | \alpha_P \rangle$, $k \in K$
 $\sum_{\alpha_P} \langle \widetilde{k} | \alpha_P \rangle \langle \alpha_P | k' \rangle = \delta_{k,k'}$
 $\gamma_P |H_{eff}^{(n=3)} |\alpha_P \rangle = \sum_{k \in K} \langle \gamma_P | (P_3 + \omega^+ \omega)^{-1/2} | \alpha_P' \rangle \langle \alpha_P' | \widetilde{k} \rangle E_k \langle \widetilde{k} | \alpha_P' \rangle \langle \alpha_P' | (P_3 + \omega^+ \omega)^{-1/2} | \alpha_P \rangle$

- Properties of $V_{3\rm eff}$
 - **•** Depends on A, N_{max} and $\hbar \Omega$
 - ► For $N_{\text{max}} \rightarrow \infty$ interaction $V_{3\text{eff}} \rightarrow V_{\text{NN}} + V_{3\text{b}}$

$n=3, V_{3eff}$: III. Transform to M-scheme



- $V_{3\text{eff}}$ calculated in Jacobi coordinate HO basis
- For *p*-shell nuclei the Slater determinant single-particle HO basis more efficient



- Complicated sum depending on
 - Products of two Brody-Moshinsky brackets (mass ratios $1, \frac{1}{2}$)
 - CFP from Jacobi coordinate antisymmetrization
 - Clebsh-Gordan coefficients



¹⁰B with the Tucson-Melbourne force



⁸Be the Tucson-Melbourne force





¹¹B with the Tucson-Melbourne force



0.345

0.440

0.526

0.525

0.461

¹³C with the Tucson-Melbourne force



¹²C with the Tucson-Melbourne force

- Binding energy increase by 6 MeV
- Improved level ordering
 - $\blacktriangleright 1^+ 0 \leftrightarrow 4^+ 0$
 - ► T=1 states
- B(GT; $0^+ 0 \rightarrow 1^+ 1$) & B(M1; $0^+ 0 \rightarrow 1^+ 1$) stronger
 - Closer to experiment





Do we really need a three-body interaction?



P. Doleschall, I. Borbely, Z. Papp and W. Plessas: Nonlocal NN interaction that fits two-nucleon data and ³H, ³He binding energies Phys. Rev. C **67**, 064005 (2003)

- Two-nucleon interaction in coordinate space
 - Local at long ranges: Yukawa tail
 - Nonlocal at shorter distances (up to 3 fm)
- Published version: Nonlocal ${}^{1}S_{0}$, ${}^{3}S_{1}$ - ${}^{3}D_{1}$ channels
 - Remaining channels taken from AV18
 - Denoted as INOY S
- Two more versions:
- i) Nonlocal in all channels containing *S*, *P* and *D* waves
 - Remaining channels taken from AV18
 - Denoted as INOY SPD
- ii) Nonlocal in all channels containing S, P and D waves
 - Triplet P waves modified to reproduce three-nucleon analysing powers
 - Remaining channels taken from AV18
 - Denoted as INOY SmodPD

Straightforward to use in the NCSM and apply to p-shell nucle

⁶Li spectrum sensitive to the NN potential



¹⁰B with the INOY nonlocal NN potential









Low-energy reactions: Cluster overlaps



Consider *a*-nucleon projectile, (*A-a*)-nucleon target and *A*-nucleon composite system

• Jacobi coordinates

- Channels described by ΓJ , $\Gamma = A \alpha \alpha I_1 \alpha \beta I_2 sl$
 - $s = I_1 + I_2$... channel spin
 - ► *l* ... orbital momentum

• Channel states

$$\begin{aligned} \left| \Phi_{\Gamma}^{JM} \right| &= \sum \left(I_{1}M_{1}I_{2}M_{2} | sm_{s} \right) (sm_{s}lm_{l} | JM) \right| A - a \alpha I_{1}M_{1} \right| a \beta I_{2}M_{2} \right\rangle Y_{lm_{l}} (\hat{\xi}_{A-a}) \\ \bullet \text{Overlap with the composite state} \\ u_{A\lambda;A-a\Gamma}^{J} (\xi_{A-a}) &= \left\langle A \lambda J M \right| A \Phi_{\Gamma}^{JM} \right) \\ \bullet Be(^{7}\text{Li}) \qquad \text{Antisymmetrizer} \end{aligned}$$

Calculation of cluster overlaps using the NCSM wave functions



a=1

Consider target, projectile and composite system as eigenstates of NCSM effective Hamiltonians with a consistent definition of basis $(N_{max}, \hbar \Omega)$

- Cluster overlap defined in Jacobi-coordinate basis
- Projectile states for a=2,3,4 are described in Jacobi-coordinate HO basis
- NCSM calculations for A>4 more efficient in single-particle Slater Determinant HO basis
 - Composite system+target in SD HO basis

Coordinate relation for
$$a=1$$

Target
center-of mass
 $\vec{r}_A = -\sqrt{\frac{A-1}{A}}\vec{\xi}_{A-1} + \sqrt{\frac{A-1}{A}}\vec{\xi}_0$
 $\vec{r}_A = -\sqrt{\frac{A-1}{A}}\vec{\xi}_{A-1} + \sqrt{\frac{1}{A}}\vec{\xi}_0$
Composite
center-of mass

• In the SD basis both the composite and the target states in the $0\hbar\Omega$ center-of-mass state

$$\varphi_{000}(\vec{R}_{A-1})\varphi_{nlm_{l}}(\vec{r}_{A}) = \langle nl00l | 00nll \rangle_{\frac{1}{A-1}} \varphi_{nlm_{l}}(\vec{\xi}_{A-1})\varphi_{000}(\vec{\xi}_{0})$$

•Cluster overlap for *a*=1

$$\langle A\lambda J | \mathbb{A}\Phi_{\Gamma}^{J} \rangle = \sum_{n} R_{nl}(\xi_{A-1}) \frac{1}{\langle nl00l | 00nll \rangle_{\frac{1}{A-1}}} \frac{1}{\hat{J}} \sum_{j} \begin{cases} I_{1} & \frac{1}{2} & s \\ l & J & j \end{cases} \hat{s}\hat{j}(-1)^{I_{1}+J-j} \\ K = \sum_{n} \langle A\lambda J | |a_{nlj}^{+}| | A - 1 \mathcal{O}I_{1} \rangle_{SD} \end{cases}$$

Generalization for a=2,3,4 straightforward

Clustering in light nuclei & resonant reactions









JLM microscopic folding optical potential

J.-P. Jeukenne, A. Lejeune and C. Mahaux, Phys. Rev. C 16, 80 (1977)

- Complex optical potential in infinite nuclear matter from BHF approximation and Reid NN potential
- Applied to finite nuclei using local density approximation
 - Non-uniform medium effects of finite range of the effective interaction included in a semiphenomenological way suggested by Hartree approximation
- Monopole diagonal optical potential:

$$U(r, E) = \frac{1}{(t\sqrt{\pi})^3} \int \rho(r') \mathcal{U}^{JLM} \left(\rho(r_i), E \right) \exp\left(-\left|\vec{r} - \vec{r'}\right| / t^2 \right) d\vec{r'}$$
$$\mathcal{U}^{JLM} \left(\rho, E\right) = V^{JLM} \left(\rho, E\right) / \rho \; ; \; r_i = \begin{cases} r \\ r' \\ (r+r') / 2 \end{cases}$$

• Transition optical potential:

$$U_{tr}(\vec{r},E) = \frac{1}{(t\sqrt{\pi})^3} \int \rho_{tr}(\vec{r}') \left(1 + \rho \frac{d}{d\rho}\right) \mathcal{U}^{JLM}(\rho,E) \Big|_{r_i} \exp\left(-\left|\vec{r} - \vec{r}'\right| / t^2\right) d\vec{r}'$$
Spin-orbit potential



- Original JLM only the central optical potential
- Complex spin-orbit potential added by E. Bauge *et al.*, Phys. Rev. C 58, 1118.

$$V_{n(p)}^{so} = \lambda_{so} \left(\frac{\hbar}{m_{\pi}c}\right)^2 \vec{l} \cdot \vec{\sigma} \frac{1}{2} \frac{1}{r} \frac{d}{dr} \left(\frac{2}{3} \rho_{p(n)} + \frac{1}{3} \rho_{n(p)}\right)$$

• Other forms available in direct reaction codes (Fresco)

• Wood-Saxon

$$V_{n(p)}^{so} = \lambda_{so} \left(\frac{\hbar}{m_{\pi}c}\right)^2 \vec{l} \cdot \vec{\sigma} \, \frac{1}{r} \frac{d}{dr} \left(\frac{1}{1 + \exp[(r-R)/a]}\right)$$

Squared Wood-Saxon

$$V_{n(p)}^{so} = \lambda_{so} \left(\frac{\hbar}{m_{\pi}c}\right)^2 \vec{l} \cdot \vec{\sigma} \, \frac{1}{r} \frac{d}{dr} \left(\frac{1}{1 + \exp[(r-R)/a]}\right)^2$$

Gaussian

$$V_{n(p)}^{so} = \lambda_{so} \left(\frac{\hbar}{m_{\pi}c}\right)^2 \vec{l} \cdot \vec{\sigma} \frac{1}{4} \frac{1}{r} \frac{d}{dr} \left(\exp\left[-(r-R)^2 / a^2\right]\right)$$

Yukawa

$$V_{n(p)}^{so} = \lambda_{so} \left(\frac{\hbar}{m_{\pi}c}\right)^2 \vec{l} \cdot \vec{\sigma} \, \frac{1}{4} \frac{1}{r} \frac{d}{dr} \left(\frac{1}{r} \exp\left[-(r-R)/a\right]\right)$$

Exponential

$$V_{n(p)}^{so} = \lambda_{so} \left(\frac{\hbar}{m_{\pi}c}\right)^2 \vec{l} \cdot \vec{\sigma} \, \frac{1}{4} \frac{1}{r} \frac{d}{dr} \left(\exp\left[-(r-R)/a\right]\right)$$

Density calculation in the NCSM



NCSM wave functions for the target nucleus

• Density operator

$$\hat{\rho}(\vec{r}) = \sum_{i=1}^{A} \delta(\vec{r} - \vec{r}_{i}) = \sum_{i=1}^{A} \frac{\delta(r - r_{i})}{rr_{i}} \sum_{Kk} Y_{Kk}(\hat{r}_{i}) Y_{Kk}^{*}(\hat{r})$$

- Standard calculation in the Slater determinant basis $\left\langle I_{f}M_{f}\left|\hat{\rho}(\vec{r})\right|I_{i}M_{i}\right\rangle = \frac{1}{\hat{I}_{f}}\sum_{Kk}\left(I_{i}M_{i}Kk\left|I_{f}M_{f}\right.\right)Y_{Kk}^{*}(\hat{r})\sum_{\substack{n_{l}l_{j}j_{1}\\n_{2}l_{2}j_{2}}}R_{n_{l}l_{1}}(r)R_{n_{2}l_{2}}(r)\frac{-1}{\hat{K}}\left\langle l_{1}j_{1}\left\|Y_{K}\right\|l_{2}j_{2}\right\rangle\left\langle I_{f}\left\|(a_{n_{1}l_{1}j_{1}}^{+}\widetilde{a}_{n_{2}l_{2}j_{2}})^{(K)}\right\|I_{i}\right\rangle$
 - Contains spurious center of mass components \otimes

Translationally invariant calculation

$$\left\langle I_{f} M_{f} \left| \hat{\rho}(\vec{r}) \right| I_{i} M_{i} \right\rangle = \left(\frac{A}{A-1} \right)^{3/2} \frac{1}{\hat{I}_{f}} \sum_{Kk} \left(I_{i} M_{i} Kk \left| I_{f} M_{f} \right\rangle Y_{Kk}^{*}(\hat{x}) \sum_{\substack{nl,n_{l}l_{1}j_{1} \\ n'l',n_{2}l_{2}j_{2}}} R_{nl}(x) R_{n'l'}(x) \right. \\ \left. \times \left(-1 \right)^{K} \frac{\hat{l}\hat{l}'(l0l'0|K0)}{\hat{l}_{1}\hat{l}_{2}(l_{1}0l_{2}0|K0)} \left(M^{K} \right)_{nln'l',n_{1}l_{1}n_{2}l_{2}}^{-1} \frac{1}{\hat{k}} \left\langle l_{1}j_{1} \right\| Y_{K} \left\| l_{2}j_{2} \right\rangle \left\langle I_{f} \left\| (a_{n_{1}l_{1}j_{1}}^{+} \widetilde{a}_{n_{2}l_{2}j_{2}})^{(K)} \right\| I_{i} \right\rangle \right.$$

$$\vec{x} = \sqrt{\frac{A}{A-1}} (\vec{r} - \vec{R}); \qquad M_{n_1 l_1 n_2 l_2, n l n' l'}^K = \sum_{N_1 L_1} (-1)^{l+l'+K+L_1} \begin{cases} l_1 & L_1 & l \\ l' & K & l_2 \end{cases} \hat{l} \hat{l} \cdot \langle n l 00l | N_1 L_1 n_1 l_1 l \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 L_1 n_2 l' \rangle_{\frac{1}{A-1}} \langle n' l' 00l' | N_1 l' \rangle_{\frac{1}{A-1}} \langle$$

Physical density ©

Importance of translational invariance





⁶He spectrum obtained in the NCSM





⁶He on polarized proton target

CNS experiment at 71 MeV/A

- NCSM ⁶He ground state density
- JLM folding optical potential
 - Parameters as obtained by earlier studies of light nuclei:
 λ_V=0.8, λ_W=0.8, *t*=1 fm,
 ρ evaluated at target position,
 original JLM parametrization
- Spin-orbit term with Wood-Saxon shape
 - Parameters:
 - λ_{SO} =5 MeV, *R*=1.3 *A*^{1/3} fm, *a*=0.8 fm
- Direct reaction code FRESCO (I. Thompson)
- Reasonable agreement with experiment also for other energies (24.5 MeV - Dubna, 40.9 MeV - Ganil)



⁶He on polarized proton target revisited



Open issues



- Description of opposite parity states, intruder states and alpha-cluster states
 - Still larger basis
 - Four-body effective interaction to describe alpha-clustering?
- Further development of effective interactions (two- and higher-body)
 - Freedom of unitary transformations
 - Reduction of the HO frequency dependence
 - Speed up of convergence
- Increase of basis in calculations with realistic three-body interaction
 - Technical issue

Collaborators



• B. R. Barrett (University of Arizona), J. P. Vary (Iowa State University), D.-C. Zheng (University of Arizona: 1993-1995)

- Started the program in 1992-1993
- E. Caurier (Strasbourg)
 - Shell model code Antoine
- A. Nogga (INT Seattle)
 - Three-body interaction, code cross-checking
- W. E. Ormand (LLNL)
 - Shell model code Redstick
- A. C. Hayes (LANL), S.A. Coon (DOE), G. P. Kamuntavicius (Vilnius)
- C. Forssen (LLNL), I. Stetcu (University of Arizona), V. Gueorguiev (LLNL)
 New postdocs
- D. C. J. Marsden (University of Arizona: 1995-2001)
 - Ph.D. student

Conclusions and outlook



- Ab initio no-core shell model
 - Method for solving the nuclear structure problem for light nuclei
 - Apart from the GFMC the only working method for A>4 at present
 - Advantages
 - applicable for any NN potential
 - → Effective field theory
 - Easily extendable to heavier nuclei
 - Calculation of complete spectra at the same time
 - Success importance of three-nucleon forces for nuclear structure

Work in progress

- Calculations with realistic three-body forces in the *p*-shell
 - Better determination of the structure of the three-body force itself
- Coupling of the NCSM to nuclear reactions theories
 - Direct reactions
 - Density from NCSM plus folding approaches
 - Low-energy resonant and nonresonant reactions
 - RGM-like approach
 - →Exotic nuclei: RIA
 - → Thermonuclear reaction rates: Astrophysics

Future plans

- Extensions to heavier nuclei
 - Effective ineraction for valence nucleons
 RIKEN, RIA

