Tensor-optimized antisymmetrized molecular dynamics (TOAMD) for light nuclei with bare interaction

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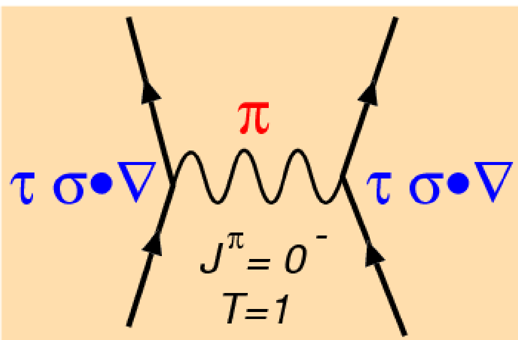
Pion exchange interaction & V_{tensor}

$$3(\vec{\sigma}_1 \cdot \hat{q})(\vec{\sigma}_2 \cdot \hat{q}) \frac{q^2}{m^2+q^2} = (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \frac{q^2}{m^2+q^2} + S_{12} \frac{q^2}{m^2+q^2}$$

$$= (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \left[\frac{m^2+q^2}{m^2+q^2} - \frac{m^2}{m^2+q^2} \right] + S_{12} \frac{q^2}{m^2+q^2}$$



δ interaction

Yukawa interaction

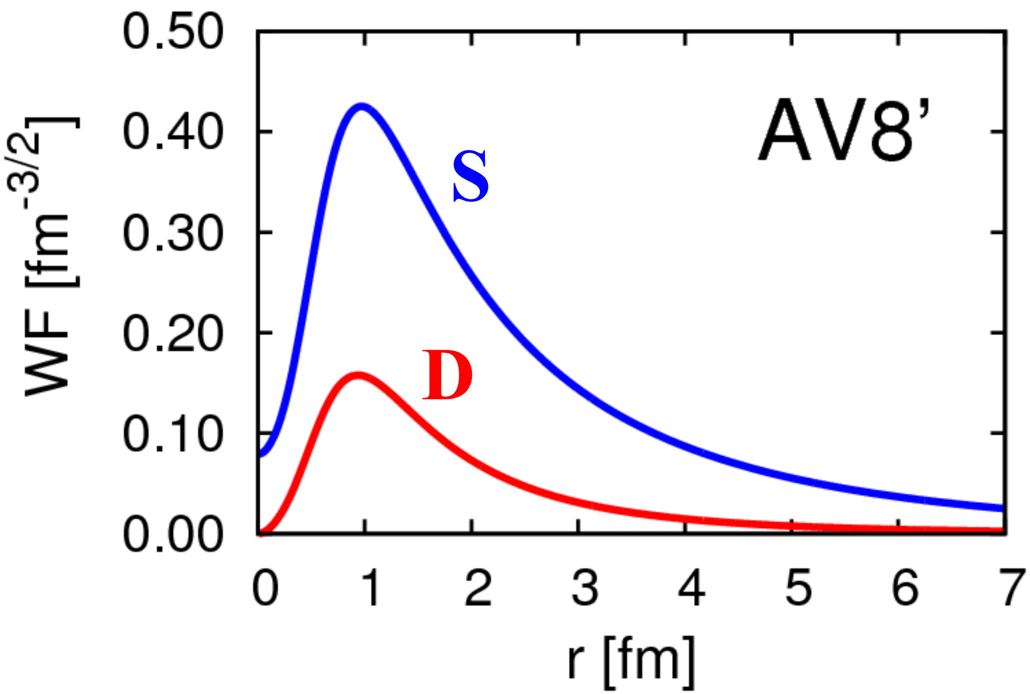
involve large momentum

Tensor operator

$$S_{12} = 3(\vec{\sigma}_1 \cdot \hat{q})(\vec{\sigma}_2 \cdot \hat{q}) - (\vec{\sigma}_1 \cdot \vec{\sigma}_2)$$

- V_{tensor} produces the high momentum component.

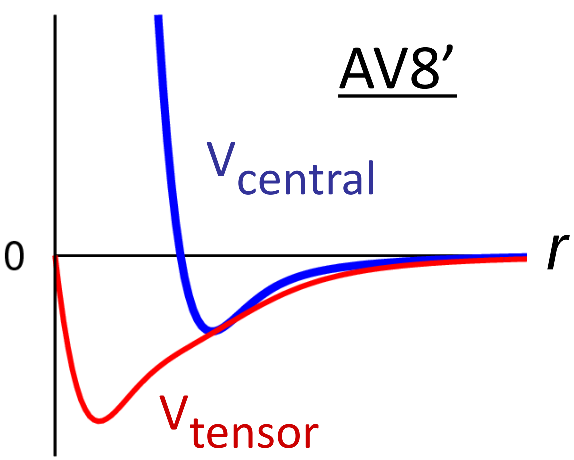
Deuteron properties & tensor force



Energy	-2.24 MeV	
Kinetic	19.88	S 11.31 D 8.57
Central	-4.46	
Tensor	**-16.64**	SD -18.93 DD 2.29
LS	-1.02	
P(L=2)	5.77%	
Radius	1.96 fm	

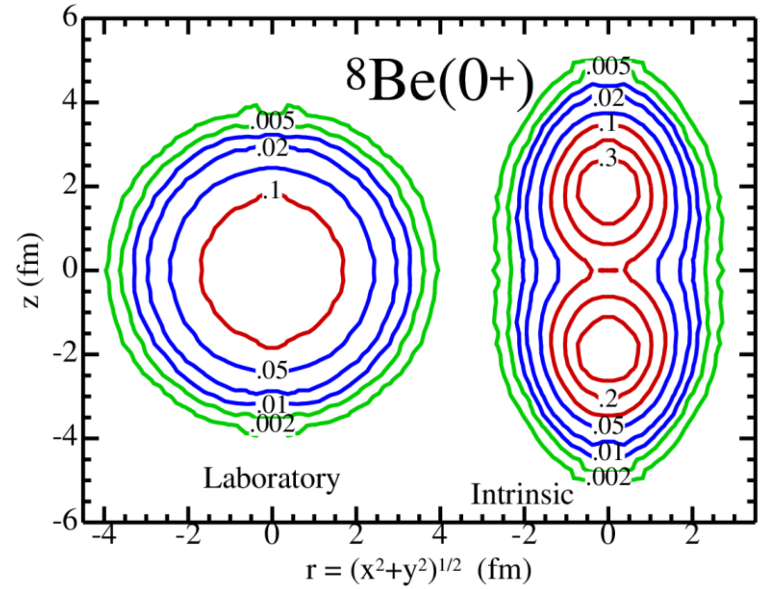
$R_m(s)$=2.00 fm

$R_m(d)$=1.22 fm



d-wave is
“**spatially compact**”
(high momentum)

Nuclear clustering & tensor force



α-α structure

- Argonne Group
  - Green's function Monte Carlo
    C.Pieper, R.B.Wiringa,
    Annu.Rev.Nucl.Part.Sci.51 (2001)
- Unitary Correlation Operator Method (**UCOM**, similar to SRG)
  - Neff, Feldmeier, NPA 713 (2004) 311.
  - Unitary transformation of V_{NN} into V_{eff} for short-range & tensor within **2-body approximation**.
  - Fermionic Molecular Dynamics (**FMD**) for nuclear w.f.
- Antisymmetrized Molecular Dynamics (**AMD**)
  - V_{eff} with central, LS, ρ-dependence.
- It is important to clarity the role of tensor force on the mechanism of nuclear clustering, such as Hoyle (triple-α) state in ^{12}C.

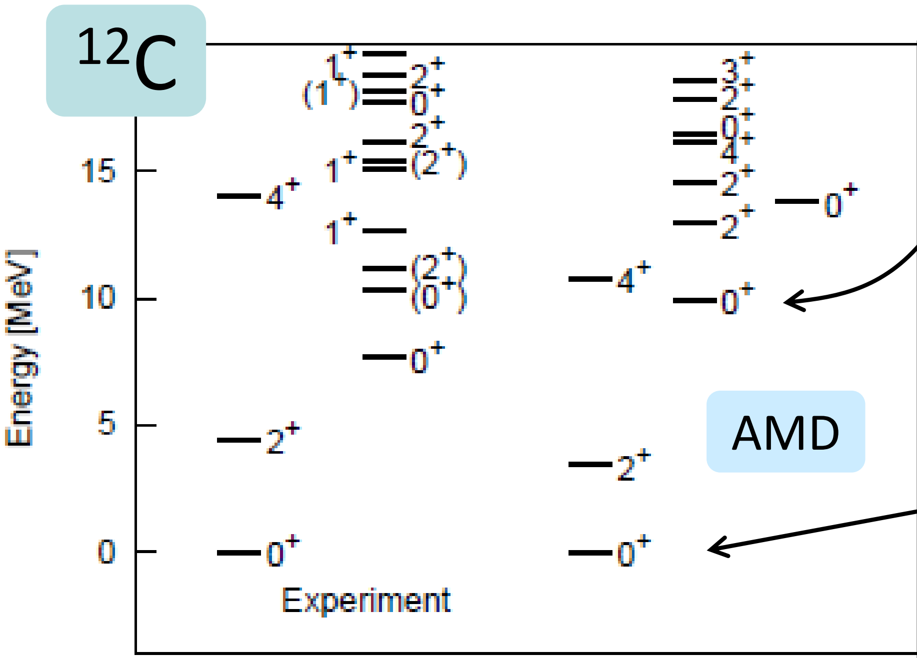
^{12}C with AMD

$$\left|\Phi_{\mathrm{AMD}}\right\rangle = \det\left\{\varphi_1 \cdots \varphi_A\right\}$$

nucleon w.f. $\quad \varphi \propto e^{-\nu(\vec{r}-\vec{Z})^2}\chi_\sigma\chi_\tau$

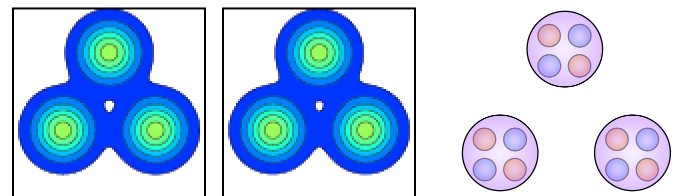
Gaussian wave packet

V_{eff} : Effective central force
+ *LS* force
(NO tensor force)



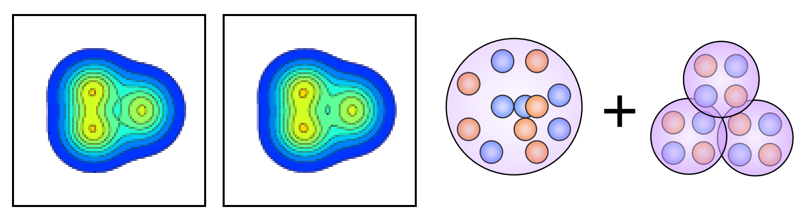
T. **Suhara**. and Y. Kanada-En'yo,
Phys. Rev. C **82,** 044301 (2010)

- 0^+(Hoyle) triple-α config.



α-particle ... s-wave state, $(0s)^4$

- 0^+(GS) shell-model-like



proton neutron

PTEP

Prog. Theor. Exp. Phys. **2015**, 073D02 (38 pages)
DOI: 10.1093/ptep/ptv087

Tensor-**O**ptimized **A**ntisymmetrized **M**olecular **D**ynamics (**TOAMD**)

TM, Hiroshi Toki, Kiyomi Ikeda, Hisashi Horiuchi, and Tadahiro Suhara

- Toward clustering description of nuclei from V_{NN} .
- Multiply tensor-type pair correlation function $\boldsymbol{F}$ to AMD w.f.
  - ✓ A. Sugie, P. E. Hodgson and H. H. Robertson, Proc. Phys. Soc. 70A, (1957) 1
  - ✓ S. Nagata, T. Sasakawa, T. Sawada, R. Tamagaki, PTP22 (1959) 274.
- Correlated Hamiltonian, $\boldsymbol{F}^{\dagger}\boldsymbol{H}\boldsymbol{F}$ generates **many-body operators** using the cluster expansion

Formulation of TOAMD

- Deuteron wave function

K. Ikeda, TM, K. Kato, H. Toki
Lecture Notes in Physics 818 (2010)

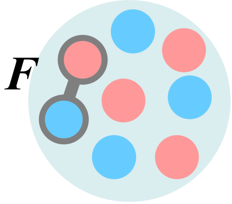
$$|\text{Deuteron}\rangle = |s\text{-wave}\rangle + |\underline{d\text{-wave}}\rangle$$

Involve high-k component induced by V_{tensor}

$$R_{d-\text{wave}} \sim 0.6 \times R_{s-\text{wave}}$$

spatially compact

- Tensor-optimized AMD (**TOAMD**)



$$|\Phi_{\text{TOAMD}}\rangle = |\Phi_{\text{AMD}}\rangle + F_D |\Phi_{\text{AMD}}\rangle$$

isospin

$$F_D = \sum_{t=0}^{1} \sum_{i<j}^{A} f_D^t(\vec{r}_i - \vec{r}_j) \cdot \left(\vec{\tau}_i \cdot \vec{\tau}_j\right)^t, \qquad f_D(\vec{r}\,) = \underline{S_{12}} \sum_{n}^{N_G} C_n e^{-a_n r^2}$$

- Pair excitation via **tensor operator** with D-wave transition
- Optimize relative motion with Gaussian expansion
- General formulation with respect to mass number A

General formulation of TOAMD

tensor

short-range (central type)

$$\left|\Phi_{\mathrm{TOAMD}}\right\rangle = (1 + F_D + F_S + F_D F_S + F_D F_D + F_S F_S + \cdots)\left|\Phi_{\mathrm{AMD}}\right\rangle$$

tensor × short-range

F_D, F_S : Gaussian expansion

- Variational principle
  - $\delta E_{\mathrm{TOAMD}} = 0$ for $E_{\mathrm{TOAMD}} = \dfrac{\langle \Phi_{\mathrm{TOAMD}} | H | \Phi_{\mathrm{TOAMD}} \rangle}{\langle \Phi_{\mathrm{TOAMD}} | \Phi_{\mathrm{TOAMD}} \rangle}$
- Variational parameters
  - AMD : ν, $\mathbf{Z}_i$ $(i=1,\dots,A)$
  - F_D : $S_{12} \sum_{n=1}^{N_G} C_n e^{-a_n r^2}$
  - F_S : $\sum_{n=1}^{N_G} C'_n e^{-a'_n r^2}$

$$\left|\Phi_{\mathrm{AMD}}\right\rangle = \det\left\{\varphi_1 \cdots \varphi_A\right\}$$

nucleon w.f. $\varphi(r) \propto e^{-\nu(\vec{r}-\vec{Z})^2} \chi_\sigma \chi_\tau$

Gaussian wave packet

$$\sum_n^N (H_{mn} - E_{\mathrm{TOAMD}} N_{mn}) C_n = 0$$

Eigenvalue problem

Matrix elements of correlated operator

Correlated Hamiltonian

$$\frac{\langle \Phi_{\mathrm{TOAMD}} | H | \Phi_{\mathrm{TOAMD}} \rangle}{\langle \Phi_{\mathrm{TOAMD}} | \Phi_{\mathrm{TOAMD}} \rangle} = \frac{\langle \Phi_{\mathrm{AMD}} | H + F^{\dagger} H F + \cdots | \Phi_{\mathrm{AMD}} \rangle}{\langle \Phi_{\mathrm{AMD}} | 1 + F^{\dagger} F + \cdots | \Phi_{\mathrm{AMD}} \rangle}$$

Correlated Norm

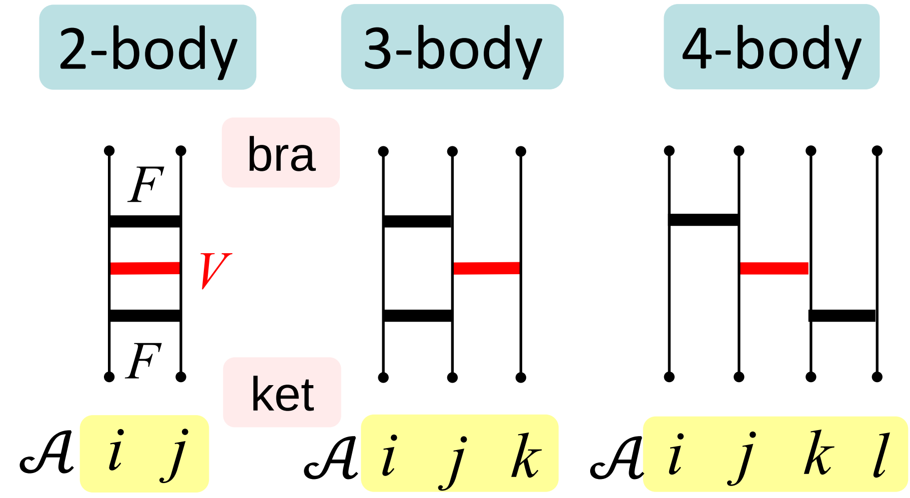
Classify the connections between F & H into **many-body operators** using cluster expansion method.

$$F^{\dagger} F = \{\text{2-body}\} + \cdots + \{\text{4-body}\}$$

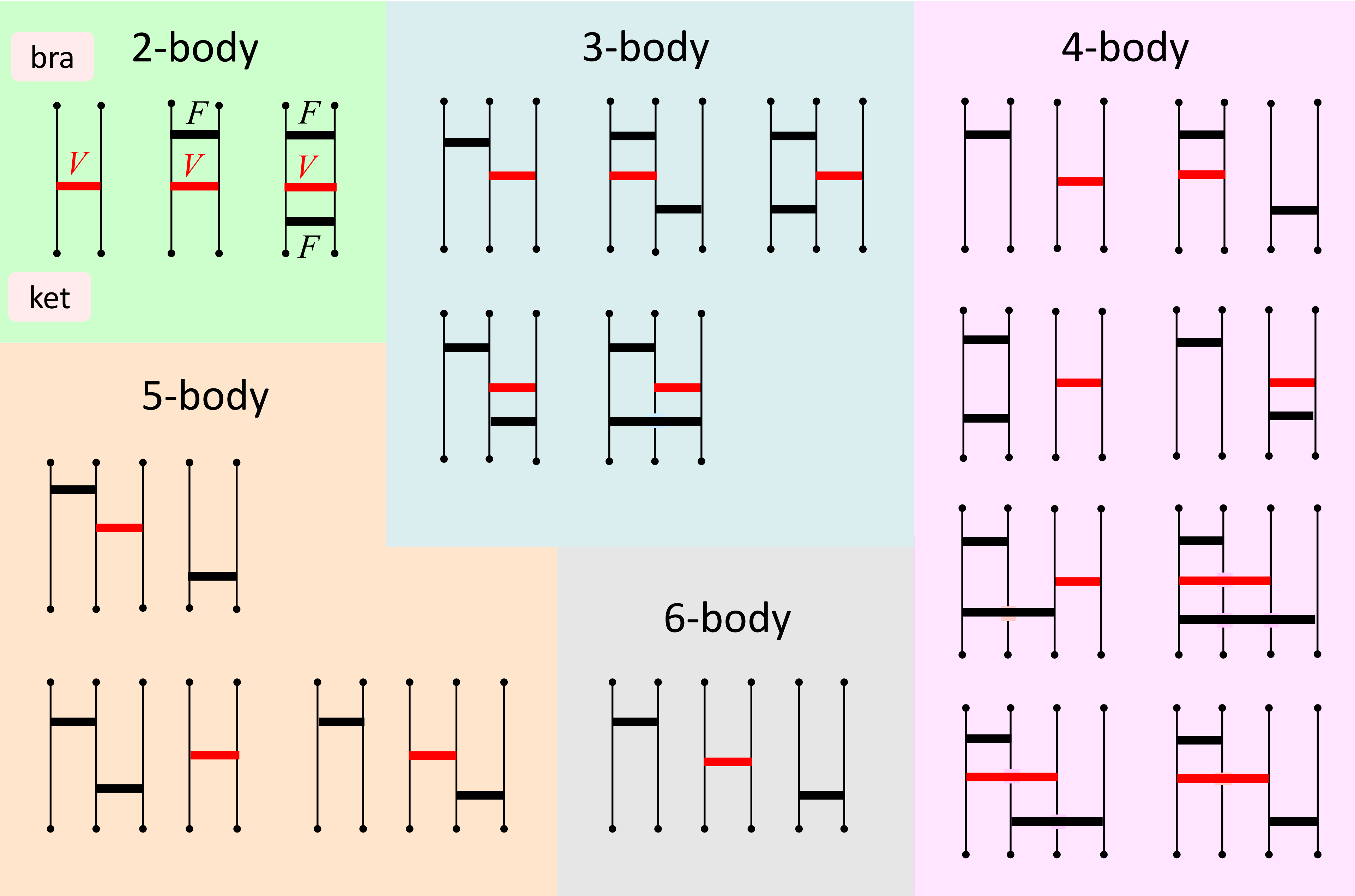
(2-body)^2

$$F^{\dagger} V F = \{\text{2-body}\} + \cdots + \{\text{6-body}\}$$

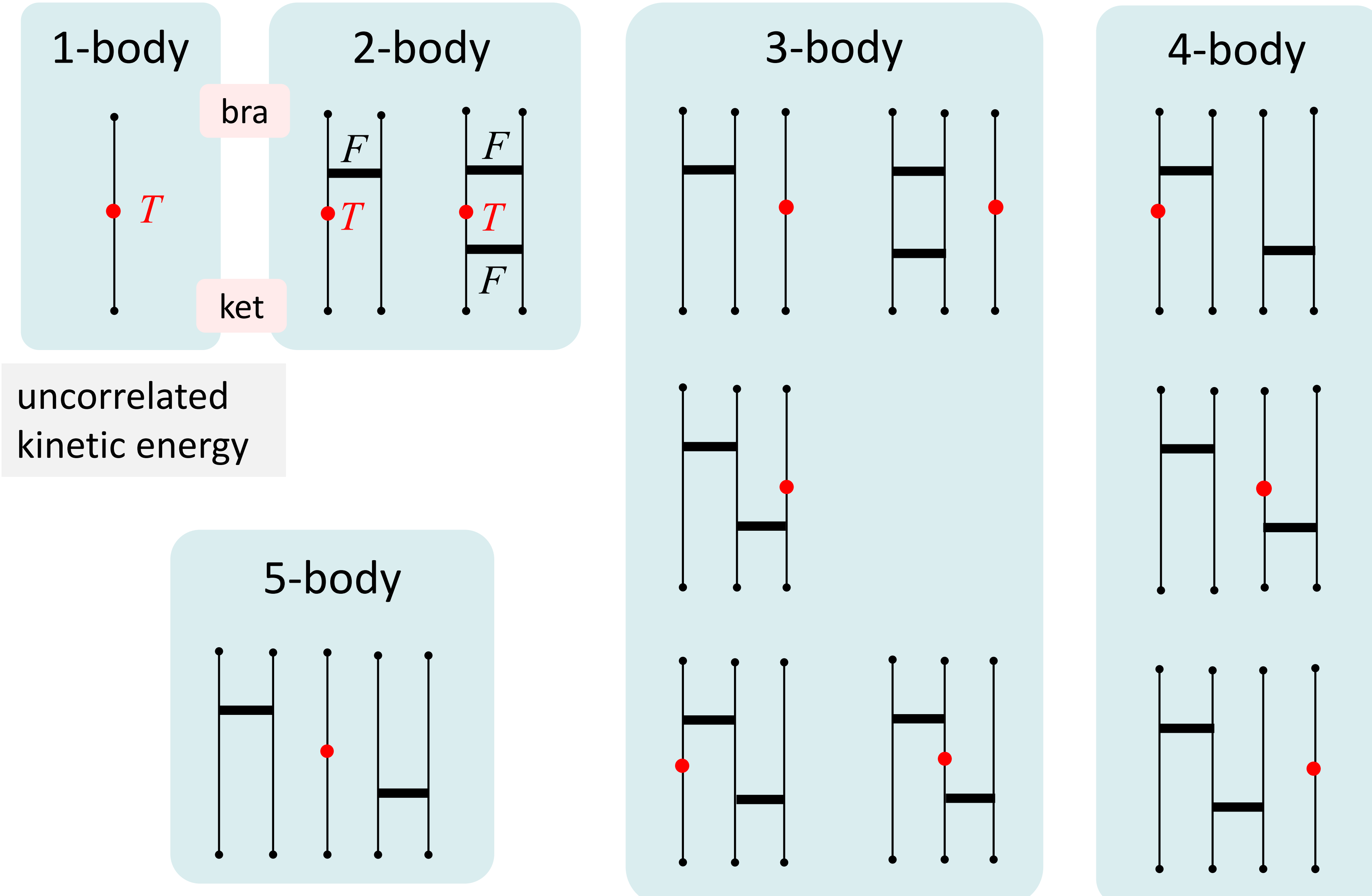
(2-body)^3



Diagrams of cluster expansion - V_{NN} -

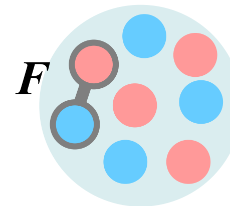


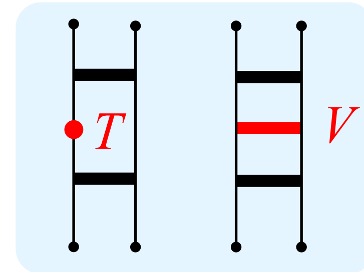
Diagrams of cluster expansion, Kinetic energy

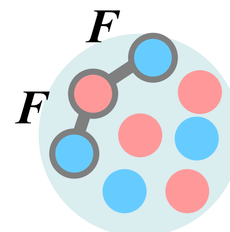


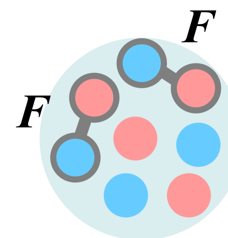
Multiple correlation functions in TOAMD

- **Signle F**
  - $|\Phi_{\mathrm{TOAMD}}\rangle = (1 + F_S + F_D)|\Phi_{\mathrm{AMD}}\rangle$
  - Correlated Hamiltonian $\widetilde{H} = F^\dagger H F$
  - Basis states are non-orthogonal.

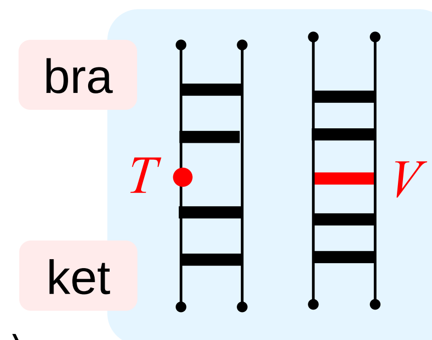








- **Double F** (Power series expansion)
  - $|\Phi_{\mathrm{TOAMD}}\rangle = (1 + F_S + F_D + \underline{F_S F_S + F_S F_D + F_D F_S + F_D F_D})|\Phi_{\mathrm{AMD}}\rangle$
  - $\widetilde{H} = F^\dagger F^\dagger H F F$ including $(S_{12})^5$
  - Each term is determined **independently**.



- **Triple F**
  - $|\Phi_{\mathrm{TOAMD}}\rangle = (1 + F_D + \cdots + \underline{F_S F_D F_D} + \cdots)|\Phi_{\mathrm{AMD}}\rangle$

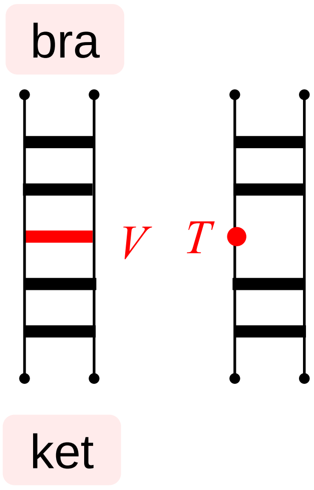
Double F effect in TOAMD

$$|\Phi_{\mathrm{TOAMD}}\rangle = (1 + \underbrace{F_S + F_D}_{\text{single}} + \underbrace{F_S F_S + F_S F_D + F_D F_S + F_D F_D}_{\text{double}})|\Phi_{\mathrm{AMD}}\rangle$$

F are independent

- Correlated Hamiltonian $\widetilde{H} = F^\dagger F^\dagger H F F$
- Number of diagrams in the cluster expansion of $\widetilde{H}$
  - $\boldsymbol{F}, \boldsymbol{V}$ ... 2-body operator, $\boldsymbol{T}$ ... 1-body operator
- We treat all the resulting diagrams for the variation.

Number of diagrams		
Operator	A=3	A=4
FVF	5	12
$FFVFF$	41	336



Number of diagrams		
Operator	A=3	A=4
FTF	5	8
$FFTFF$	41	224

Matrix elements with Fourier trans.

- Fourier transformation of the interaction V_{NN} & F_D, $F_{S.}$
  - Y. Goto and H. Horiuchi, Prog. Theor. Phys., **62** (1979) 662
  - Gaussian expansion of V_{NN}, F_D, F_S for **relative motion** .
  - Multi-body operators are represented in the separable form with respect to **the single particle coordinates**.
  - Three-body interaction can be treated in the same manner.

relative

$$e^{-a(\vec{r}_i-\vec{r}_j)^2} = \frac{1}{(2\pi)^3}\left(\frac{\pi}{a}\right)^{3/2}\int d\vec{k}\; e^{-\vec{k}^2/4a} \times e^{i\vec{k}\vec{r}_i} \times e^{-i\vec{k}\vec{r}_j}$$

single particle (separable)

$$r_{ij}^2 S_{12}(\vec{r})\, e^{-a(\vec{r}_i-\vec{r}_j)^2} = \frac{1}{(2\pi)^3}\left(\frac{\pi}{a}\right)^{3/2}\left(\frac{i}{2a}\right)^{2}\int d\vec{k}\; e^{-\vec{k}^2/4a} \times e^{i\vec{k}\vec{r}_i} \times e^{-i\vec{k}\vec{r}_j} \times \vec{k}^2 S_{12}(\vec{k})$$

tensor-type

one-body ME in AMD

$$\langle \mathbf{Z} | e^{i\vec{k}r} | \mathbf{Z}' \rangle = \langle \mathbf{Z} | \mathbf{Z}' \rangle \cdot \exp\left(-\vec{k}^2/8\nu + i\vec{k}(\mathbf{Z}+\mathbf{Z}')/2\right)$$

Gaussian wave packet

overlap

Quadratic + Linear terms of k

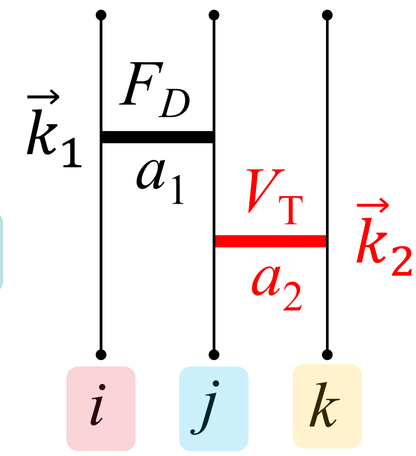
Matrix elements with Fourier trans.

- Example : $F_D \times V_{\rm T} \;\propto (S_{12})^2$

(2-body)×(2-body)

= (2-body)+(3-body)+(4-body)

3-body



$$\langle \Phi_{\rm AMD} | (F_D V_{\rm T})_3 | \Phi_{\rm AMD} \rangle \propto \iint d\vec{k}_1 d\vec{k}_2 \; e^{-\vec{k}_1^2/4a_1} e^{-\vec{k}_2^2/4a_2}$$

k-integral

$$\times \sum_{\rm ijk,\, i'j'k'} \langle \mathbf{Z}_i | e^{i\vec{k}_1 r} | \mathbf{Z}'_i \rangle \langle \mathbf{Z}_j | e^{-i\vec{k}_1 r} e^{i\vec{k}_2 r} | \mathbf{Z}'_j \rangle \langle \mathbf{Z}_k | e^{-i\vec{k}_2 r} | \mathbf{Z}'_k \rangle$$

spatial part

$$\times \sum_{\substack{xyx'y' \\ uvu'v'}} k_{1x} k_{1y} k_{2u} k_{2v} \left(3\delta_{xx'}\delta_{yy'} - \delta_{xy}\delta_{x'y'} \right) \left(3\delta_{uu'}\delta_{vv'} - \delta_{uv}\delta_{u'v'} \right)$$

(tensor)^2

$$\times \langle \chi_i | \sigma_{x'} | \chi'_i \rangle \langle \chi_j | \sigma_{y'} \sigma_{u'} | \chi'_j \rangle \langle \chi_k | \sigma_{v'} | \chi'_k \rangle \cdot \det \left| B^{-1}_{i'i} B^{-1}_{j'j} B^{-1}_{k'k} \right|$$

$B_{ij} = \langle \varphi_i | \varphi_j \rangle$

spin-isospin part

antisymmetrization

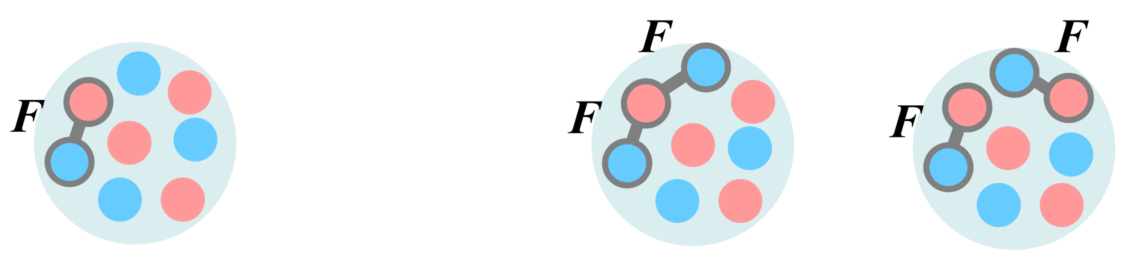
overlap

Results

- ^{3}H, ^{4}He, ^{6}He, ^{6}Li
- V_{NN} : AV8' (central, LS, tensor)
- 7 Gaussians for F_D, F_S to converge the solution.
- Full treatment of many-body operators (all diagrams) to retain the variational principle.
- Successively increase the correlation terms

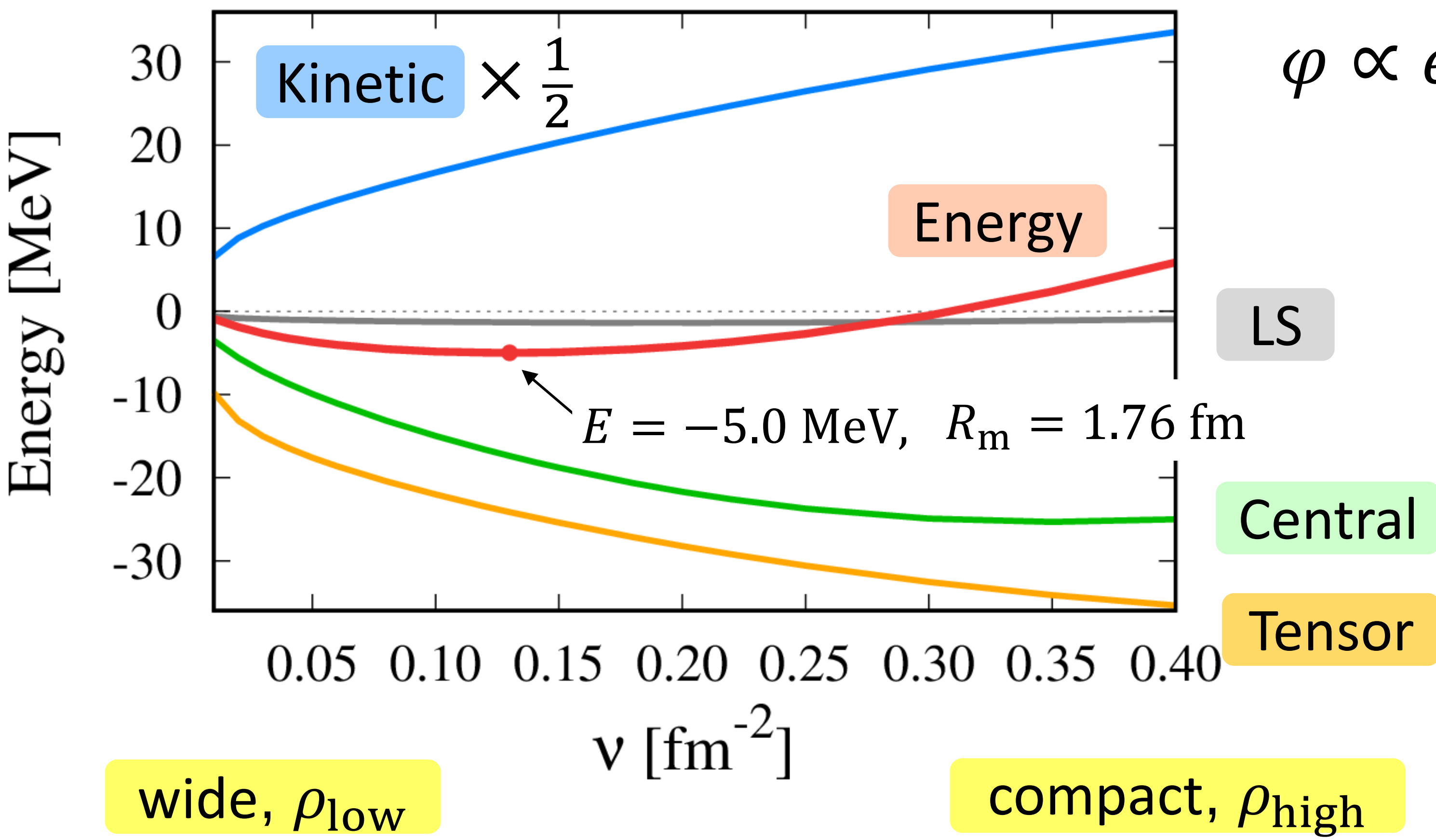
$$|\Phi_{\mathrm{TOAMD}}\rangle = (1 + F_D + F_S + F_S F_S + F_S F_D + F_D F_S + F_D F_D)|\Phi_{\mathrm{AMD}}\rangle$$

Single F | **Double F** |



^{3}H in TOAMD with single F

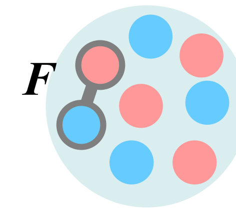
$(1 + F_D + F_S)|\Phi_{\mathrm{AMD}}\rangle$



$$\varphi \propto e^{-\nu(\vec{r}-\vec{Z})^2}$$

$$\nu = \frac{1}{2b^2}$$

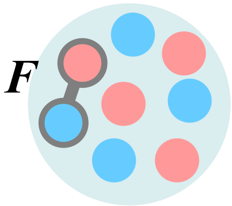
$$\frac{\hbar^2}{m}\nu = \frac{\hbar\omega}{2}$$

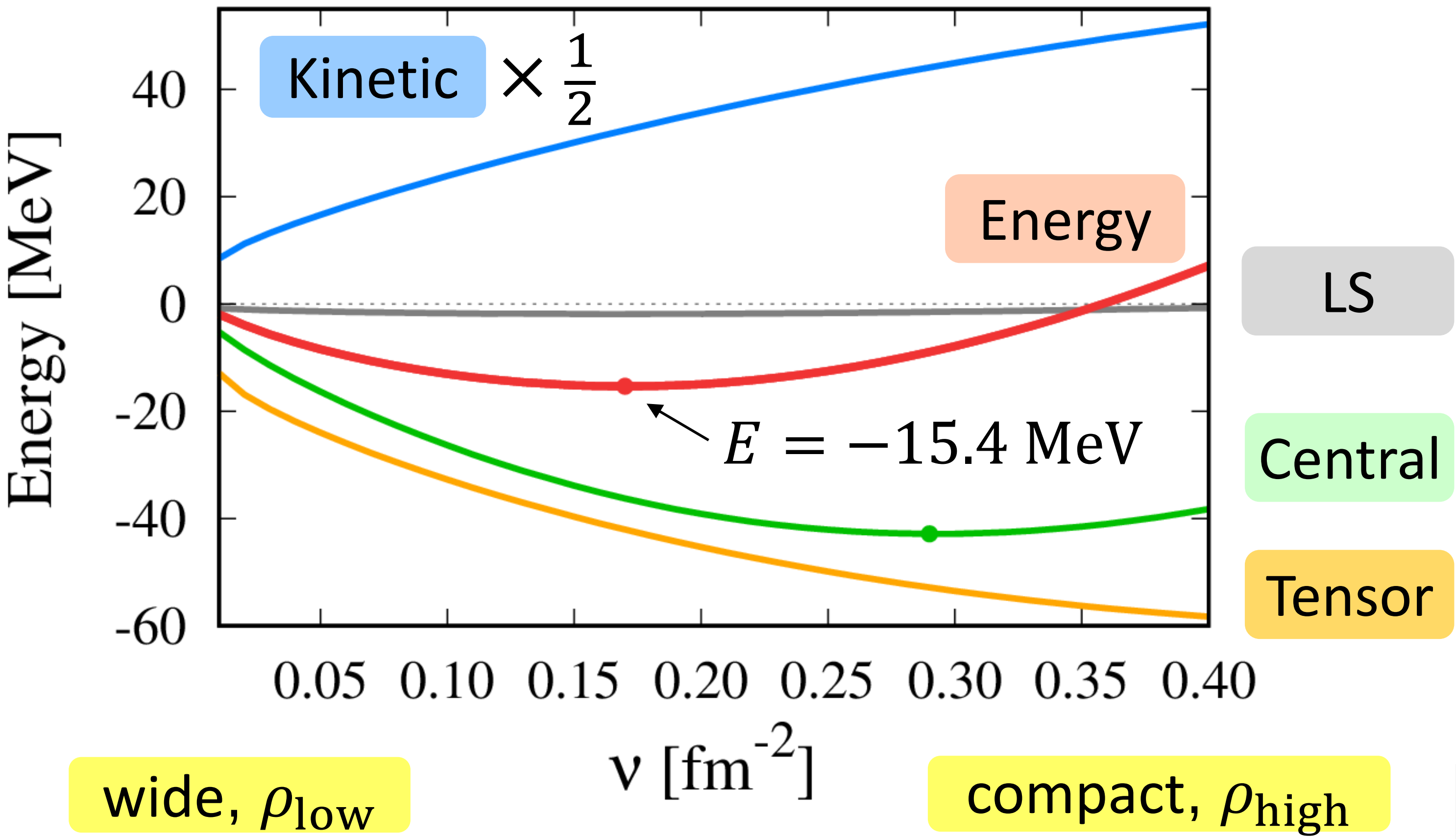


- Large cancelation of T & V makes the small total energy.
- $\vec{Z}_1 = \vec{Z}_2 = \vec{Z}_3 = 0$, s-wave configuration of AMD w.f.

^{4}He in TOAMD with single F

$(1 + F_D + F_S)|\Phi_{\mathrm{AMD}}\rangle$





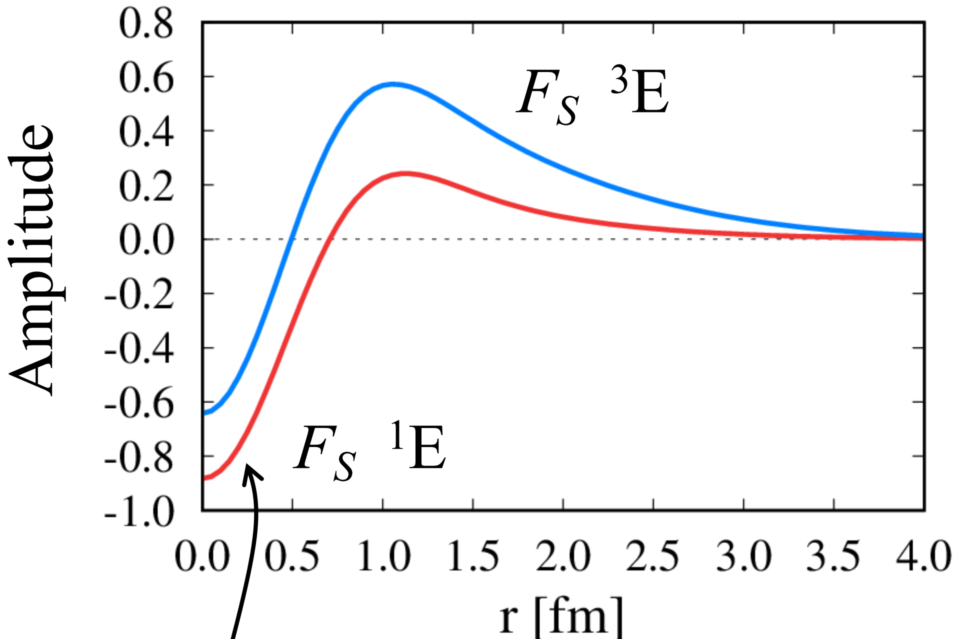
$$\frac{\hbar^2}{m}\nu = \frac{\hbar\omega}{2}$$

AMD...$(0s)^4$

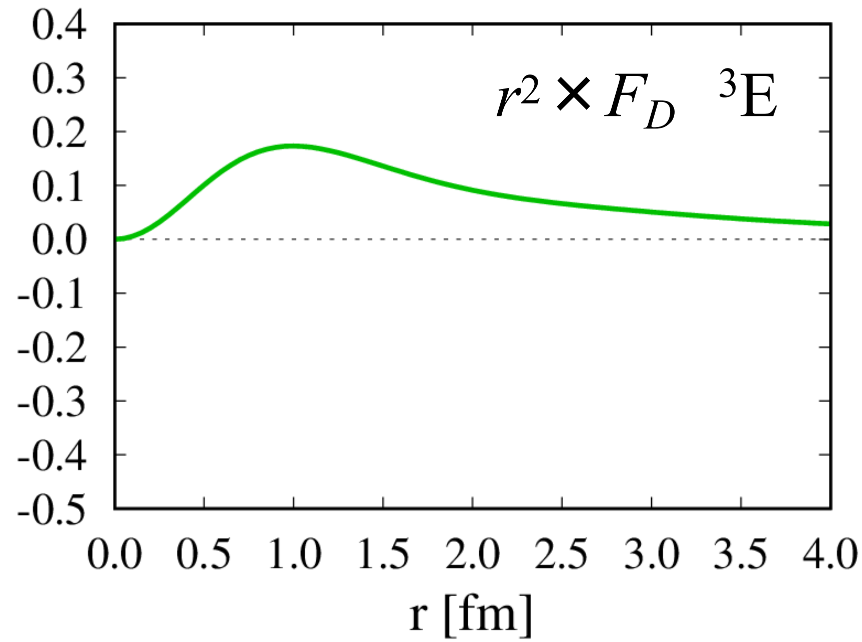
- Large cancelation of T & V makes the small total energy.
- Need $F_S \times F_D$-type correlation to gain the energy more.

Correlation functions F_D , F_S in ^{3}H

short-range $F_S(r)$



tensor $F_D(r)$



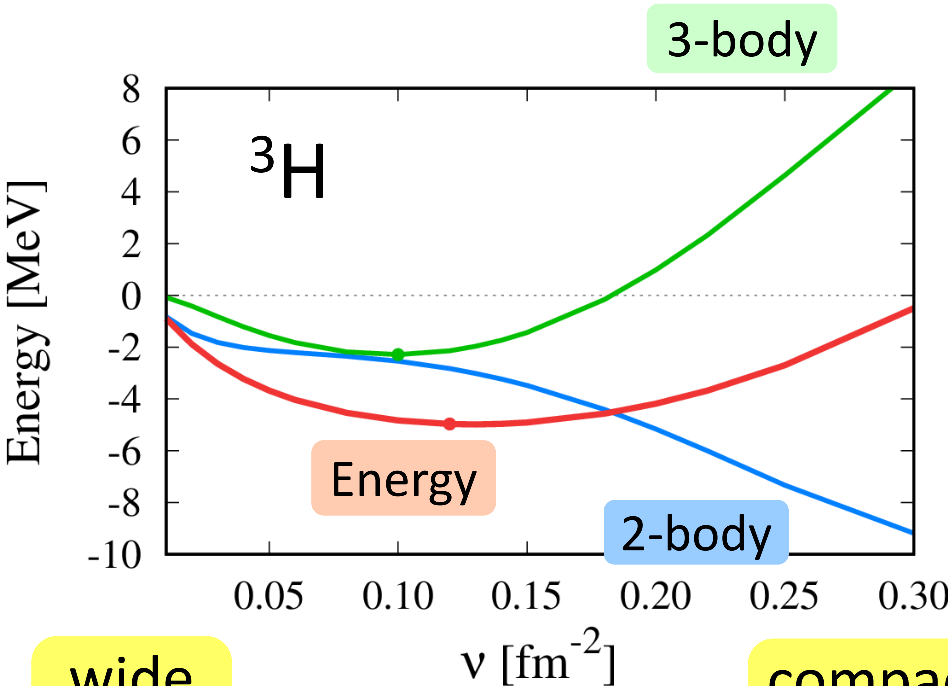
- Negative sign in F_S to avoid short-range repulsion in V_{NN}
- Ranges of F_D, F_S are NOT short.
- Range b of $F_D \Phi_{\text{AMD}} \approx 0.6\ b_{\text{AMD}}$ $\rightarrow$ spatially compact, high-k

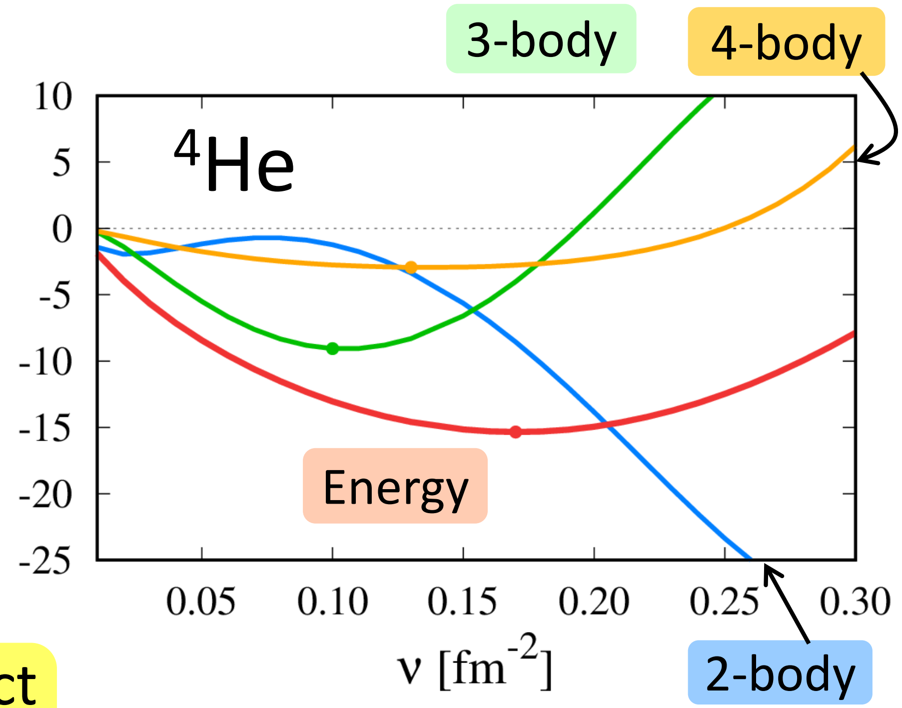
  $(= 1/\sqrt{2a + \nu})$ $(1/\sqrt{\nu})$

Tensor-optimized shell model

TM, K. Kato, K. Ikeda PTP113 (2005) 763

Many-body operators of $F^\dagger HF$ in ^{3}H, ^{4}He





wide ρ_{low}

compact ρ_{high}

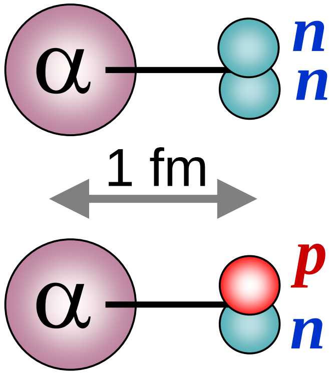
NO energy saturation within 2-body

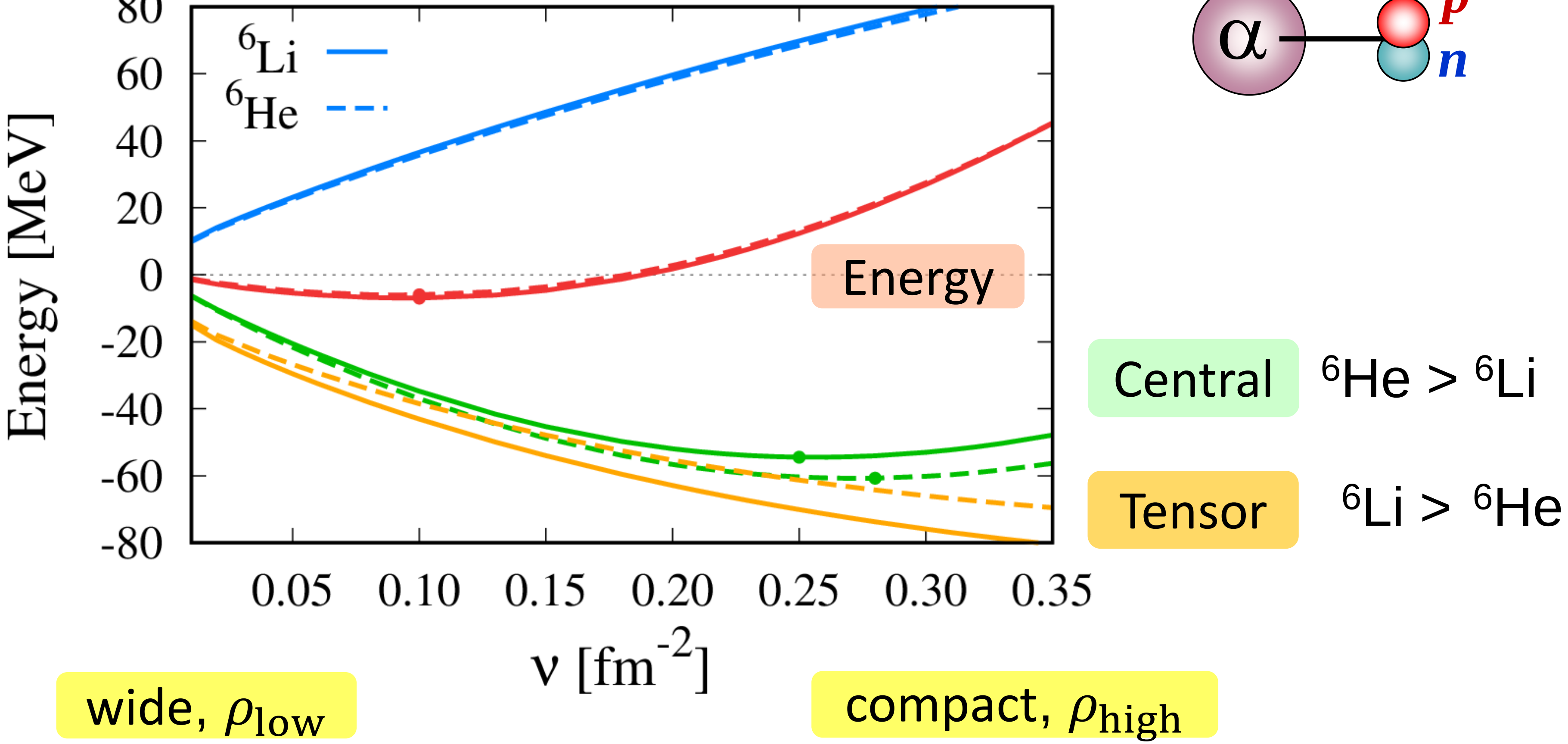
$$\nu = \frac{1}{2b^2}, \quad \frac{\hbar^2}{m}\nu = \frac{\hbar\omega}{2}$$

$$\{\vec{Z}_i\} = 0$$

- Many-body term plays a decisive role for energy saturation.
  - Similar to Bethe-Brueckner-Goldstone approach with *G*-matrix (Baldo)

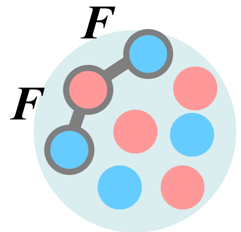
Hamiltonian components in ^{6}He & ^{6}Li





- Larger tensor contribution in ^{6}Li due to last ***pn*** pair

Double F_S effect in TOAMD

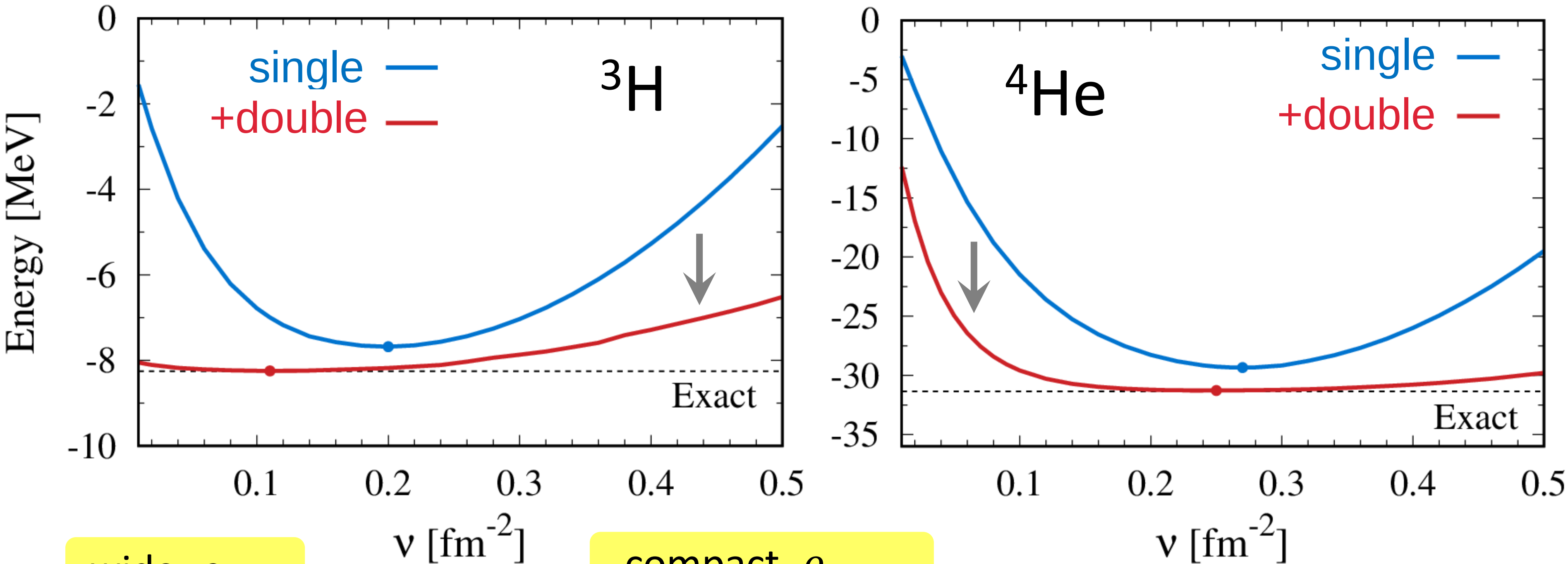


Malfliet-Tjon V
(central short-range)

$$(1 + F_{S1} + F_{S2}F_{S3})|\Phi_{\mathrm{AMD}}\rangle$$

single double

F are independent



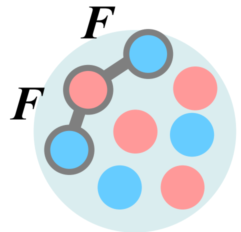
wide, ρ_{low}

compact, ρ_{high}

- Double F_S reproduces the exact energy .
- Small ν-dependence indicates the flexibility of F_S.

$$\frac{\hbar^2}{m}\nu = \frac{\hbar\omega}{2}$$

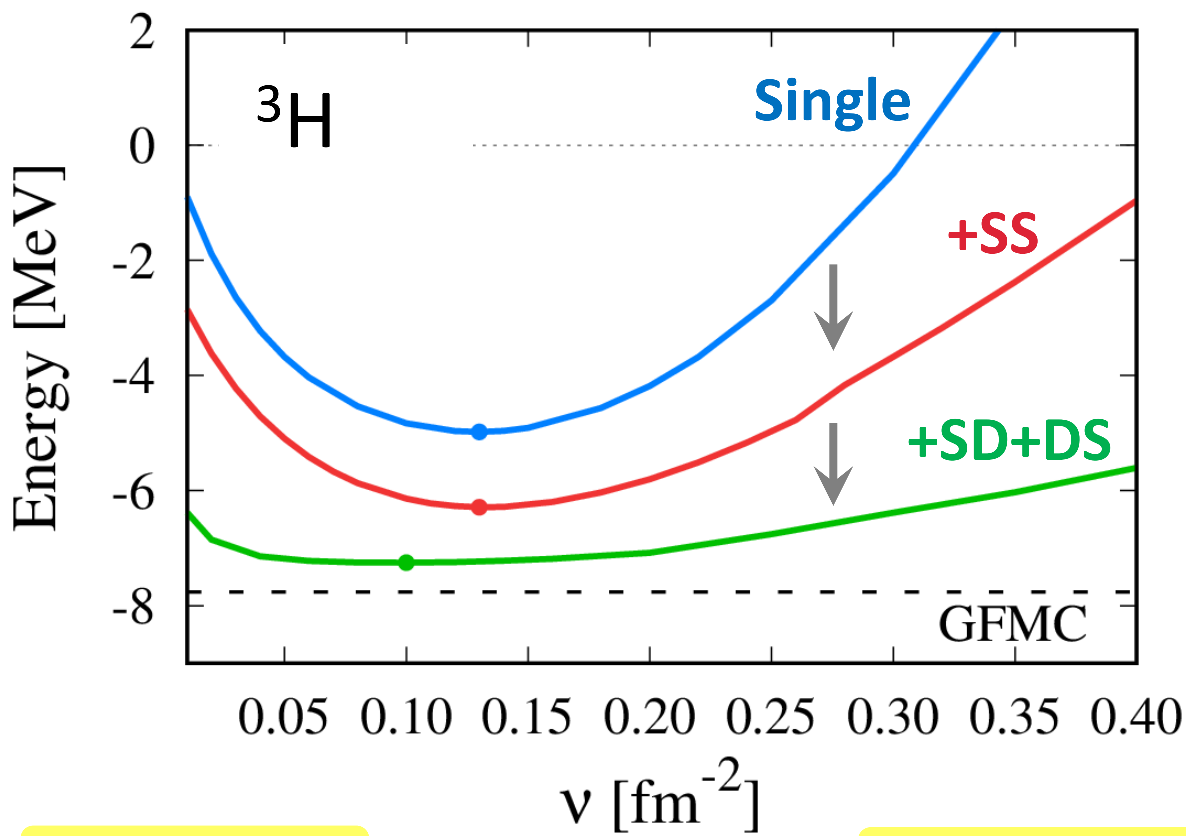
Double F effect in TOAMD



AV8’ $(1 + \underbrace{F_S + F_D}_{\text{single}} + \underbrace{F_S F_S}_{\text{SS}} + \underbrace{F_S F_D}_{\text{SD}} + \underbrace{F_D F_S}_{\text{DS}})|\Phi_{\text{AMD}}\rangle$

$$\varphi \propto e^{-\nu(\vec{r}-\vec{Z})^2}$$

$$\nu = \frac{1}{2b^2} \qquad \frac{\hbar^2}{m}\nu = \frac{\hbar\omega}{2}$$



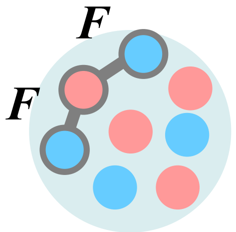
wide, ρ_{low}

compact, ρ_{high}

F are independent

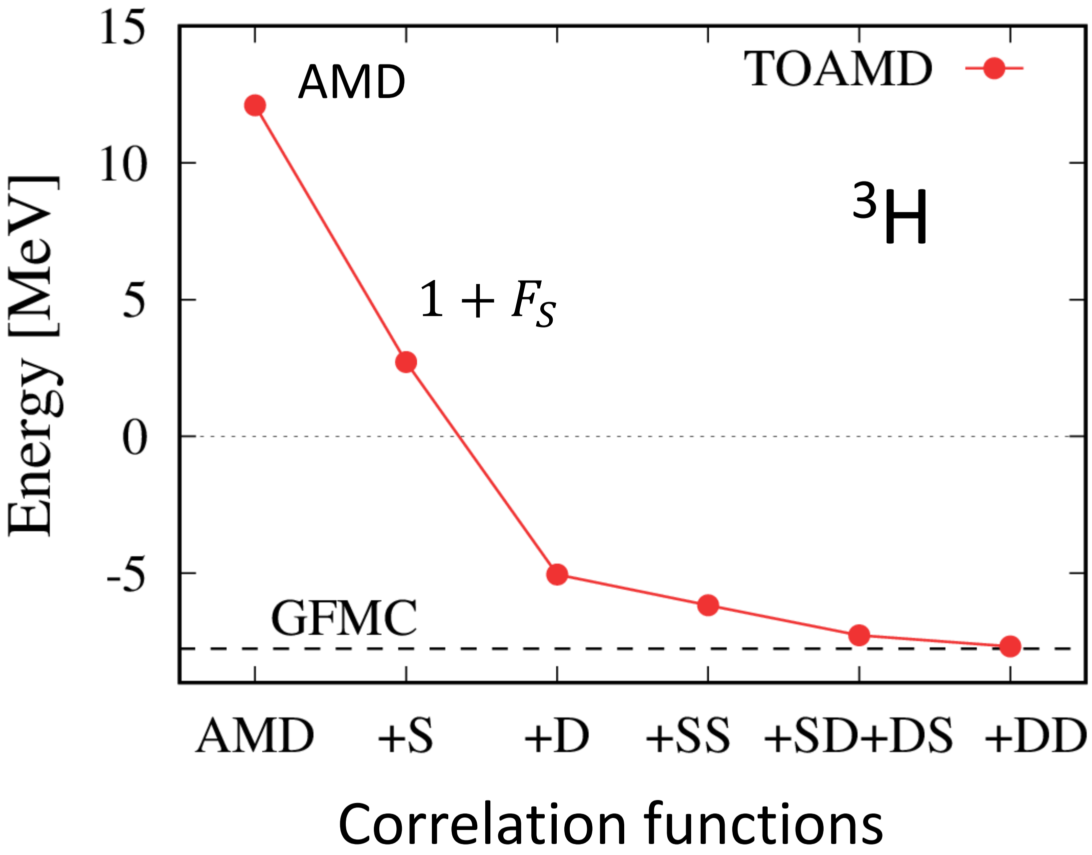
- Get close to the GFMC energy.
- ν-dependence is small due to the flexibility of F.

Double F effect in TOAMD



AV8'

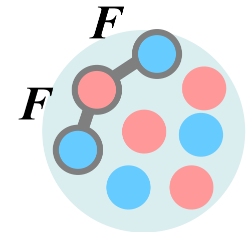
$$(1 + \underbrace{F_S}_{S} + \underbrace{F_D}_{D} + \underbrace{F_S F_S}_{SS} + \underbrace{F_S F_D}_{SD} + \underbrace{F_D F_S}_{DS} + \underbrace{F_D F_D}_{DD})|\Phi_{\mathrm{AMD}}\rangle$$



F are independent

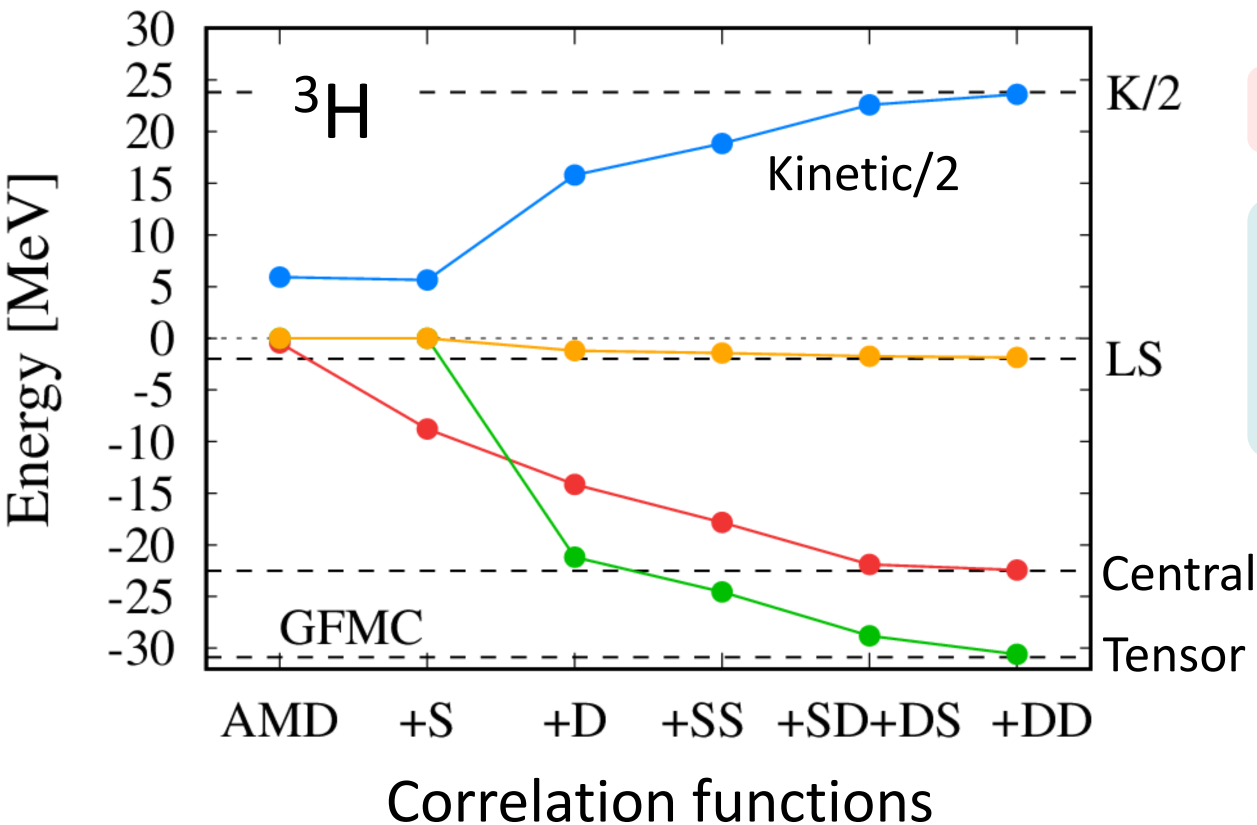
- Reproduce the GFMC energy
- Small curvature as F^2 terms increase $\rightarrow$ good convergence
- $\sqrt{\langle r^2 \rangle} = 1.75$ fm

Double F effect in TOAMD



AV8’ $$(1 + F_S + F_D + F_S F_S + F_S F_D + F_D F_S + F_D F_D)|\Phi_{\rm AMD}\rangle$$

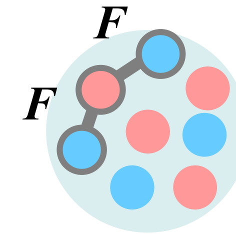
S D SS SD DS DD



F are independent

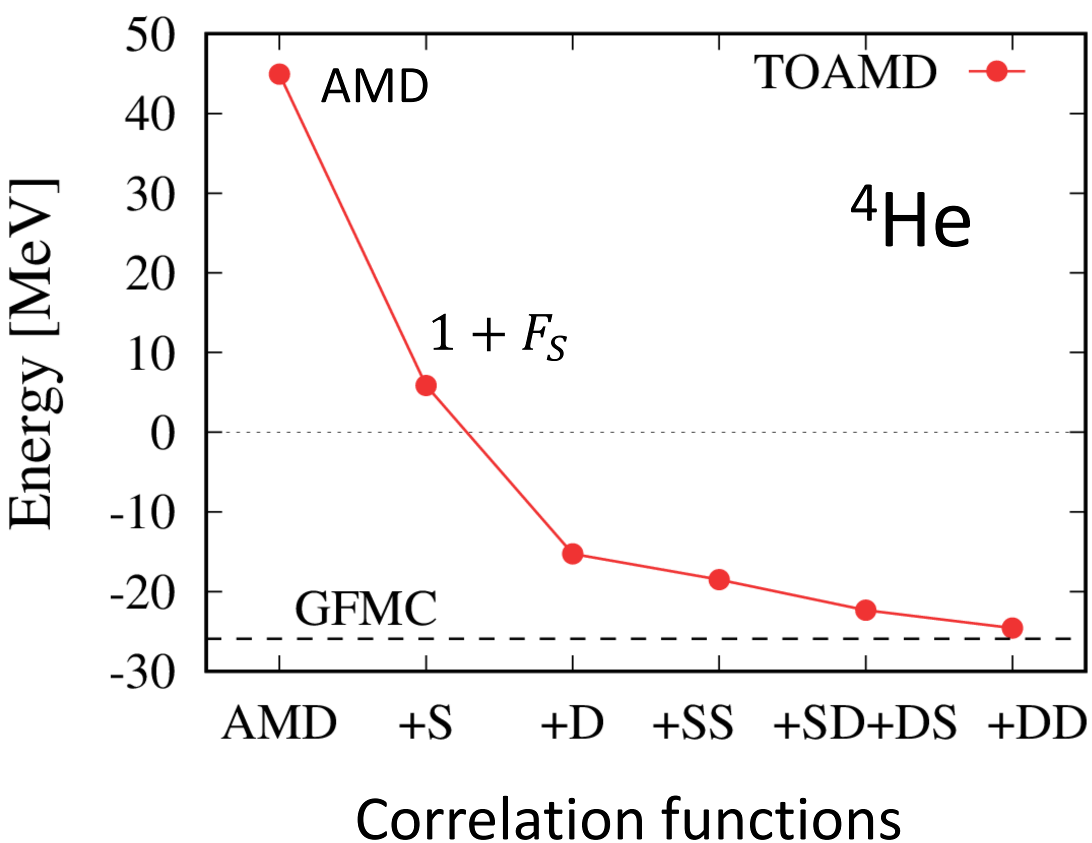
- Reproduce the Hamiltonian components of ^{3}H

Double F effect in TOAMD



AV8'

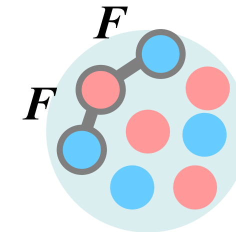
$$(1 + \underbrace{F_S}_{\text{S}} + \underbrace{F_D}_{\text{D}} + \underbrace{F_S F_S}_{\text{SS}} + \underbrace{F_S F_D}_{\text{SD}} + \underbrace{F_D F_S}_{\text{DS}} + \underbrace{F_D F_D}_{\text{DD}})|\Phi_{\text{AMD}}\rangle$$



F are independent

- Good energy with F^2
- Small curvature as F^2 terms increase $\rightarrow$ good convergence
- $\sqrt{\langle r^2 \rangle} = 1.50$ fm
- Next order is triple-F such as $F_D\ F_D F_S$.

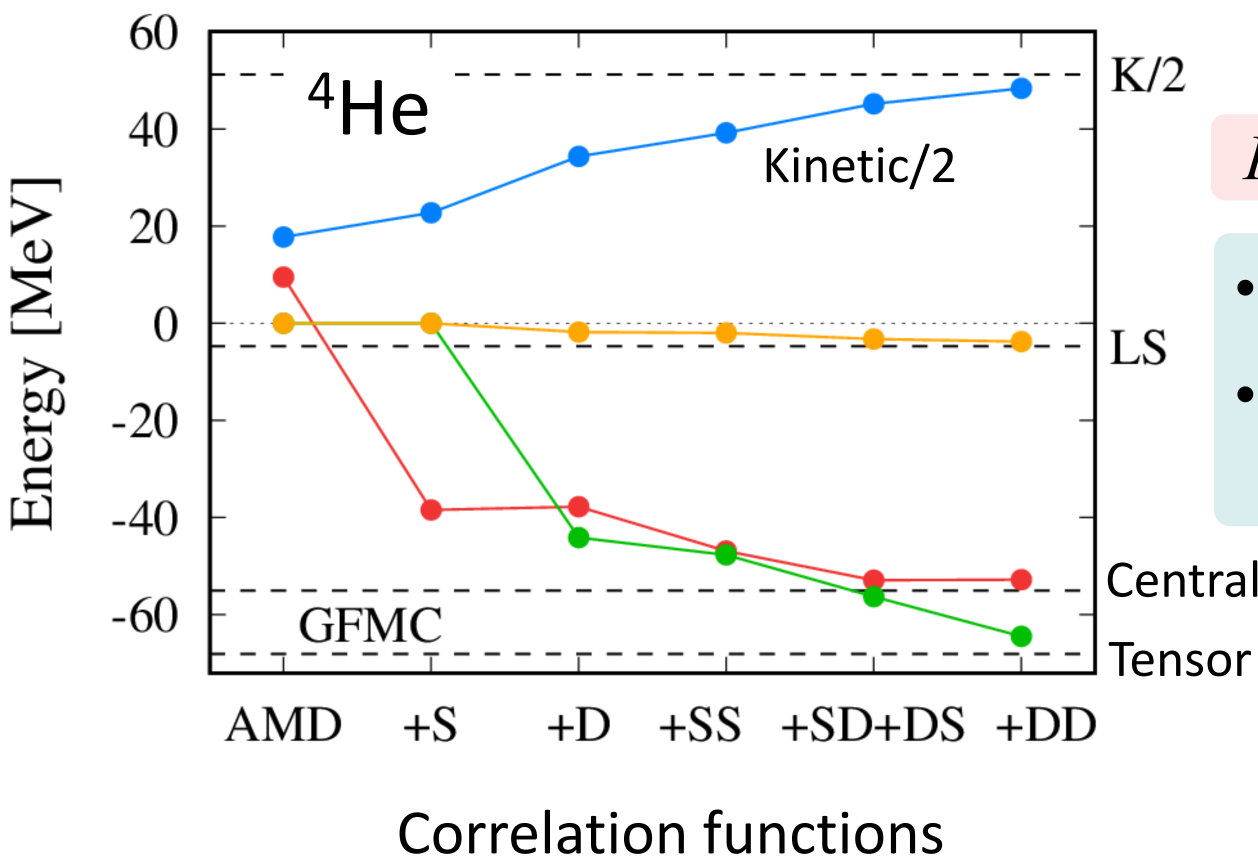
Double F effect in TOAMD



AV8'

$$(1 + F_S + F_D + F_S F_S + F_S F_D + F_D F_S + F_D F_D)|\Phi_{\rm AMD}\rangle$$

S D SS SD DS DD



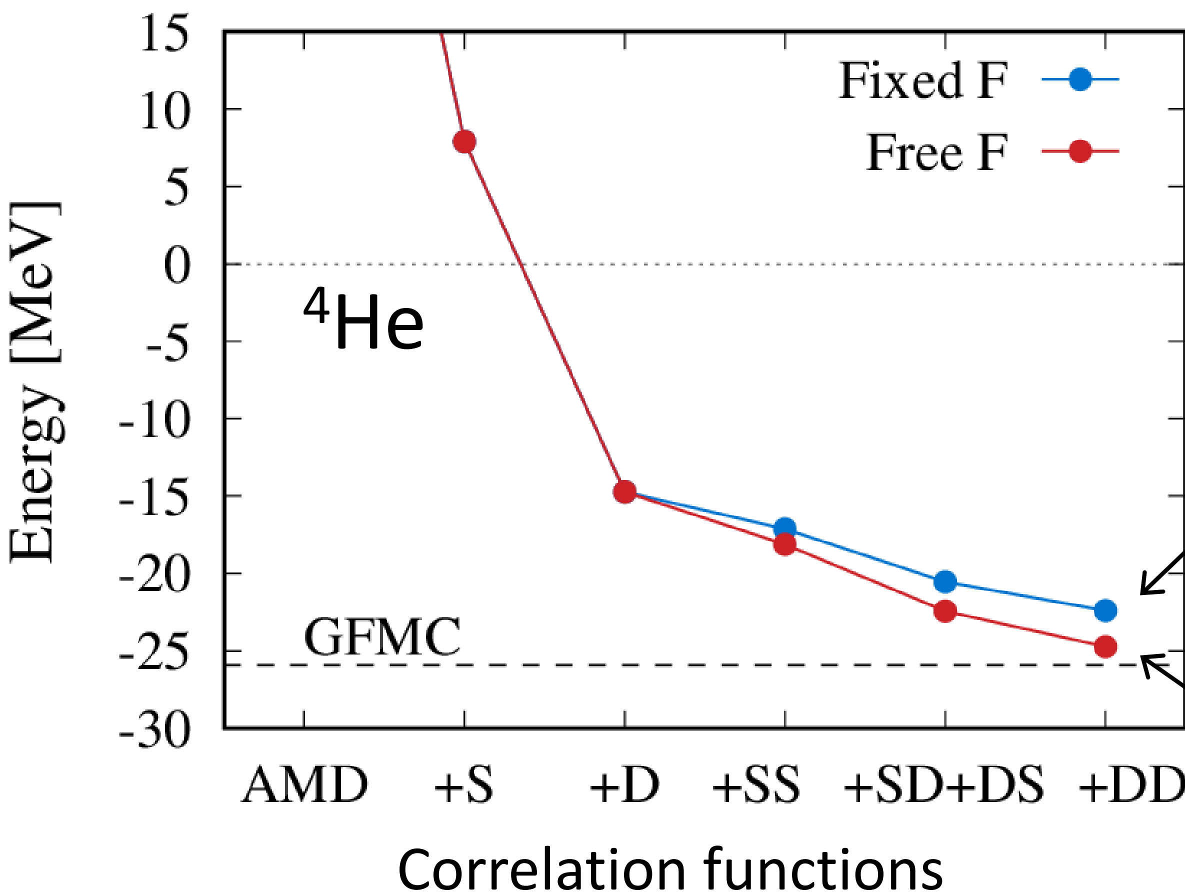
F are independent

- Good energy with F^2
- Next order is triple-F such as $F_D\, F_D\, F_S$.

Variation of multi-F in TOAMD

AV8'

$$(1 + \underbrace{F_S}_{S} + \underbrace{F_D}_{D} + \underbrace{F_S F_S}_{SS} + \underbrace{F_S F_D}_{SD} + \underbrace{F_D F_S}_{DS} + \underbrace{F_D F_D}_{DD})|\Phi_{\mathrm{AMD}}\rangle$$



cf. Jastrow ansatz

$F_D(r), F_S(r)$ are fixed at single level, and used in F^2 terms

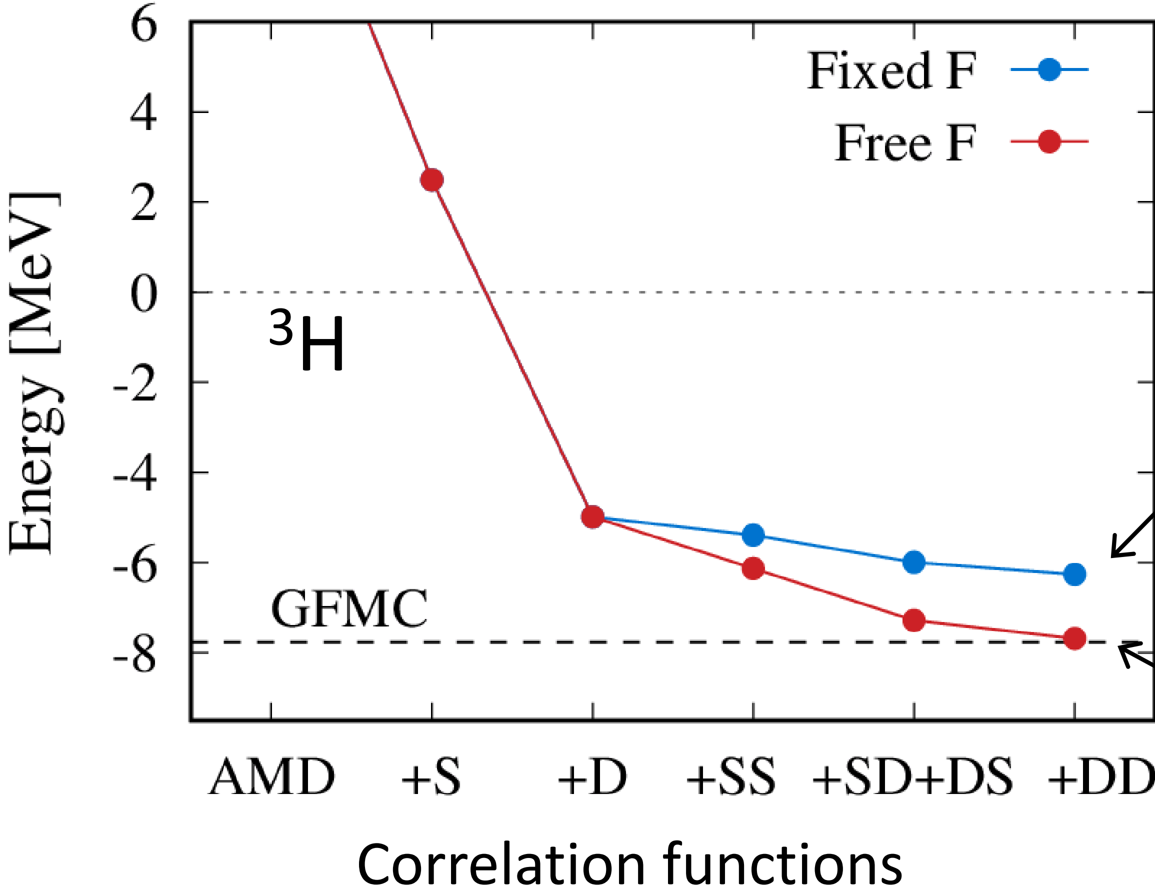
ΔE=2.3 MeV

F are independent as a full variation

Variation of multi-F in TOAMD

AV8'

$$(1 + \underbrace{F_S}_{S} + \underbrace{F_D}_{D} + \underbrace{F_S F_S}_{SS} + \underbrace{F_S F_D}_{SD} + \underbrace{F_D F_S}_{DS} + \underbrace{F_D F_D}_{DD})|\Phi_{\rm AMD}\rangle$$



cf. Jastrow ansatz

$F_D(r), F_S(r)$ are fixed at single level, and used in F^2 terms

ΔE=1.4 MeV

F are independent as a full variation

Summary

- **Tensor-Optimized AMD (TOAMD).**
  - Successive variational method for nuclei to treat V_{NN} directly.
  - Correlation functions, F_D (tensor) , F_S (short-range).
  - Full treatment of many-body operators in the cluster expansion.
  - At F^2 level, good reproduction of *s*-shell nuclei.
    Next, we shall apply TOAMD to *p*-shell nuclei.
  - We can increase multiple correlation functions systematically, such as $F_D F_D F_S$.
  - We can include V_{NNN} such as Fujita-Miyazawa type in the same manner of many-body operators.