Tensor Optimized Shell Model

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T. Myo, S, Sugimoto, K. Katō, H. Toki and K. Ikeda. Prog.Theor.Phys. **117**:257 (2007)
T. Myo, H. Toki and K. Ikeda. Prog.Theor.Phys. **121**:511 (2009)

QCD and nuclear physics used to be somehow disconnected

QCD

- DIS
- Lattice
- Chiral simmetry approaches (Mostly at hadron level)

Nuclear Physics

- Shell model (phenomenological potentials)
- Bruckner-Hartree-Fock (G-matrix)
- Density functional theory
- Ab initio: GFMC, Non-core shell model, GEM . . .

Some new approaches:

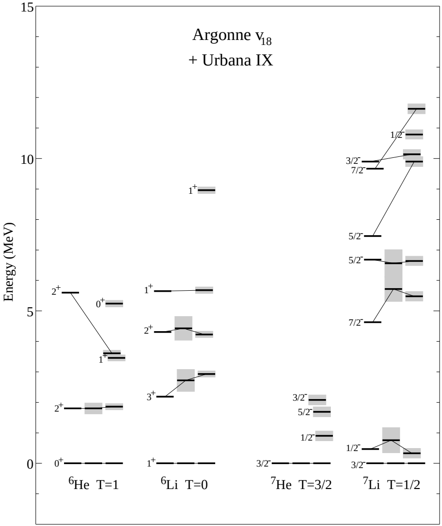
- D. Vretenar, W. Weise, Lect. Notes Phys. **641**, 65-117 (2004).
- J. A. Oller, A. Lacour, U. -G. Meissner, J. Phys. G **G37**, 015106 (2010).
- Y. Ogawa, H. Toki, in preparation.

The main feature of low-energy QCD are:

- Confinement (Still lacking easy explanation)
- Chiral symmetry

Chiral simmetry is realized in the Nambu-Goldstone boson: PION!
But pion is pseudo-scalar particle, very difficult to handle in shell model for nuclei

Nowadays we have ab initio approach to nuclear structure:
GFMC relies on nucleon-nucleon interaction



AV'18 is sophisticated nucleon-nucleon interaction

- Intermediate range and short-range hardcore:
  (40 free parameters, 18 operators)
- Fit to Nijmegen *NN*-scattering data: $\chi^2/\text{dof} = 1.09$
- Three body interactions for bound state problem (Urbana IX)
- Long range interaction: One pion exchange

$$V_\pi(\mathbf{r}) = \frac{1}{3}\frac{f^2}{4\pi}\left(\frac{e^{-m_\pi r}}{r} - \frac{4\pi}{m_\pi^2}\right)\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\tau}_1\boldsymbol{\tau}_2 + \frac{1}{3}\frac{f^2}{4\pi}\left(1 + \frac{3}{m_\pi r} + \frac{3}{m_\pi^2 r^2}\right)\frac{e^{-m_\pi r}}{r} S_{12}(\hat{\mathbf{r}})\boldsymbol{\tau}_1\boldsymbol{\tau}_2$$

$$V_\pi(\mathbf{q}) = -\frac{g^2}{4f_\pi}\frac{\boldsymbol{\sigma}_1\cdot\mathbf{q}\boldsymbol{\sigma}_2\cdot\mathbf{q}}{m_\pi^2 + \mathbf{q}^2}$$

The tensor force is crucial in light nuclei

- D-wave components: 6-7% in ^{2}H, 15% in ^{4}He
- OPE provides 70-80% of two-body attraction
- Tensor interaction: 50% of two-body matrix element
- *np* pair momentum distribution

If we want nuclear model with realistic NN interaction (long-range) we must include tensor interactions

Main features of NN potential

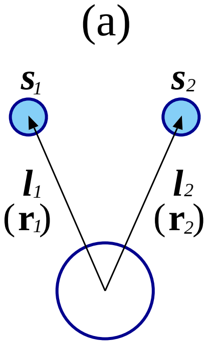
Tensor interaction: Tensor Optimized Shell Model (TOSM)

- Shell model-like space
- Variational calculation for configuration mixing
- No mean field interaction
  NN interaction with realistic tensor interaction

Short-range hard core

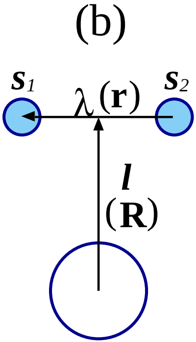
- Use effective interaction (G-matrix)
- Unitarized Correlated Operator Method (UCOM)

V-type coordinates
dof $\sim A$

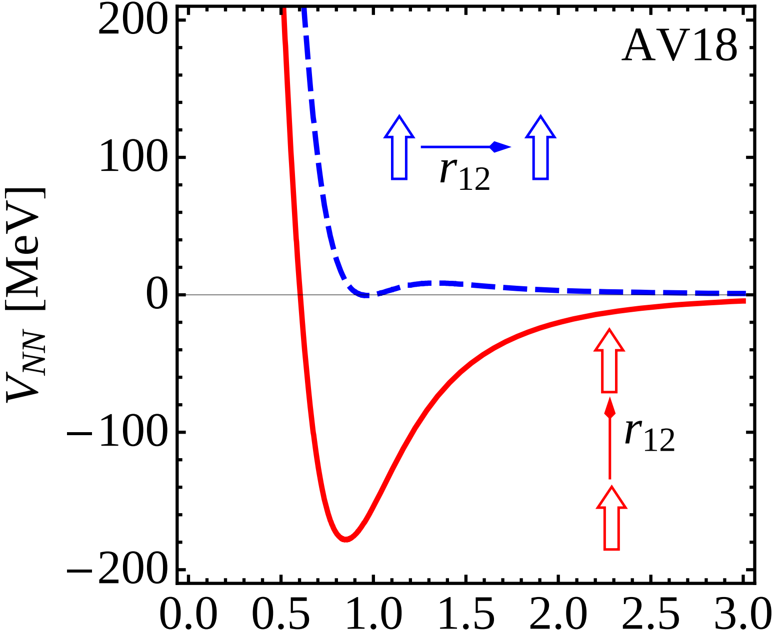


S_{12} and SR force renormalized into the central and spin-orbit terms (G-matrix, ...)

T-type coordinates
dof $\sim A^2$



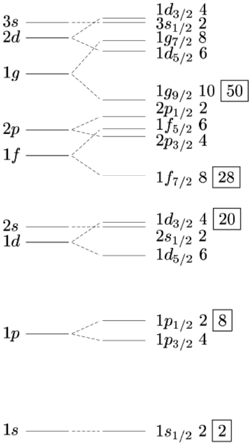
Beyond $A \sim 10$ unfeasible
Allows for Jastrow-type correlation function



AV18
V_{NN} [MeV]
200
100
0
−100
−200
0.0
0.5
1.0
1.5
2.0
2.5
3.0
r_{12}
r_{12}

TOSM model space for tensor force

$$S_{12} = \frac{3\left(\boldsymbol{\sigma}_1 \cdot \mathbf{r}\right)\left(\boldsymbol{\sigma}_2 \cdot \mathbf{r}\right)}{r^2} - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 = \sqrt{24\pi}\left[\left[\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2\right]_2, Y_2\left(\hat{\mathbf{r}}\right)\right]_0$$



Independent particle Hilbert space

$0p0h$ plus $2p2h$ configurations

$$\Psi^{0^+}(^4\mathrm{He}) = \Phi^{0^+}\left((0s)^4\right) + \Phi^{0^+}\left((0s)^2(0p)^2\right)$$

Bruckner Hartree-Fock

This is related to the Bruckner G-matrix model
We substitute $\langle ab|V|cd\rangle$ with a renormalized interaction $\langle ab|G|cd\rangle$

$$G^E_{ab,cd} = v_{ab,cd} + \frac{1}{2}\sum_{mn>\epsilon_F} v_{ab,mn}\frac{G^E_{mn,cd}}{E-\epsilon_m-\epsilon_n+i\epsilon}$$

Configuration mixing for ^{4}He

$$\Psi(^4\mathrm{He}) = \sum_{i=1}^{N_{cf}} C_p\,\Phi_i \qquad \begin{cases} \Phi_1 = (0s_{1/2})^4_{00} \\ \Phi_2 = \left[(0s_{1/2})^2_{01}, (0p_{1/2})^2_{01}\right]_{00} \\ \Phi_3 = \left[(0s_{1/2})^2_{10}, (0p_{1/2})^2_{10}\right]_{00} \\ \Phi_4 = \left[(0s_{1/2})^2_{01}, (0p_{3/2})^2_{01}\right]_{00} \\ \Phi_5 = \left[(0s_{1/2})^2_{10}, (0p_{3/2})^2_{10}\right]_{00} \\ \Phi_6 = \left[(0s_{1/2})^2_{10}, \left[(0p_{1/2})(0p_{3/2})\right]_{10}\right]_{00} \end{cases}$$

TOSM wave function

Each configuration is a Slater determinant of single particle states

$$\Phi_p = \mathcal{A}\left\{\prod_{k=1}^{A} \psi_{\alpha_k}^{n_k}\right\}$$

There are a few possible model choices for single particle wf

- Harmonic Oscillator, w/wo different length for each orbit
- Gaussian expansion method
  (E.Hiyama, et al. PPNP **51** 223,(2003))

Modified HO wf

$$\phi_i = \phi_{nljm}(\mathbf{r}_i, b_{nl})\chi_i^\tau$$
$$\phi_{nljm}(\mathbf{r}, b_{nlj}) = \phi_{nl}(r, b_{nl})\left[Y_{lm} \cdot \chi^\sigma\right]_{nljm}$$

We modify ϕ_{1s} by hand so we keep orthogonality $\langle \phi_i \mid \phi_j \rangle = \delta_{ij}$

GEM

$$\phi_{nlm}(\mathbf{r}) = \sum_{i=1}^{N} C_i^l u_{nlm,i}(\mathbf{r}, a_i)$$
$$u_{nlm}(\mathbf{r}, a) = u_{nl}(r, a) Y_{lm}(\hat{\mathbf{r}})$$
$$u_{nl}(r, a) \sim r^l \exp\left[-\frac{1}{2} a r^2\right]$$

Hamiltonian

$$H = \sum_{i=1}^{A} t_i - T_G + \sum_{\{i,j\}}^{A} v_{ij} + H_{\text{cm}}$$

with

$$v_{ij} = v_{ij}^{C} + v_{ij}^{T} + v_{ij}^{LS} + v_{ij}^{Clmb}$$

Furthermore we must extract Center of Mass excitation

$$H_{\text{cm}} = \lambda \left(\frac{P_{\text{cm}}^2}{2M_G} + \frac{1}{2}\, M_G\, \omega_G\, \mathbf{r}_G^2 - \frac{3}{2}\hbar\omega \right)$$

Variational calculation

To calculate the wf we adopt variatonal approach

$$\delta \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0$$

leads to the following equations

$$\frac{\partial \langle \Psi | H - E | \Psi \rangle}{\partial b_{\alpha,m}} = 0 \ , \quad \frac{\partial \langle \Psi | H - E | \Psi \rangle}{\partial C_p} = 0$$

The free parameters are configuration mixing parameters C_p
length parameters of the wave functions b_α

Eigenvalue problem in GEM

For the configuration mixing parameters C_p we must take into account the wf normalization

This means

$$\mathcal{H}_{ij} = \left\langle \phi_i \middle| \widehat{H} \middle| \phi_j \right\rangle , \quad \mathcal{N}_{ij} = \langle \phi_i | \phi_j \rangle$$

$$0 = \frac{\partial}{\partial \widetilde{C}_i} \langle \Psi | H - E | \Psi \rangle = \frac{\partial}{\partial \widetilde{C}_i} \left[\sum_{i'j} \widetilde{C}_{i'} \cdot C_j \left(\mathcal{H}_{i'j} - \mathcal{N}_{i'j} \right) \right]$$

$$\sum_{j}^{N} \left(\mathcal{H}_{ij} - E\, \mathcal{N}_{ij} \right) C_j = 0$$

Hill-Wheeler equation

$$\sum_{j}^{N} (\mathcal{H}_{ij} - E\ \mathcal{N}_{ij})\ C_j = 0$$

- First diagonalize norm matrix

$$\sum_{j=1}^{N} \mathcal{N}_{ij}\ n_{jk} = \mu_k\ n_{ik}$$

- Renormalize Hamiltonian

$$\widetilde{\mathcal{H}}_{ij} = \left\langle \widetilde{\phi}_i \middle| \widehat{H} \middle| \widetilde{\phi}_j \right\rangle = \sum_{k,k'=1}^{N} \widetilde{n}^*_{ki}\ \widetilde{n}_{k'j}\ \left\langle \phi_k \middle| \widehat{H} \middle| \phi_{k'} \right\rangle$$

- Diagonalize new hamiltonian

$$\sum_{j=1}^{N_1} \widetilde{\mathcal{H}}_{ij}\ D_{j\alpha} = E_\alpha\ D_{i\alpha}$$

2p-2h matrix elements computations

$$\mathcal{H}_{ij} = \left\langle 2p - 2h \middle| V \middle| 2p - 2h' \right\rangle$$

Many methods for calculation

- Slater determinants
- Coefficients of Fractional-Parentage
- Generalized Pandya transformations

Complicated because it is a full Hilbert space calculation:
All A nucleons are active!!

Results for ^{4}He

Phenomenological potential (tamed hard-core repulsion)

Tensor part

AK [Akaishi, NPA **738**,80:2004]
G-matrix force based on AV'8

Central part

GPT [Gogny et al. PLB **32**,591:1990]
Understimates tensor contribution

Optimized length parameters (b_α) of single-particle states ^{4}He

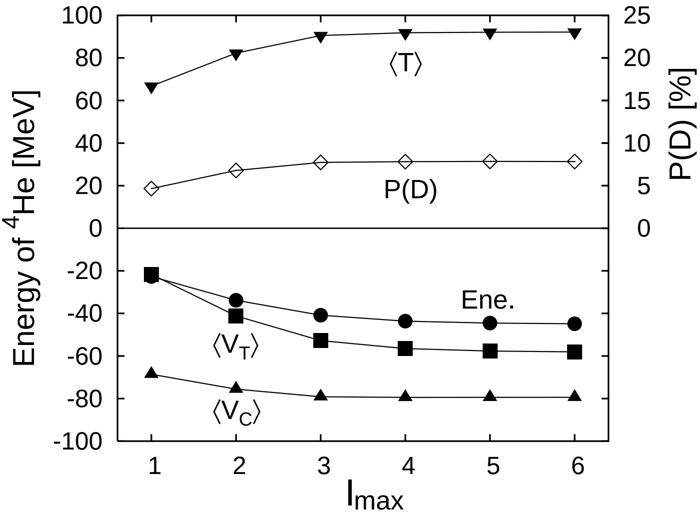
l_{max}	$0s_{1/2}$	$0p_{1/2}$	$0p_{3/2}$	$1s_{1/2}$	$0d_{3/2}$	$0d_{5/2}$	$0f_{5/2}$	$0f_{7/2}$
1	1.26	0.75	0.69	—	—	—	—	—
2	1.19	0.78	0.75	0.76	0.69	0.62	—	—
3	1.16	0.74	0.66	0.73	0.67	0.62	0.77	0.66
4	1.16	0.75	0.67	0.73	0.67	0.61	0.77	0.67
5	1.16	0.76	0.67	0.73	0.67	0.61	0.77	0.64
6	1.16	0.76	0.67	0.73	0.67	0.61	0.77	0.64

l_{max}	$0g_{7/2}$	$0g_{9/2}$	$0h_{9/2}$	$0h_{11/2}$	$0i_{11/2}$	$0i_{13/2}$
4	0.70	0.67	—	—	—	—
5	0.70	0.68	0.70	0.67	—	—
6	0.70	0.67	0.70	0.69	0.71	0.65

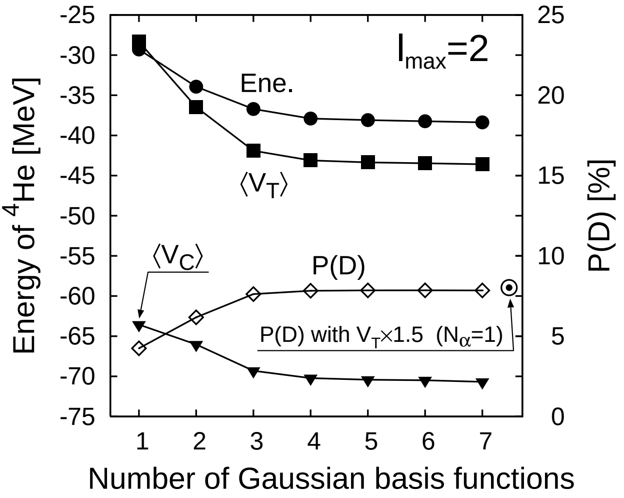
The properties of ^{4}He for each $l_{\max}$

l_{max}	1	2	3	4	5	6
E	-22.66	-33.82	-40.85	-43.65	-44.55	-44.85
$\langle T \rangle$	66.77	82.25	90.53	91.83	92.08	92.16
$\langle V_C \rangle$	-68.59	-75.57	-79.16	-79.46	-79.43	-79.40
$\langle V_T \rangle$	-21.65	-41.17	-52.80	-56.52	-57.67	-58.06
$\langle V_{LS} \rangle$	-0.67	-0.20	-0.30	-0.36	-0.39	-0.40
$\langle V_{Clmb} \rangle$	0.87	0.87	0.88	0.87	0.86	0.86
R_m	1.34	1.27	1.24	1.24	1.24	1.24
$P(D)$	4.66	6.78	7.73	7.82	7.85	7.83
$\frac{\langle H_G \rangle}{1.5\hbar\omega}$	1.067	1.048	1.024	1.021	1.017	1.016

^{4}He Properties



Results with GEM



^{4}He with GEM (4-dim basis and $l_{max} = 5$)

E	-27.89
$\langle T \rangle$	75.85
$\langle V_C \rangle$	-44.57
$\langle V_T \rangle$	-58.97
$\langle V_{LS} \rangle$	-0.98
$\langle V_{Clmb} \rangle$	0.78
$\langle H_G \rangle / (1.5\hbar\omega)$	1.011
R_m	1.47

$P(D)$	9.13
$0p0h$	85.02
$(0p_{1/2})^2_{10}$	3.40
$(1s_{1/2})(0d_{3/2})_{10}$	2.35
$(0p_{3/2})(0f_{5/2})_{10}$	2.21
$(0p_{1/2})(0p_{3/2})_{10}$	1.61
$(0d_{5/2})(0g_{7/2})_{10}$	0.83
$(0d_{3/2})^2_{10}$	0.60
$(0p_{3/2})^2_{10}$	0.53

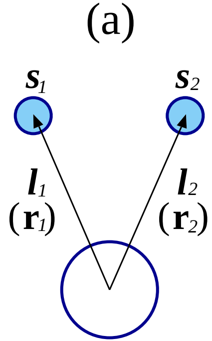
TOSM conclusions

- High partial waves are shrinked ($\sim 60\%$) with respect $0s$ orbit
- 10% of the $P(D)$
- $V_C \lesssim V_T \sim E$

However, so far this is purely academical
We use a not very realistic interaction
We still need to understand short range interactions!!

V-type coordinates
dof $\sim A$

T-type coordinates
dof $\sim A^2$



S_{12} and SR force renormalized into the central and spin-orbit terms (G-matrix, ...)

Beyond $A \sim 10$ unfeasible
Allows for Jastrow-type correlation function

UCOM

$$C = \exp(-i \sum_{i<j} g_{ij}) = \prod_{i<j} c_{ij}$$

UCOM method

$\hat{H}\Phi = E\Phi$

$\hat{H} = C^\dagger H C$

$$\delta \frac{\langle \Phi | \hat{H} | \Phi \rangle}{\langle \Phi | \Phi \rangle} = 0$$

Schrödinger equation

$H\Psi = E\Psi$

$$\delta \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0$$

- Φ is simple wf (Slater determinant)
- We impose C is unitary (g is Hermitian)

$$C^\dagger = C^{-1}, \qquad g = g^\dagger$$

H.Feldmeier *et al.* NPA **632**91, 1998

The correlation generator

$$C = \exp(-i \sum_{i<j} g_{ij} - i \sum_{i<j<k} g_{ijk})$$

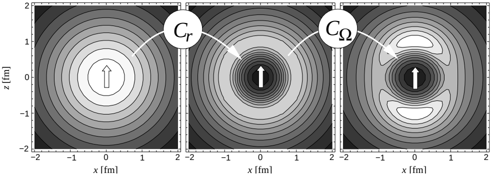
$$B^{[n]} \rightarrow \hat{B} = C^\dagger B C = \hat{B}^{[n]} + \hat{B}^{[n+1]} + \ldots$$

We limit ourselves up to two-body effects
(We are neglecting 3-body potential...)

$T = \sum_i^A t_i - T_{\text{cm}} \rightarrow$

$$\hat{T} = C^\dagger T C = \underbrace{\sum_i^A t_i - T_{\text{cm}}}_{\text{Original term}} + \underbrace{\sum_{i<j} C^\dagger t_{\text{rel}} C - t_{\text{rel}}}_{\text{Correlated part}}$$

Correlation as coordinate shift



The most general correlator would be $C = C_r C_\Omega$

C_r

$$g_{ij} = \frac{1}{2}\left\{p_r s(r) + s(r) p_r\right\}$$

C_Ω

$$g_{ij} = \frac{3}{2}\theta(\mathbf{r})\left\{(\sigma_\mathbf{i}\cdot\mathbf{p}_\perp)(\sigma_\mathbf{j}\cdot\mathbf{r}) + (\sigma_\mathbf{i}\cdot\mathbf{r})(\sigma_\mathbf{j}\cdot\mathbf{p}_\perp)\right\}$$

$g_{ij}^{[2]} = \sum_{S,T}^{(0,1)} g_{ST}(\mathbf{r},\mathbf{q})\Pi_S \otimes \Pi_T$

Relative distance correlation

Relative distance shift

$r \longrightarrow R_+(r)$ and $R_+(R_-(r)) = r$

$$c^\dagger r c = R_+(r)\,, \qquad c^\dagger p_r c = \frac{1}{\sqrt{R'_+(r)}} p_r \frac{1}{\sqrt{R'_+(r)}},$$
$$c^\dagger \mathbf{l} c = \mathbf{l}\,, \qquad c^\dagger \mathbf{s} c = \mathbf{s}\,, \qquad c^\dagger S_{12} c = S_{12}\,,$$

A most general transformation would be $\mathbf{R}_-(\mathbf{r}, \boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2)$

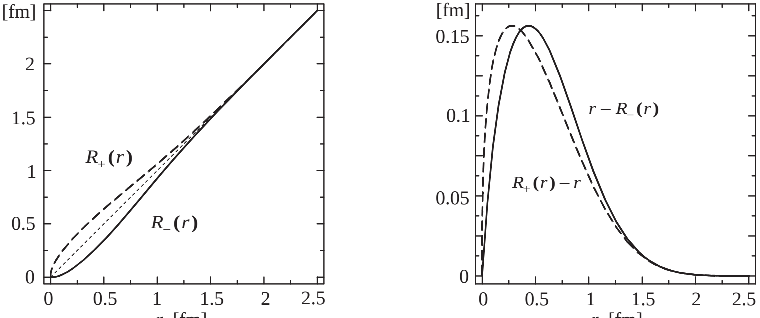
Choice of correlation function $R_\pm(r)$

We have introduced C in terms of $s(r)$ but it is more useful to define

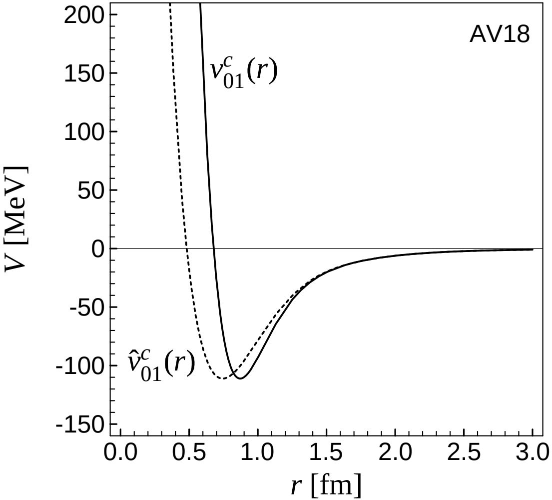
Variational input

$$R_+^{\text{even}}(r) = r + \alpha \left(\frac{r}{\beta}\right)^\gamma \exp[-\exp(r/\beta)]$$

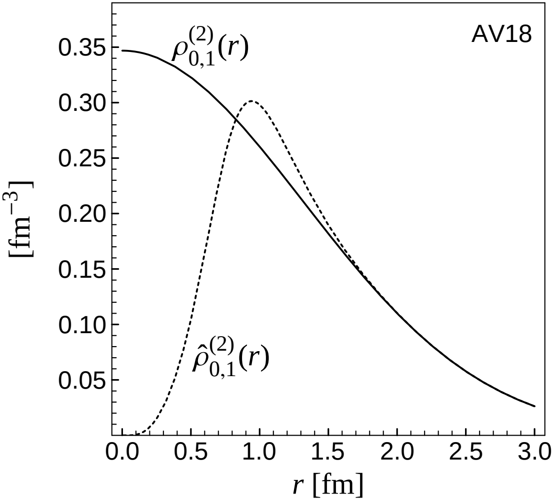
From Feldmeier *et al.*, where it was fit to the exact two body case



UCOM effect on potential

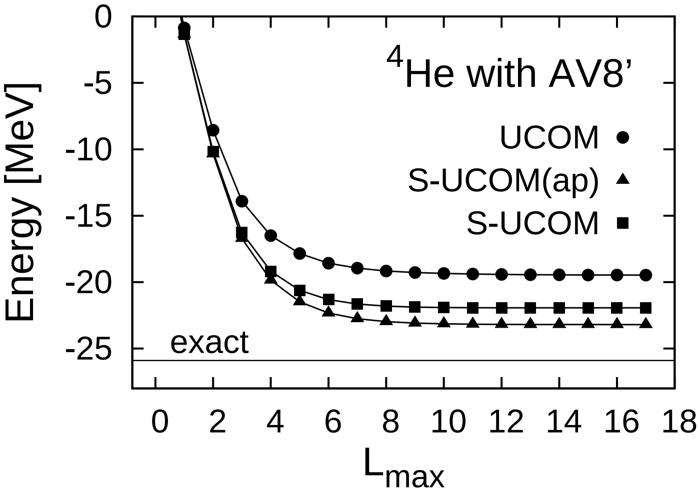


UCOM effect on densities

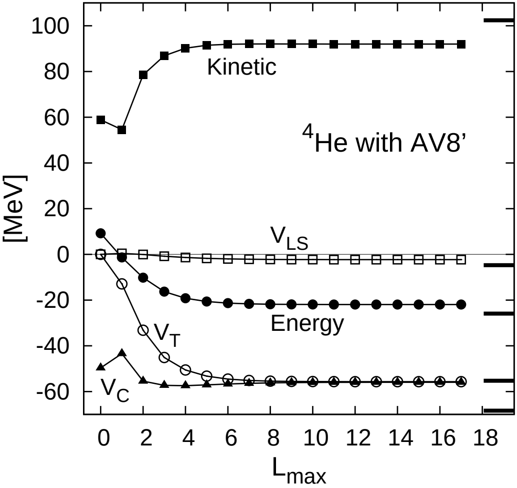


TOSM + UCOM with AV'8

(s-UCOM) approximation
Only introduce correlator in relative s-wave



TOSM + UCOM with AV'8 (S-UCOM)



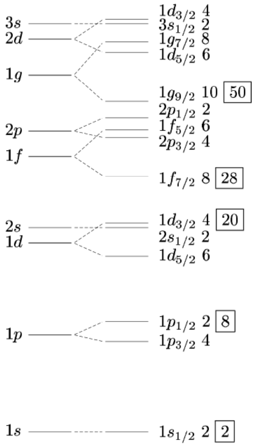
TOSM + UCOM with AV'8 (S-UCOM)

Units: MeV, fm

	Energy	Kinetic	Central	Tensor	LS	Radius
TOSM	-27.89	75.85	-44.57	-58.97	-0.98	1.47
UCOM	-19.46	88.64	-56.81	-50.05	-1.24	1.555
S-UCOM	-22.30	90.50	-55.71	-54.55	-2.53	1.546
FY	-25.94	102.39	-55.26	-68.35	-4.72	1.485

Extension to heavier nuclei

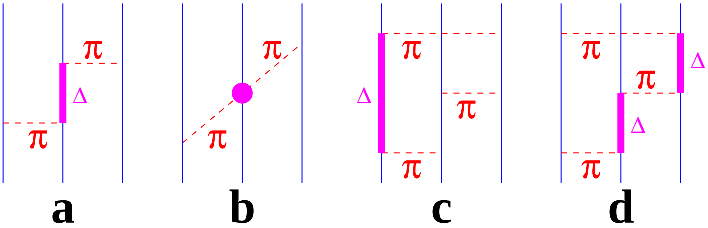
We want to extend our model to heavier nuclei
namely ^{12}C and ^{16}O



Shell structure explained by $L \cdot S$ splitting
But not fundamental explanation
Some models (Walecka σ-ω)...
What about tensor interaction?

Three body operators

GFMC studies show that 3 body forces are needed to describe ground state energies of light nuclei (AV'18 fit to NN scattering)



Conclusions

- Tensor part is crucial in realistic model of nuclear forces
- Hints of its important role in $L \cdot S$ splitting
- Subtle interplay with short range correlation (UCOM)

Outlook

We want to study nuclei $A \gtrsim 10$
The model is already set, but there are some issues

- Include 3-body correlations
- Then we will need 3-body interactions
- Introduce tensor correlation by UCOM
- Gamow-Teller operators