Nuclear matter calculation with the tensor optimized Fermi sphere method (TOFS)

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Outline of the talk

1. Introduction
2. Formulation of the tensor optimized Fermi sphere method (TOFS)
3. A linked cluster expansion theorem in TOFS
4. Frist application of TOFS to nuclear matter with AV4' force
5. Summary

◎Interests in nuclear matter study

（1）High-density region： Neutron star, EOS

Roepke et al. PRL80 (1998)

（2）Low-density region： Alpha condensation（$\rho < \rho_0/4$）

Alpha cluster structure in finite nuclei (ex. Hoyle state)

◎Study of nuclear matter with realistic forces

- Non relativistic： ex. Pandharipande et al. with VCS, FHNC/SOC
- Relativistic： ex. Brocmann et al. with Relativistic BHF

Comparative study of various methods：Baldo et al. PRC86 (2012)

◎Tensor optimized Fermi sphere method（TOFS）

A new nuclear matter calculation method

Nuclear matter w.f.

T. Yamada, Annals of Physics 403 (2019), 1.

＝ Power-series-type and/or Exponential-type correlated w.f.s

supported by a linked cluster expansion theorem in TOFS

⇔ The TOFS method is contrast to FHNC/0,/4,/SOC, using Jastrow-type w.f. supported by a linked cluster expansion theorem by Fantoni & Rosati

Nuclear matter studies

- **Non relativistic:**

  Brueckner-Hartree-Fock cal. (BHF) — Brueckner et al., PR97 (1955); Brueckner PR100 (1955); Goldstone Proc. Roy. Soc. A239 (1957)

  Brueckner-Bethe-Goldstone approach to third order in hole-line expansion (BBG) — Song et al., PRL81 (1998)

  Variational method based on hypernetted chain summation method (VCS, FHNC/SOC) — Pandharipande et al., RMP51 (1979), Akmal et al., PRC56(1997)

  Self-consistent Green's function (SCGF) — Fantoni & Rosati, NC43A (1978); Frick et al., PRC71 (2005),Rios et al., PRC79 (2009)

  Auxiliary field diffusion Monte Carlo (AFDMC) — Gandolfi et al., PRL98 (2007), PRC79 (2009)

  Green's function Monte Carlo (GFMC) — Carlson et al., PRC68 (2003)

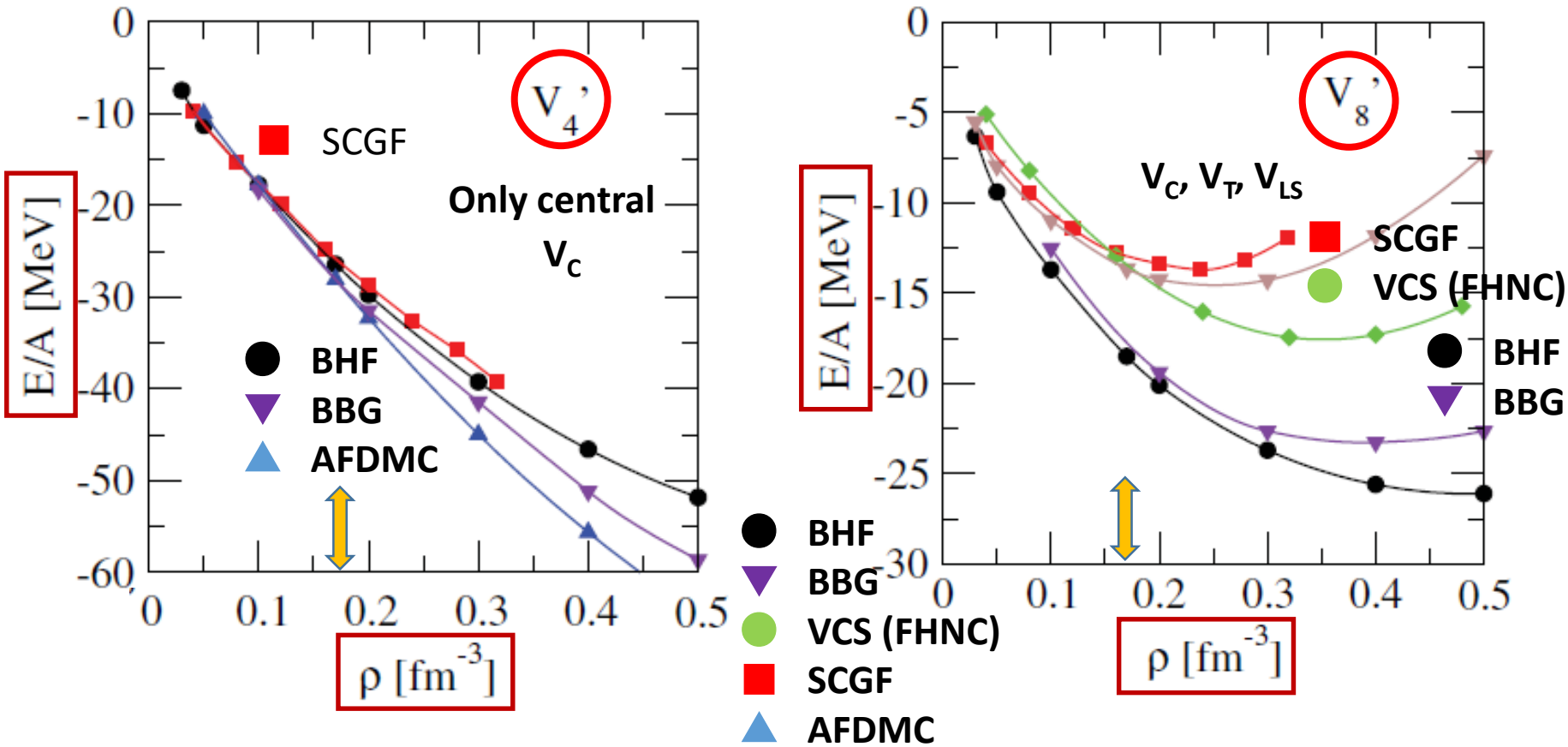
  Lattice calculation — Abe & Seki (2007)

- **Relativistic :** Brockmann et al. PRC42 (1990)

  Relativistic Brueckner Hartree Fock calculation

  3-body force caused by anti-particle and Δ-particle ?

Symmetric nuclear matter : Argonne potentials (no 3N force)



Baldo et al., PRC86 (2012)

- Dependence on calculation methods.
- A problem of numerical convergence .

It is important to study the nuclear matter with a new method.

FHNC(/0, /4, /SOC)

Linked cluster expansion theory

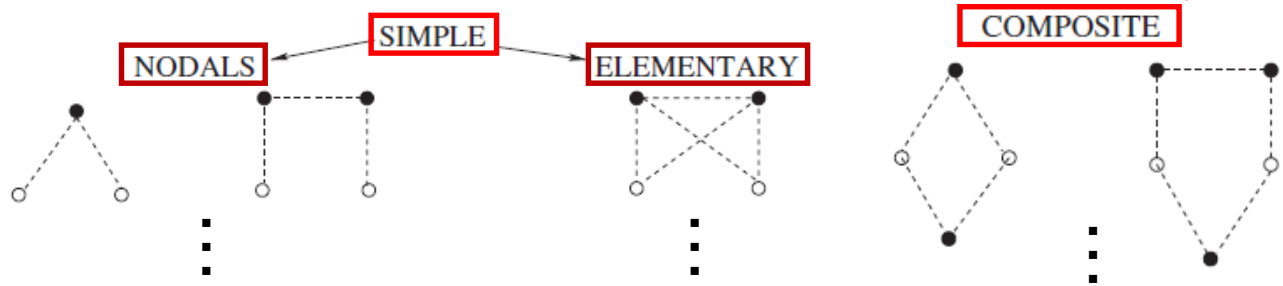
Diagram representation:

Fantoni et al. Nuovo Cimento A 20(1974)

Jastrow-type Iwamoto, Yamada PTP17(1957)

$$\Psi = \left(\mathcal{S} \prod_{i<j} f_{ij} \right) \Phi_0$$

$$-B = \frac{E}{A} = \frac{1}{A} \times \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle},$$



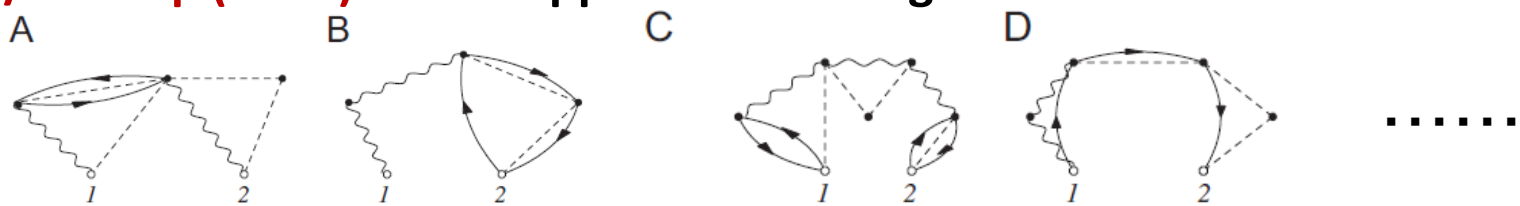
(1) " f_{ij} " independent of operators: Fantoni & Rosati NC A43, (1978) etc.

FHNC/0 eq. : "NODAL"+ "COMPOSITE" : Integral equations (FHNC eq.)

FHNC/4 eq. : "NODALS" + "COMPOSIT" +"Lowest ELEMENTARY (only 4th term)"

(2) " f_{ij} " dependent on operators: Pandharipande et al., RMP51 (1979)

FHNC/SOC eq. (=VCS) : "SOC-approximable diagrams of NODALS"+"COMPOSITE"



・Variation for two-body cluster energy ⇒ determination of " f "

⇒ estimation of many-body terms by SOC eq.

・Neglection of "ELEMENTARY" diagrams: But, possible effects in 16O and 40Ca

G. Co et al, 1994

TOFS

$$\Psi = \left[1 + F + \frac{1}{2!} F^2 + \frac{1}{3!} F^3 + \cdots \right] \Phi_0$$

: Power-series (or Exponential) correlated w.f.

energy variation with Ψ

⇒ "NODALS", "COMPOSITE", and "ELEMENTARY" are computable.

Formulation of TOFS and Linked cluster expansion theorem

Formulation of TOFS method (on Hermitian form)

◎Power-series type (*N*th order)

T. Yamada, Annals of Physics 403 (2019), 1.

$$\Psi_N = \left[\sum_{k=0}^{N} \frac{1}{k!} F^k\right] \Phi_0 \qquad \rho = \frac{2k_F^3}{3\pi^2}$$

$$F = F_S + F_D$$

$$F_S = \frac{1}{2}\sum_{i\neq j} f_S(i,j) = \frac{1}{2}\sum_{s=0}^{1}\sum_{t=0}^{1}\sum_{i\neq j} f_S^{(st)}(i,j) P_{ij}^{(st)},$$ **Central-force type**

$$F_D = \frac{1}{2}\sum_{i\neq j} f_D(i,j) = \frac{1}{2}\sum_{s=0}^{1}\sum_{t=0}^{1}\sum_{i\neq j} f_D^{(st)}(i,j) r_{ij}^2 S_{12}(i,j) P_{ij}^{(st)} \delta_{s,1},$$ **Tensor-force type**

$$\Phi_0 = \frac{1}{\sqrt{A!}} \det\left|\phi_{\gamma_1}(1)\phi_{\gamma_2}(2)\cdots\phi_{\gamma_A}(A)\right|$$

Fermi-sphere w.f.

$$\phi_{\gamma_n}(n) = \phi_{\boldsymbol{k}_n}(\boldsymbol{r}_n)\chi_{m_{s_n}}(n)\xi_{m_{t_n}}(n)$$

$$\phi_{\boldsymbol{k}_n}(\boldsymbol{r}_n) = \frac{1}{\sqrt{\Omega}}\exp(i\boldsymbol{k}_n\cdot\boldsymbol{r}_n)$$

◎Exponential type

$$\Psi_{\mathrm{ex}} = \exp(F)\,\Phi_0 = \lim_{N\to\infty}\left[\sum_{k=0}^{N}\frac{1}{k!}F^k\right]\Phi_0 = \lim_{N\to\infty}\Psi_N$$

Expectation value in nuclear matter: Cluster expansion

Arbitrary *M*-body operator（Hermite, translationally invariant, symmetric）

$$\hat{O} = \sum_{i_1 \neq i_2 \neq \cdots \neq i_M}^{A} \hat{O}(i_1, i_2, \cdots, i_M)$$

Exponential type w.f.

$$\Psi_{\mathrm{ex}}(\alpha) = \exp(\alpha F)\,\Phi_0 = \lim_{N\to\infty}\left[\sum_{k=0}^{N}\frac{1}{k!}(\alpha F)^k\right]\Phi_0$$

$$O_{\mathrm{ex}}(\alpha) \equiv \frac{\langle\Psi_{\mathrm{ex}}(\alpha)|\hat{O}|\Psi_{\mathrm{ex}}(\alpha)\rangle}{\langle\Psi_{\mathrm{ex}}(\alpha)|\Psi_{\mathrm{ex}}(\alpha)\rangle} = \frac{\sum_{n=0}^{\infty} a_n \alpha^n}{\sum_{n=0}^{\infty} b_n \alpha^n} = \sum_{n=0}^{\infty} B_n \alpha^n$$

α is a real number

$$B_n = \frac{a_0}{b_0} - \sum_{k=1}^{n}\frac{b_k}{b_0}B_{n-k}$$

$$a_n = \sum_{k=0}^{n}\frac{1}{(n-k)!\,k!}\langle\Phi_0|F^{n-k}\hat{O}F^k|\Phi_0\rangle$$

$$b_n = \frac{2^n}{n!}\langle\Phi_0|F^n|\Phi_0\rangle$$

Setting $\alpha = 1$,

$$\langle\hat{O}\rangle_{ex} = \frac{\langle\Psi_{\mathrm{ex}}|\hat{O}|\Psi_{\mathrm{ex}}\rangle}{\langle\Psi_{\mathrm{ex}}|\Psi_{\mathrm{ex}}\rangle} = \frac{\langle\Phi_0|\exp(F^\dagger)\hat{O}\exp(F)|\Phi_0\rangle}{\langle\Phi_0|\exp(F^\dagger)\exp(F)|\Phi_0\rangle} = \sum_{n=0}^{\infty} B_n$$

Correlated Hamiltonian $\exp(F^\dagger)\hat{O}\exp(F)$ **= Hermit**

Difference from "Coupled-cluster theory"

A-fermion wave function: exponential ansatz

$$|\Psi\rangle \equiv e^{\hat{T}}|\Phi_0\rangle$$

$$\hat{T} = \sum_{m=1}^{A} \hat{T}_m$$

$$\hat{T}_m = \left(\frac{1}{m!}\right)^2 \sum_{\substack{\boldsymbol{k}_{i_1}\cdots\boldsymbol{k}_{i_m} \\ \boldsymbol{k}_{a_1}\cdots\boldsymbol{k}_{a_m}}} t_{\boldsymbol{k}_{i_1}\cdots\boldsymbol{k}_{i_m}}^{\boldsymbol{k}_{a_1}\cdots\boldsymbol{k}_{a_m}} c_{\boldsymbol{k}_{a_1}}^{\dagger} \cdots c_{\boldsymbol{k}_{a_m}}^{\dagger} c_{\boldsymbol{k}_{i_m}} \cdots c_{\boldsymbol{k}_{i_1}}$$

***m*-particle m-hole**

H. Kummel et al., Phys. Rep. 36 (1978)
G. Baardsen et al., PRC88, (2013)
G. Hagen et al., Rep. Progr. Phys. 77 (2014)

A-particle Schrodinger eq. or CC energy eq.

$$E = \langle\Phi_0|e^{-\hat{T}}\hat{H}e^{\hat{T}}|\Phi_0\rangle$$

Correlated Hamiltonian $e^{-\hat{T}}\hat{H}e^{\hat{T}}$ **= "Non-Hermit"**

$$\hat{H}\Psi = E\Psi \quad \rightarrow \hat{H}e^{\hat{T}}\Phi_0 = Ee^{\hat{T}}\Phi_0$$

In TOFS, $\exp(F^{\dagger})\hat{O}\exp(F)$ **= "Hermit"**

Set of CC amplitude equations:

$$\left\langle \Psi_{\boldsymbol{k}_{i_1}\cdots\boldsymbol{k}_{i_m}}^{\boldsymbol{k}_{a_1}\cdots\boldsymbol{k}_{a_m}} \middle| e^{-\hat{T}}\hat{H}e^{\hat{T}} \middle| \Phi_0 \right\rangle = 0$$

$$|\Psi_{\boldsymbol{k}_{i_1}\cdots\boldsymbol{k}_{i_m}}^{\boldsymbol{k}_{a_1}\cdots\boldsymbol{k}_{a_m}}\rangle = c_{\boldsymbol{k}_{a_1}}^{\dagger} \cdots c_{\boldsymbol{k}_{a_m}}^{\dagger} c_{\boldsymbol{k}_{i_m}} \cdots c_{\boldsymbol{k}_{i_1}}|\Phi_0\rangle,$$

***m*-particle *m*-hole**

Expectation value of $\hat{O}$ with power-series-type w.f. Ψ_N

Arbitrary *M*-body operator（Hermite, translationally invariant, symmetric）

$$\hat{O} = \sum_{i_1 \neq i_2 \neq \cdots \neq i_M}^{A} \hat{O}(i_1, i_2, \cdots, i_M)$$

Power-series type w.f.

$$\Psi_N(\alpha) = \left[\sum_{k=0}^{N} \frac{1}{k!} (\alpha F)^k \right] \Phi_0,$$

α is a real number

$$O_N(\alpha) \equiv \frac{\langle \Psi_N(\alpha) | \hat{O} | \Psi_N(\alpha) \rangle}{\langle \Psi_N(\alpha) | \Psi_N(\alpha) \rangle} = \frac{\sum_{n=0}^{2N} a_n \alpha^n}{\sum_{n=0}^{2N} b_n \alpha^n} = \sum_{n=0}^{\infty} A_n \alpha^n$$

$$A_n = \frac{a_n}{b_0} - \frac{b_1}{b_0} A_{n-1} - \cdots - \frac{b_{2N}}{b_0} A_{n-2N}$$

where $A_i = 0$ for $i < 0$, $b_0 = 1$,
and $a_n = b_n = 0$ for $n > 2N$

$$a_n = \sum_{k=0}^{n} \frac{1}{(n-k)!\, k!} \langle \Phi_0 | F^{n-k} \hat{O} F^k | \Phi_0 \rangle$$

$$b_n = \frac{2^n}{n!} \langle \Phi_0 | F^n | \Phi_0 \rangle$$

Setting $\alpha = 1$,

$$\langle \hat{O} \rangle_N = \frac{\langle \Psi_N | \hat{O} | \Psi_N \rangle}{\langle \Psi_N | \Psi_N \rangle} = \sum_{n=0}^{\infty} A_n$$

$$A_n = B_n \quad \text{for } 0 \leq n \leq N$$

Linked cluster expansion theorem in TOFS

We will show that a linked cluster expansion theorem is established in the exponential type w.f. Ψ_{ex}

T. Yamada, Annals of Physics 403 (2019), 1.

Expectation value of $\hat{O}$ with exponential type w.f. Ψ_{ex}

Arbitrary *M*-body operator（Hermite, translationally invariant, symmetric）

$$\hat{O} = \sum_{i_1 \neq i_2 \neq \cdots \neq i_M}^{A} \hat{O}(i_1, i_2, \cdots, i_M)$$

Exponential type w.f.

$$\Psi_{\mathrm{ex}} = \exp(F)\,\Phi_0 = \lim_{N\to\infty}\left[\sum_{k=0}^{N}\frac{1}{k!}F^k\right]\Phi_0$$

$$\langle\hat{O}\rangle_{ex} = \frac{\langle\Psi_{\mathrm{ex}}|\hat{O}|\Psi_{\mathrm{ex}}\rangle}{\langle\Psi_{\mathrm{ex}}|\Psi_{\mathrm{ex}}\rangle} = \frac{\langle\Phi_0|\exp(F^\dagger)\hat{O}\exp(F)|\Phi_0\rangle}{\langle\Phi_0|\exp(F^\dagger)\,\exp(F)|\Phi_0\rangle} = \sum_{n=0}^{\infty}\boldsymbol{B_n}$$

$$B_n = \frac{a_0}{b_0} - \sum_{k=1}^{n}\frac{b_k}{b_0}B_{n-k}$$

$$a_n = \sum_{k=0}^{n}\frac{1}{(n-k)!\,k!}\langle\Phi_0|\boldsymbol{F^{n-k}\hat{O}F^k}|\Phi_0\rangle$$

$$b_n = \frac{2^n}{n!}\langle\Phi_0|\boldsymbol{F^n}|\Phi_0\rangle$$

We have to evaluate the expectation value of the operator products, for example,

$$\boxed{\langle \Phi_0 | \boldsymbol{F^{n-k}\hat{O}F^k} | \Phi_0 \rangle \text{ and } \langle \Phi_0 | \boldsymbol{F^n} | \Phi_0 \rangle}$$

The operator products, $\boldsymbol{F^{n-k}\hat{O}F^k}$ and $\boldsymbol{F^n}$, can be expanded as the sum of the multi-body operators. For example,

$$F^2 = \left(\frac{1}{2} \sum_{i \neq j}^{A} f(ij) \right) \left(\frac{1}{2} \sum_{i \neq j}^{A} f(ij) \right)$$

$$= \frac{1}{2} \sum_{i \neq j}^{A} f^2(ij) + \sum_{i \neq j \neq k}^{A} f(ij) f(ik) + \frac{1}{4} \sum_{i \neq j \neq k \neq l}^{A} f(ij) f(kl)$$

$$= \text{ 2-body term} + \text{3-body term} \quad + \quad \text{4-body term}$$

In general, if $\boldsymbol{\hat{O}}$ is a 2-body operator, $\boldsymbol{F^{n-k}\hat{O}F^k}$ is expressed as the summation from the 2-body to (2*n*+2)-body terms.

Furthermore, the matrix element of the *m*-body term with respect to Φ_0 has an (*m*-1)-power dependence with density $\boldsymbol{\rho}$.

For example, a correlated Hamiltonian with tensor force V_T, having 5-operator product, is expressed as

$$F_D F_S V_T F_S F_D = \left(\sum_{i<j} f_D(ij)\right)\left(\sum_{i<j} f_S(ij)\right)\left(\sum_{i<j} V_T(ij)\right)\left(\sum_{i<j} f_S(ij)\right)\left(\sum_{i<j} f_D(ij)\right)$$

$$= \text{2-body terms} + \cdots + \textbf{5-body terms} + \cdots + \text{10-body terms}$$

Next, we will show one example of the 5-body terms.

One example of the 5-body terms in the previous-slide correlated Hamiltonian is given as

$$O_5 = \sum_{i_1 \neq i_2 \neq i_3 \neq i_4 \neq i_5} f_D(i_1 i_2) f_S(i_3 i_4) V_T(i_3 i_4)\, f_S(i_3 i_4) f_D(i_3 i_5) \equiv (12)(34)^3(35)$$

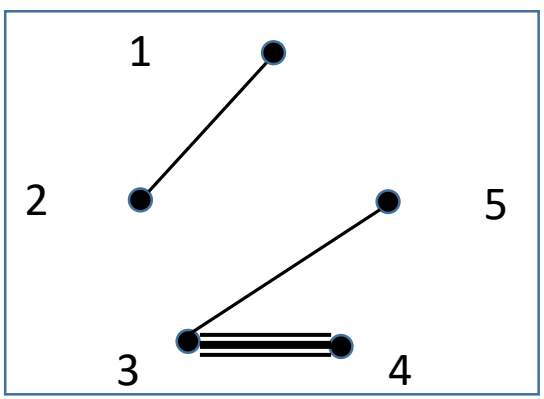
Matrix element of the 5-body term: composed of 5！=120 integrals（=12-dim. integral）

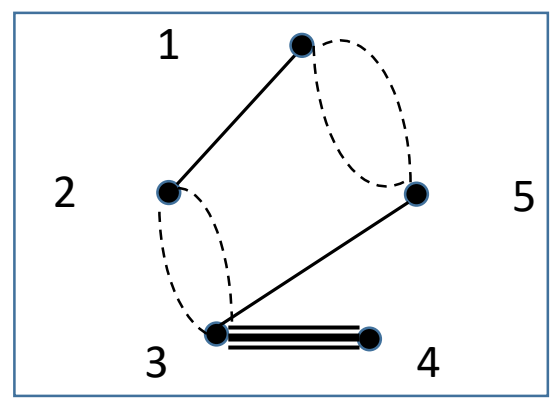
$$\langle \Phi_0 | O_5 | \Phi_0 \rangle = A \times \boldsymbol{\rho}^4 \times \sum_{\beta} \mathrm{sgn}(\beta) \int d\boldsymbol{r}_{12} d\boldsymbol{r}_{34} d\boldsymbol{r}_{35} d\boldsymbol{r}_{14} G_\beta(\boldsymbol{r}_{12}, \boldsymbol{r}_{34}, \boldsymbol{r}_{35}, \boldsymbol{r}_{14}),$$

β: permutation

$$G_\beta(\{\boldsymbol{r}\}) = \sum_{s_1 t_1 s_2 t_2 s_3 t_3} \delta_{s_1,1} \delta_{s_2,1} \delta_{s_3,1} \times \frac{1}{4^5} \sum_{xyuvpq} F_\beta^{(5)(12:34:35)}(s_1 s_2 s_3) F_\beta^{(5)(12:34:35)}(t_1 t_2 t_3)$$
$$\times f_D^{(s_1 t_1)}(r_{12})(\boldsymbol{r}_{12})_x (\boldsymbol{r}_{12})_y f_S^{(s_2 t_2)}(r_{34}) V_T^{(s_2 t_2)}(r_{34})(\boldsymbol{r}_{34})_u (\boldsymbol{r}_{34})_v\, f_S^{(s_2 t_2)}(r_{34}) f_D^{(s_3 t_3)}(r_{35})(\boldsymbol{r}_{35})_p (\boldsymbol{r}_{35})_q g_\beta(\{\boldsymbol{r}\})$$

Each integral (5！=120) can be shown graphically, and is classified into linked and unlinked diagrams: One ex. of unlinked (linked) diagrams





Unlinked (divergent) $\propto$ volume $\boldsymbol{\Omega} \to \infty$

$$\beta = \begin{pmatrix} 12345 \\ 12345 \end{pmatrix}$$

Linked (convergent)

$$\beta = \begin{pmatrix} 12345 \\ \mathbf{53241} \end{pmatrix}$$

Decomposition into linked and unlinked diagrams

$$\left\langle \Phi_0 \middle| F^{n_1}\, \hat{O} F^{n_2} \middle| \Phi_0 \right\rangle = \left\langle \Phi_0 \middle| F^{n_1}\, \hat{O} F^{n_2} \middle| \Phi_0 \right\rangle_{\mathrm{c}} + \left\langle \Phi_0 \middle| F^{n_1}\, \hat{O} F^{n_2} \middle| \Phi_0 \right\rangle_{\mathrm{dis}}$$

First term in R.H.S: linked (=sum of linked diagrams): convergent
Second in R.H.S.: unlinked (=sum of unlinked diagrams): divergent ($\propto \boldsymbol{\Omega^m}$)

(Volume $\Omega \longrightarrow \infty$)

We can prove the following **recurrence formulas**:

$$\langle \Phi_0 | F^n | \Phi_0 \rangle = \sum_{k=0}^{n-1} \frac{(n-1)!}{k!\,(n-k-1)!} \langle \Phi_0 | F^{n-k} | \Phi_0 \rangle_{\mathrm{c}} \langle \Phi_0 | F^k | \Phi_0 \rangle,$$

$$\left\langle \Phi_0 \middle| F^{n_1}\, \hat{O} F^{n_2} \middle| \Phi_0 \right\rangle$$

$$= \sum_{k=0}^{n_1+n_2} \sum_{\substack{k_1,k_2 \\ k_1+k_2=k}} \frac{n_1!}{k_1!\,(n_1-k_1)!} \frac{n_2!}{k_2!\,(n_2-k_2)!} \left\langle \Phi_0 \middle| F^{k_1}\, \hat{O} F^{k_2} \middle| \Phi_0 \right\rangle_{\mathrm{c}} \langle \Phi_0 | F^{n_1+n_2-k} | \Phi_0 \rangle$$

We can prove them by the characters of operator products and antisymmetrization of Fermi-sphere w.f. Φ_0. See 'T. Yamada, Annals of Physics 403 (2019), 1.'

In general, B_n has linked diagrams and unlinked diagrams.
But, applying the recurrence formulas shown in previous slide to a_n and b_n, we can prove that all of the unlinked diagrams in B_n are canceled out. Consequently, we only have to evaluate the linked diagrams in the present framework:

$$\boxed{B_n = \frac{a_0}{b_0} - \sum_{k=1}^{n} \frac{b_k}{b_0} B_{n-k} = \cdots\cdots = (a_n)_{\mathbf{c}}}$$

Eventually, we get the final expression as

$$\langle \hat{O} \rangle_{\mathrm{ex}} = \frac{\langle \Psi_{\mathrm{ex}} | \hat{O} | \Psi_{\mathrm{ex}} \rangle}{\langle \Psi_{\mathrm{ex}} | \Psi_{\mathrm{ex}} \rangle} = \frac{\langle \Phi_0 | \exp(F^\dagger) \hat{O} \exp(F) | \Phi_0 \rangle}{\langle \Phi_0 | \exp(F^\dagger) \exp(F) | \Phi_0 \rangle}$$

$$= \sum_{n=0}^{\infty} B_n = \sum_{n=0}^{\infty} (a_n)_{\mathbf{c}} = \sum_{n=0}^{\infty} \sum_{\substack{n_1, n_2 \\ n_1 + n_2 = n}} \frac{1}{n_1!\, n_2!} \left\langle \Phi_0 \middle| F^{n_1}\, \hat{O} F^{n_2} \middle| \Phi_0 \right\rangle_{\mathbf{c}}$$

This equation means that the expectation value of operator $\hat{O}$ with the exponential-type correlated wave function Ψ_{ex} is given as the sum of the linked diagrams.

In other word, a linked cluster expansion theorem is established.

Next, we will discuss the expectation value of $\hat{O}$, $\langle \hat{O} \rangle_N$, with *N*th power-series correlated nuclear-matter wave function $\Psi_N = \left[\sum_{k=0}^{N} \frac{1}{k!} F^k\right] \Phi_0$.

Taking into account the fact that Ψ_N is the *N*th order polynomial with respect to *F*, one may take the following expression for $\langle \hat{O} \rangle_N$ as an approximation of the exponential-type case $\langle \hat{O} \rangle_{ex}$,

$$\langle \hat{O} \rangle_N = \frac{\langle \Psi_N | \hat{O} | \Psi_N \rangle}{\langle \Psi_N | \Psi_N \rangle} \cong \sum_{n_1=0}^{N} \sum_{n_2=0}^{N} \frac{1}{n_1!\, n_2!} \left\langle \Phi_0 \middle| F^{n_1}\, \hat{O} F^{n_2} \middle| \Phi_0 \right\rangle_{\mathbf{c}}$$

$$\xrightarrow[N \to \infty]{} \quad \langle \hat{O} \rangle_{\mathbf{ex}} = \frac{\langle \Phi_0 | \exp(F^\dagger) \hat{O} \exp(F) | \Phi_0 \rangle}{\langle \Phi_0 | \exp(F^\dagger)\, \exp(F) | \Phi_0 \rangle}$$

$$= \sum_{n=0}^{\infty} \sum_{\substack{n_1, n_2 \\ n_1+n_2=n}} \frac{1}{n_1!\, n_2!} \left\langle \Phi_0 \middle| F^{n_1}\, \hat{O} F^{n_2} \middle| \Phi_0 \right\rangle_{\mathbf{c}}$$

In the actual numerical calculation, the calculation of exponential-type $\langle \hat{O} \rangle_{ex}$ is difficult. Therefore, we will use power-series-type $\langle \hat{O} \rangle_N$ in the actual calculation.

Binding energy per particle in nuclear matter with TOFS

Hamiltonian

$$H = \sum_{i=1}^{A} t_i + \frac{1}{2}\sum_{i\neq j}^{A} v_{ij} + \frac{1}{6}\sum_{i\neq j\neq k}^{A} V_{ijk}$$

Binding energy per particle in n.m. with power-series-type Ψ_N

$$-B_N = \frac{1}{A}\frac{\langle\Psi_N|H|\Psi_N\rangle}{\langle\Psi_N|\Psi_N\rangle} \cong \frac{1}{A}\sum_{n_1=0}^{N}\sum_{n_2=0}^{N}\frac{1}{n_1!\,n_2!}\left\langle\Phi_0\middle|F^{n_1}\,HF^{n_2}\,\middle|\Phi_0\right\rangle_{\mathbf{c}}$$

We refer to evaluate B_N as the Nth-order TOFS calculation.

1st order TOFS cal.

$$-B_{N=1} = \frac{1}{A}\left[\langle\Phi_0|H|\Phi_0\rangle_{\mathbf{c}} + \langle\Phi_0|FH+HF|\Phi_0\rangle_{\mathbf{c}} + \langle\Phi_0|FHF|\Phi_0\rangle_{\mathbf{c}}\right]$$

2nd order TOFS cal.

$$-B_{N=2} = \frac{1}{A}\left[\begin{array}{c}\langle\Phi_0|H|\Phi_0\rangle_{\mathbf{c}} + \langle\Phi_0|FH+HF|\Phi_0\rangle_{\mathbf{c}} + \left\langle\Phi_0\middle|\frac{1}{2!}F^2H + FHF + \frac{1}{2!}HF^2\middle|\Phi_0\right\rangle_{\mathbf{c}} \\ + \left\langle\Phi_0\middle|\frac{1}{2!}F^2HF + \frac{1}{2!}FHF^2\middle|\Phi_0\right\rangle_{\mathbf{c}} + \left\langle\Phi_0\middle|\frac{1}{2!^2}F^2HF^2\middle|\Phi_0\right\rangle_{\mathbf{c}}\end{array}\right]$$

Gaussian expansion of F_S and F_D

$$F = F_S + F_D$$

$$F_S = \frac{1}{2}\sum_{i\neq j} f_S(i,j) = \frac{1}{2}\sum_{s=0}^{1}\sum_{t=0}^{1}\sum_{i\neq j} f_S^{(st)}(r_{ij}) P_{ij}^{(st)},$$ **Central type**

$$f_S^{(st)}(r) = \sum_{\mu} C_S^{(st)} \exp\left[-a_{S,\mu}^{(st)} r^2\right],$$

$a_{S,\mu}^{(st)} = a_{S,0}^{(st)} \times \gamma^{\mu-1}$: size parameter

$C_S^{(st)}$: expansion coefficient

$$F_D = \frac{1}{2}\sum_{i\neq j} f_D(i,j) = \frac{1}{2}\sum_{s=0}^{1}\sum_{t=0}^{1}\sum_{i\neq j} f_D^{(st)}(r_{ij}) r_{ij}^2 S_{12}(i,j) P_{ij}^{(st)} \delta_{s,1},$$ **Tensor type**

$$f_D^{(st)}(r) = \sum_{\mu} C_D^{(st)} \exp\left[-a_{D,\mu}^{(st)} r^2\right],$$

$a_{D,\mu}^{(st)} = a_{D,0}^{(st)} \times \gamma^{\mu-1}$: size parameter

$C_D^{(st)}$: expansion coefficient

Variational condition of the binding energy B_N

$$\frac{\partial B_N}{\partial C_{S,\mu}^{(st)}} = 0, \qquad \frac{\partial B_N}{\partial C_{D,\mu}^{(st)}} = 0$$

→ determination of $C_{S,\mu}^{(st)}$ and $C_{D,\mu}^{(st)}$

1st order TOFS calculation with central *NN* force

$$\Psi_N = (1 + F_S)\Phi_0$$

$$F_S = \sum_{s,t,\mu} C_{S,\mu}^{(s,t)} F_{S,\mu}^{(st)}, \qquad F_{S,\mu}^{(st)} = \frac{1}{2}\sum_{i\neq j}^{A} \exp\left(-a_{S,\mu}^{(st)} r_{ij}^2\right) P_{ij}^{(st)}$$

$$-B_{N=1} = \frac{1}{A}\left[\langle\Phi_0|H|\Phi_0\rangle_{\mathbf{c}} + \langle\Phi_0|F_S H + H F_S|\Phi_0\rangle_{\mathbf{c}} + \langle\Phi_0|F_S H F_S|\Phi_0\rangle_{\mathbf{c}}\right]$$

$$= \frac{1}{A}\left[\begin{array}{l} \langle\Phi_0|H|\Phi_0\rangle_{\mathbf{c}} + \sum_{s,t,\mu}\left\langle\Phi_0\left|F_{S,\mu}^{(st)} H + H F_{S,\mu}^{(st)}\right|\Phi_0\right\rangle_{\mathbf{c}} C_{S,\mu}^{(s,t)} \\ + \sum_{\boldsymbol{s,t,\mu}}\sum_{\boldsymbol{s',t',\mu'}}\left\langle\Phi_0\left|F_{S,\mu}^{(st)} H F_{S,\mu'}^{(s't')}\right|\Phi_0\right\rangle_{\mathbf{c}} C_{S,\mu}^{(s,t)} C_{S,\mu'}^{(s',t')} \end{array}\right]$$

Quadratic form with $C_{S,\mu}^{(s,t)}$

From the variational condition, $\dfrac{\partial B_{N=1}}{\partial C_{S,\mu}^{(st)}} = 0,$

$$\sum_{s',t',\mu'}\left\langle\Phi_0\left|F_{S,\mu}^{(st)} H F_{S,\mu'}^{(s't')}\right|\Phi_0\right\rangle_{\mathbf{c}} C_{S,\mu'}^{(s',t')} = -\frac{1}{2}\left\langle\Phi_0\left|F_{S,\mu}^{(st)} H + H F_{S,\mu}^{(st)}\right|\Phi_0\right\rangle_{\mathbf{c}}$$

Simultaneous linear equations with respect to $\left\{C_{S,\mu}^{(s,t)}\right\}$

In the 1st order TOFS calculation,
we have to expand the operator products:

$$H = T + V = \sum_{i=1}^{A} t(i) + \frac{1}{2}\sum_{i\neq j}^{A} v(i,j)$$

$$F_S T = \left(\frac{1}{2}\sum_{i\neq j} f_S(i,j)\right)\left(\sum_{i=1}^{A} t(i)\right) = \sum_{i\neq j} f_S(i,j)t(i) + \frac{1}{2}\sum_{i\neq j\neq k} f_S(i,j)t(k)$$

2-body term **3-body term**

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

$$F_S V F_S = \left(\frac{1}{2}\sum_{i\neq j} f_S(i,j)\right)\left(\frac{1}{2}\sum_{i\neq j}^{A} v(i,j)\right)\left(\frac{1}{2}\sum_{i\neq j} f_S(i,j)\right)$$

$$= \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

= **2-body term** + **3-body terms** + ··· + **6-body term**

In the TOFS calculation, we estimate the contributions from all of the many-body terms, i.e., matrix elements up to the 6-body term.

2nd order TOFS calculation with central *NN* force

$$\Psi_N = \left(1 + F_S + \frac{1}{2!}F_S^2\right)\Phi_0$$

$$F_S = \sum_{s,t,\mu} C_{S,\mu}^{(s,t)} F_{S,\mu}^{(st)}, \qquad F_{S,\mu}^{(st)} = \frac{1}{2}\sum_{i\neq j}^{A} \exp\left(-a_{S,\mu}^{(st)} r_{ij}^2\right) P_{ij}^{(st)}, \qquad a_{S,\mu}^{(st)} = a_{S,0}^{(st)} \times \gamma^{\mu-1}$$

$$-B_{N=2} = \frac{1}{A}\left[\begin{array}{c}\langle\Phi_0|H|\Phi_0\rangle_{\mathbf{c}} + \langle\Phi_0|F_S H + H F_S|\Phi_0\rangle_{\mathbf{c}} + \left\langle\Phi_0\left|\frac{1}{2!}{F_S}^2 H + F_S H F_S + \frac{1}{2!}H{F_S}^2\right|\Phi_0\right\rangle_{\mathbf{c}} \\ + \left\langle\Phi_0\left|\frac{1}{2!}{F_S}^2 H F_S + \frac{1}{2!}F_S H {F_S}^2\right|\Phi_0\right\rangle_{\mathbf{c}} + \left\langle\Phi_0\left|\frac{1}{2!^2}{F_S}^2 H {F_S}^2\right|\Phi_0\right\rangle_{\mathbf{c}}\end{array}\right]$$

We have to estimate the matrix element up to 10-body term arising from ${F_S}^2 V {F_S}^2$

$${F_S}^2 V {F_S}^2 = \left(\frac{1}{2}\sum_{i\neq j} f_S(i,j)\right)\left(\frac{1}{2}\sum_{i\neq j} f_S(i,j)\right)\left(\frac{1}{2}\sum_{i\neq j}^{A} v(i,j)\right)\left(\frac{1}{2}\sum_{i\neq j} f_S(i,j)\right)\left(\frac{1}{2}\sum_{i\neq j} f_S(i,j)\right)$$

$$= \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

$$= \text{2-body term} + \text{3-body terms} + \cdots + \text{10-body term}$$

From the variational condition, $\dfrac{\partial B_{N=2}}{\partial C_{S,\mu}^{(st)}} = 0,$

one should solve non-linear equations with respect to $\left\{C_{S,\mu}^{(s,t)}\right\}$**.**

Difference from TOAMD (tensor optimized AMD)

TOAMD : Variational framework for ab initio description of light nuclei

T. Myo et al., Prog. Thor. Exp. Phys. 2017 (2017)

Lyu-san's talk

$$\Psi(\mathrm{TOAMD}) = \left(\text{Arbitrary power-series form of } F_S \text{ and } F_D \right) \times \Phi(\mathrm{AMD})$$

For example,

$$\Psi = (1 + F_S)(1 + F_D)\Phi_0$$
$$\Psi = (1 + F_S + F_D)^2\Phi_0$$
$$\Psi = (1 + F_S + F_D + F_S^2 + F_D^2 + F_S F_D + F_D F_S)\Phi_0$$

These w.f.s successfully reproduce the properties of s-shell nuclei.

However, they are not allowed in nuclear matter calculation, because unlinked diagrams are not canceled out in their calculations.

In nuclear matter, the following type w.f. is allowed

$$\Psi = \left[1 + (F_S + F_D) + \frac{1}{2!}(F_S + F_D)^2 + \frac{1}{3!}(F_S + F_D)^3 + \cdots\right]\Phi_0$$

In this w.f., all of unlinked diagrams are canceled out, and only linked diagrams remain.

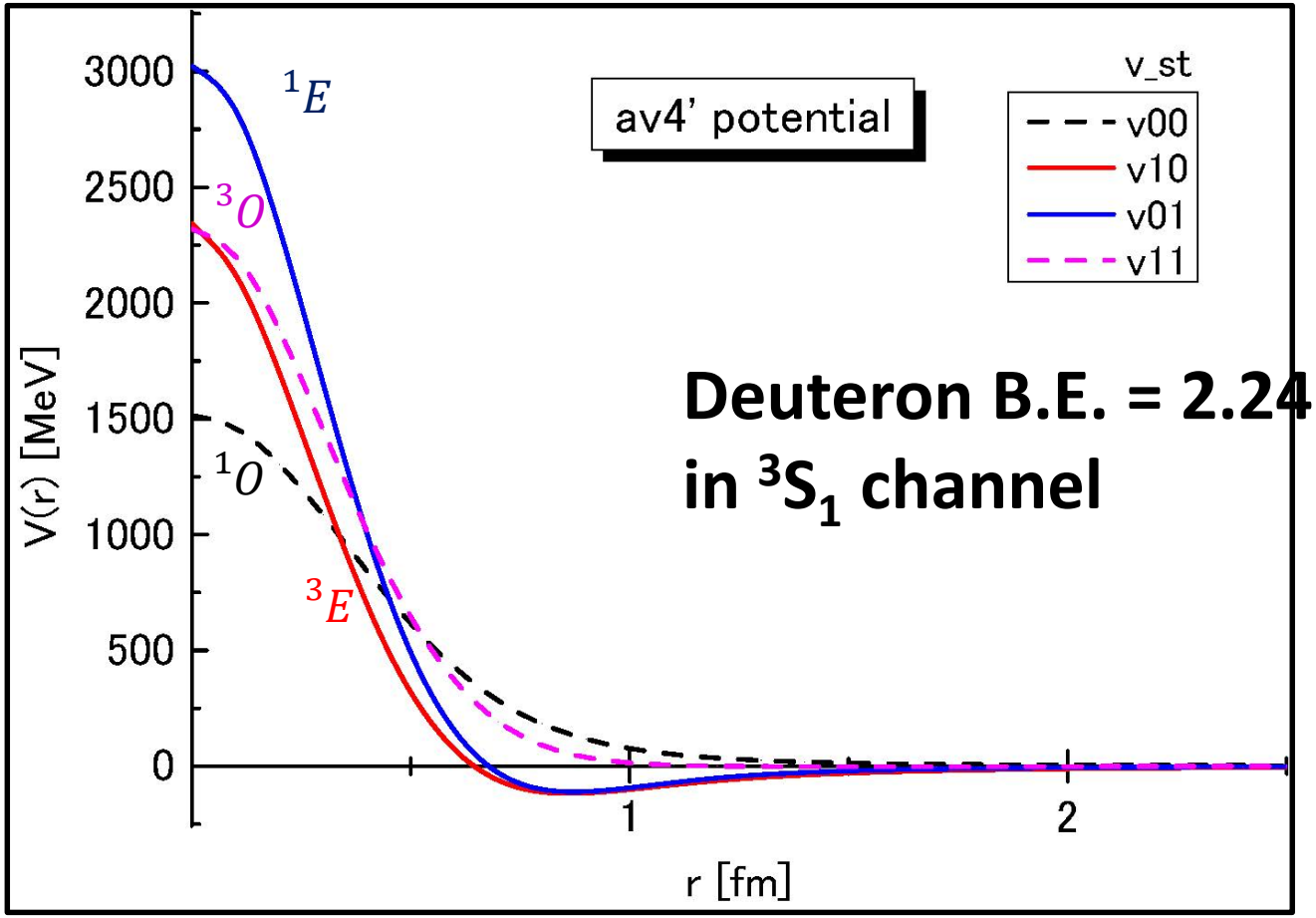
1st order TOFS calculation with AV4' force

Yamada, Myo, Toki, Horiuchi, Ikeda, arXiv1808.08120.

Nuclear force : AV4' (only central)

R.B. Wiringa et al., PRC51 (1985)

3 GeV



Deuteron B.E. = 2.24 MeV in $^3S_1$ channel

The NN phase shifts of $^1S_0$, $^3S_1$, and $^1P_1$ channels are reasonably reproduced up to 350 MeV/c. But, those of $^3S_{3,2}$ and $^3P_{0,1,2}$ are not because of no tensor coupling etc.

1st order TOFS cal. (symmetric nuclear matter)

$$-B_{N=1} = \frac{1}{A}[\langle\Phi_0|H|\Phi_0\rangle_{\mathbf{c}} + \langle\Phi_0|F_S H + H F_S|\Phi_0\rangle_{\mathbf{c}} + \langle\Phi_0|F_S H F_S|\Phi_0\rangle_{\mathbf{c}}]$$

= Kinetic （1-body + 2-body + 3-body + 4-body + 5-body ）terms

$\rho^{2/3}$ $\rho, \rho^{5/3}$ $\rho^2, \rho^{8/3}$ $\rho^3, \rho^{11/3}$ $\rho^4, \rho^{14/3}$

＋ Potential (2-body + 3-body + 4-body + 5-body + 6-body ）

ρ ρ^2 ρ^3 ρ^4 ρ^5

How to calculate the matrix elements of many-body terms arising from operator products.

Ex.

$$F_S V F_S = \left(\frac{1}{2}\sum_{i\neq j} f_S(i,j)\right)\left(\frac{1}{2}\sum_{i\neq j}^{A} v(i,j)\right)\left(\frac{1}{2}\sum_{i\neq j} f_S(i,j)\right)$$

$$= \text{2-body term} + \text{3-body terms} + \cdots + \textbf{6-body term}$$

6-body term $= \dfrac{1}{8}\displaystyle\sum_{i\neq j\neq k\neq l\neq m\neq n} f_S(i,j)v(k,l)f_S(m,n) \equiv \frac{1}{8}(12)(34)(56)$

$$\left\langle \Phi_0 \middle| \frac{1}{8}(12)(34)(56) \middle| \Phi_0 \right\rangle = A \times \rho^5 \times \sum_{\beta} \mathrm{sgn}(\beta) \int d\{\boldsymbol{r}\}\, G_\beta(\{\boldsymbol{r}\}),$$

$$G_\beta(\{\boldsymbol{r}\}) = \frac{1}{8}\sum_{s_1,t_1}\sum_{s_2,t_2}\sum_{s_3,t_3} \frac{1}{4^6} F_\beta^{(6)(12:34:56)}(s_1,s_2,s_3) F_\beta^{(6)(12:34:56)}(t_1,t_2,t_3)$$

$$\times f_S^{(s_1,t_1)}(r_{12})\, v^{(s_2,t_2)}(r_{34})\, f_S^{(s_3,t_3)}(r_{56}) \prod_{n=1}^{6} h\big(k_F \rho_n(\beta)\big),$$

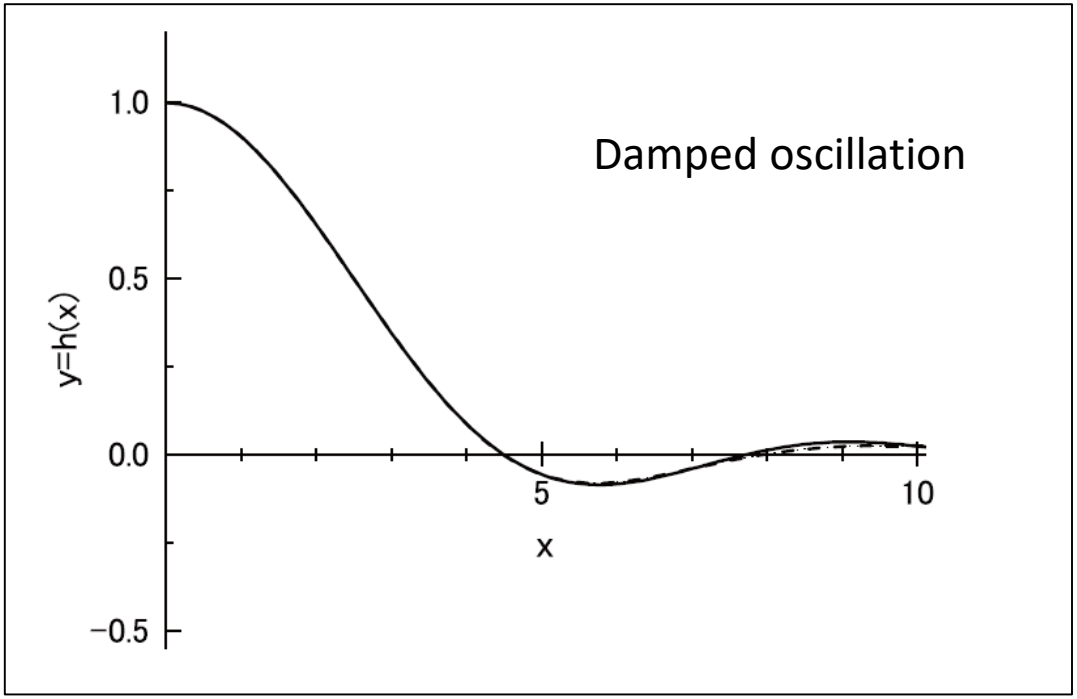
$h(x) = \dfrac{j_1(x)}{x}$: slater function, $\beta = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ \beta_1 & \beta_2 & \beta_3 & \beta_4 & \beta_5 & \beta_6 \end{pmatrix}$, $\boldsymbol{\rho}_n(\beta) = \displaystyle\sum_{j=1}^{6} \delta_{n\beta_j}\boldsymbol{r}_j - \boldsymbol{r}_n$

$j_1(x)$: spherical Bessel function

Gaussian expansion of $h(x) = \frac{j_1(x)}{x}$

$j_1(x)$: spherical Bessel function

$$h(x) = \frac{j_1(x)}{x} = \sum_n c_n \exp(-\nu_n x^2)\,, \qquad x = k_F \times r$$



$\left\langle \Phi_0 \middle| \frac{1}{8}(12)(34)(56) \middle| \Phi_0 \right\rangle$ = multi-dimensional (15th dim.) integral = **Gaussian Integral**

This reduces a lot of the computation cost.

1st order TOFS cal. (symmetric nuclear matter)

$$-B_{N=1} = \frac{1}{A}[\langle\Phi_0|H|\Phi_0\rangle_{\mathbf{c}} + \langle\Phi_0|F_S H + H F_S|\Phi_0\rangle_{\mathbf{c}} + \langle\Phi_0|F_S H F_S|\Phi_0\rangle_{\mathbf{c}}]$$

= Kinetic （1-body + 2-body + 3-body + 4-body + 5-body ）terms

$\rho^{2/3}$ $\rho, \rho^{5/3}$ $\rho^2, \rho^{8/3}$ $\rho^3, \rho^{11/3}$ $\rho^4, \rho^{14/3}$

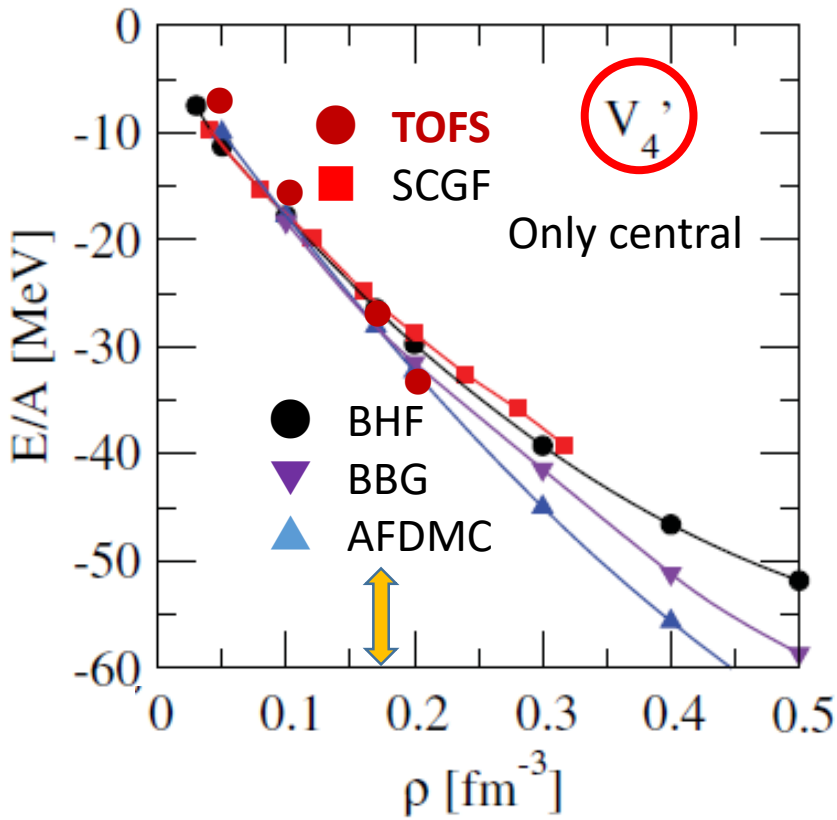
＋ Potential (2-body + 3-body + 4-body + 5-body + 6-body ）

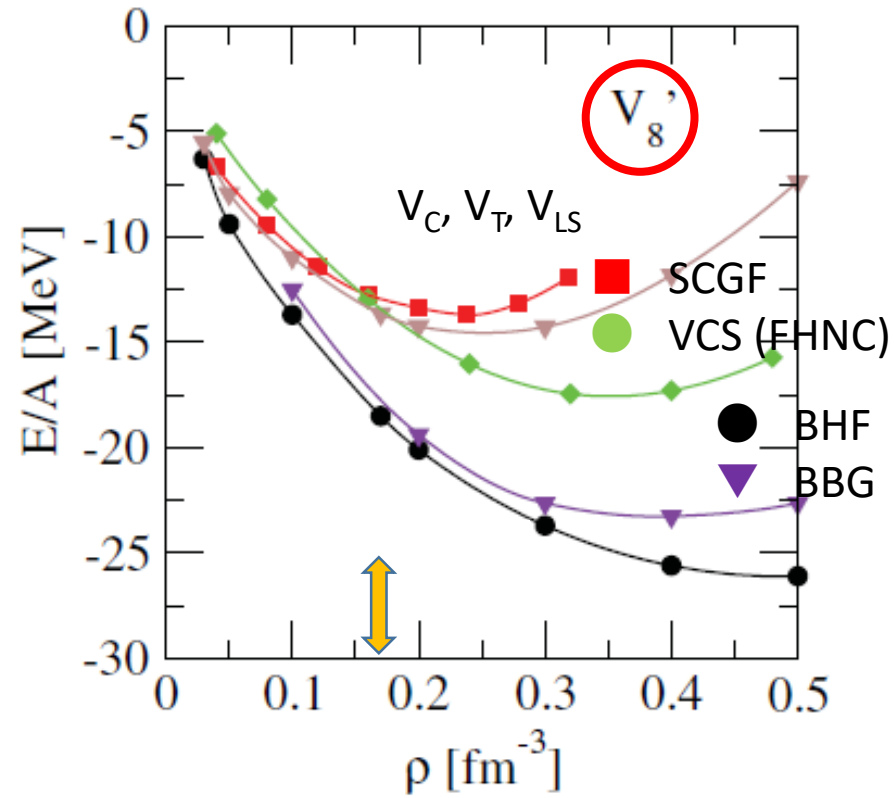
ρ ρ^2 ρ^3 ρ^4 ρ^5

ρ [fm^{-3}]	0.03	0.05	0.10	0.17	0.20
$-B_{N=1}$	-4.1	-7.4	-15.1	-26.6	-35.4
BHF	-7.4	-11.2	-17.7	-26.4	-29.7

BHF results from "Baldo et al., PRC86 (2012)", including the contribution from 3-hole lines

Symmetric nuclear matter : Argonne potentials (no 3N force)





● **1st order TOFS**

● BHF
▼ BBG
● VCS (FHNC)
■ SCGF
▲ AFDMC

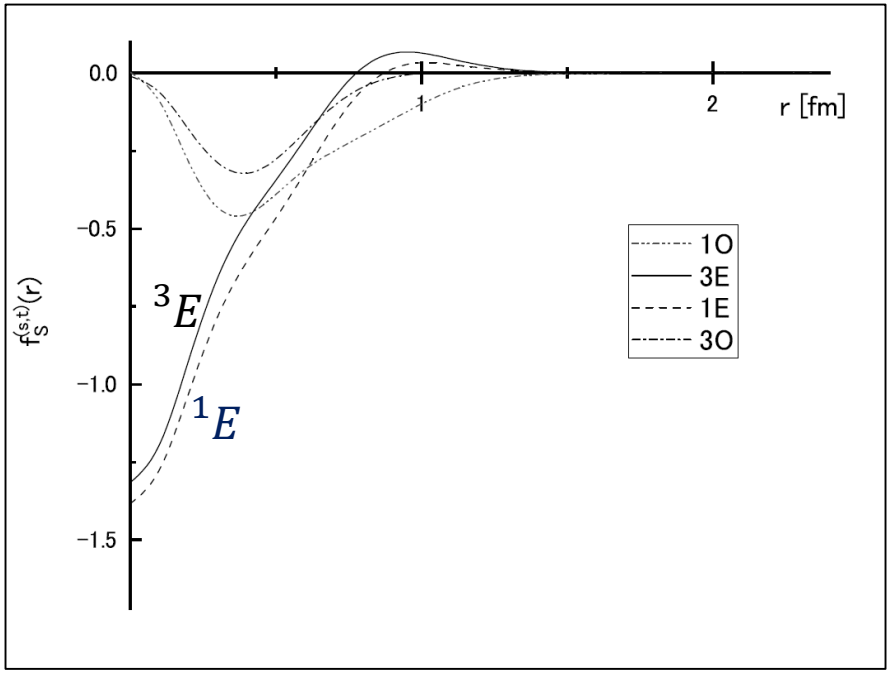
Baldo et al., PRC86 (2012)

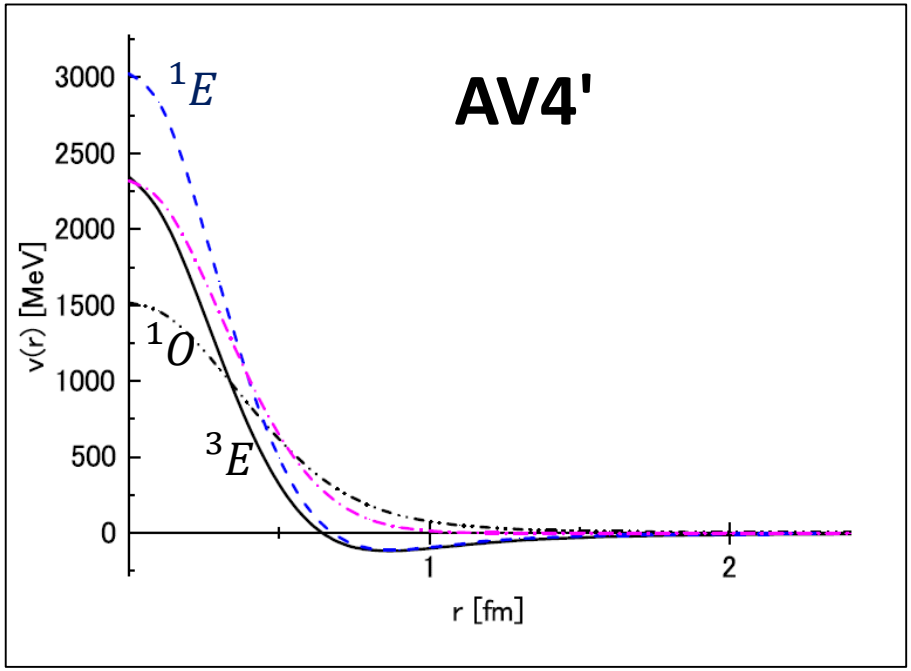
Yamada, Myo, Toki, Horiuchi, Ikeda, arXiv1808.08120.

Radial behaviors of spin-isospin correlated functions

$$F_S = \frac{1}{2}\sum_{s,t}\sum_{i\neq j}^{A} f_S^{(st)}(r_{ij})P_{ij}^{(st)}$$

ρ=0.170 fm^{-3}





Deuteron B.E. = 2.24 MeV

Contributions from many-body terms at $\rho = 0.170\text{fm}^{-3}$

$\langle O \rangle = \langle \Phi_0 \| O \| \Phi_0 \rangle$	One-body	Two-body		Three-body	Four-body	Five-body	Six-body	total
$\langle T \rangle$	○							
$\langle F_S T \rangle$			○	○				
$\langle T F_S \rangle$			○	○				
$\langle F_S T F_S \rangle$			○	○	○	○		
$\langle V \rangle$		○						
$\langle F_S V \rangle$			○	○	○			
$\langle V F_S \rangle$			○	○	○			
$\langle F_S V F_S \rangle$			○	○	○	○	○	
	23.0	-21.9	-25.5	11.6	-9.9	1.3	-5.3	
$-B_{N=1}$ [MeV]								-26.6

We can see important contributions from many-body terms.

Summary

- **The tensor optimized Fermi sphere (TOFS) method based on Hermite form has been newly proposed. In this formalism, the correlated nuclear matter w.f. is taken to be the power-series-type (and exponential-type) of the correlation function F. This was ensured by the linked cluster expansion theorem established in TOFS.**
- **In TOFS, the correlation function is optimally determined in the variation of the energy with respect to the nuclear matter w.f.**
- **We have performed the 1st order TOFS calculation with AV4' force, where we took into account the contributions from all the many-body terms (up to 6-body term).**
- **We found the density dependence of E/A in nuclear matter is reasonably reproduced up to $\rho = 0.20$ fm^{-3}, in comparison with the other methods such as the BHF approach. We found important contributions from the many-body terms.**
- **Future plans: nuclear matter calculations with AV6', AV8' etc.**

  2nd order TOFS calculation etc.