# Unitary Model Operator Approach with Two-Nucleon and Three-Nucleon Forces

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The National Institute for Nuclear theory's Program

Nuclear Many-Body Approaches for the 21st Century

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# Overview

1. Introduction
2. Short review of UMOA with 2NF
3. Formulation of UMOA with 2NF and 3NF
4. Calculation procedure
5. Summary and discussion

# 1. Introduction-motivations-

## Missing Correlations!

A. Bhagwat, R. Wyss, W. Satula, J. Meng, Y. K. Gambhir,
Deficiency of Spin Orbit Interaction in Relativistic Mean Filed Theory
nucl-th/0605009；

the need of extensions either by considering new coupling terms
like the tensor interactions
or to go beyond the Hartree approximation

T. Lesinski, M. Bender, K. Bennceu, T. Duguet, J. Meyer,
The tensor part of the Skyrme energy density functional.
I. Spherical nuclei. nucl-th/0704073

... We conclude that the currently used central and
spin-orbit parts of the Skyrme energy density functional are not flexible
enough to allow for the presence of large tensor terms.

as residual interactions

⇨ Need of alternative studies

## Need of genuine three-nucleon force not only in few-nucleon systems but also in medium-mass nuclei

(1)few-nucleon systems,
H. Kamada et al.,
*Benchmark test calculations of a four-nucleon bound state*
Phys. Rev. C64, 044001(2001) and references-therein
Lack of B.E.

(2)S. Fujii, R. Okamoto, K. Suzuki, PRC (2004),
Lack of B.E. of $^{16}$O, $^{40}$Ca

(3)A. Nogga, P. Navratil, B. R. Barrett, J. P. Vary,
Phy. Rev. C73, 064002(2006), arXIV: nucl-th/0511082
$^{7}$Li

(4)E. Caurier et al,
*The shell model as a unified view of nuclear structure*,
Rev. Mod. Phys. 77, 428-488(2006)

(5)T. Otsuka, talk for JUSTIPEN-LACM Meeting at Oak Ridge National laboratory, Tennessee, USA, March 5-8, 2007.

# Progress in our understanding of nuclear forces

**Phenomenological three-nucleon force**

↓

**Chiral Nuclear Force**

**As a recent review:**

**R. Machliedt**
**nucl-th/07040807**
***Nuclear forces from chiral effective field theory***

http://www.int.washington.edu/talks/WorkShops/int_07_3/

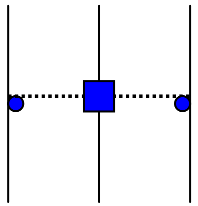
# Explicit expressions for the Chiral 3NF

A. Nogga, P. Navratil, B. R. Barrett, J. P. Vary, Phys. Rev. **C73**, 064002(2006)

Notations follows the ref. J. L. Friar, D. Hueber, U. van Kolck, Phys. Rev. **C59**, 53(1999)

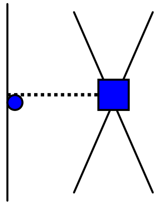
## The 2π exchange part

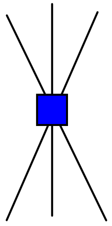
$$V_{ijk}^{(k);2\pi} \equiv \sum_{i\neq j\neq k} \frac{1}{2}\left(\frac{g_A}{2F_\pi}\right)^2 \times \frac{(\vec{\sigma}_i \bullet \vec{q}_i)(\vec{\sigma}_j \bullet \vec{q}_j)}{(\vec{q}_i^{\,2} + m_\pi^2)(\vec{q}_j^{\,2} + m_\pi^2)} F_{ijk}^{\alpha\beta} \cdot \tau_i^\alpha \tau_j^\beta,$$



$$\vec{q}_j = \text{the momentum of the pion exchanged between nucleons i and k}$$

$$F_{ijk}^{\alpha\beta} \equiv \delta^{\alpha\beta}\left[-\frac{4c_1 m_\pi^2}{F_\pi^2} + \frac{2c_3}{F_\pi^2}(\vec{q}_i \bullet \vec{q}_j)\right] + \sum_\gamma \frac{c_4}{F_\pi^2}\varepsilon^{\alpha\beta\gamma} \cdot \tau_k^\gamma \vec{\sigma}_k \bullet (\vec{q}_i \times \vec{q}_j)$$





## The new terms

$$V_{ijk}^{(k);1\pi} \equiv -\sum_{i\neq j\neq k}\left(\frac{g_A}{8F_\pi^2}\right)\left(\frac{c_D}{F_\pi^2 \Lambda_\chi}\right) \times \frac{(\vec{\sigma}_j \bullet \vec{q}_j)}{(\vec{q}_j^{\,2} + m_\pi^2)} \cdot (\boldsymbol{\tau}_i \bullet \boldsymbol{\tau}_j)(\vec{\sigma}_i \bullet \vec{q}_j),$$

$$V_{ijk}^{(k);\text{contact}} \equiv \frac{1}{2}\sum_{i\neq j\neq k}\left(\frac{c_E}{F_\pi^4 \Lambda_\chi}\right)(\boldsymbol{\tau}_j \bullet \boldsymbol{\tau}_k),$$

Some mistakes are corrected following

A. Nogga, P. Navratil, B. R. Barrett, J. P. Vary nucl-th/0511082v1!

$$\Lambda_\chi = 700\text{ MeV},\ g_A = 1.29,\ F_\pi = 92.4\text{ MeV},\ m_\pi = 183.03\text{ MeV},$$

the cutoff for regularization of the 3NF, Λ=500 MeV.

# However, the 3NF has not yet been completely determined!

The low-energy constants, $C_i$'s, included in the 3NF at NNLO, are needed to be determined by structure calculations.

The famous '$A_y$ puzzle' of nucleon-deuteron scattering is not resolved by the 3NF at NNLO.

Thus, one important outstanding issue is the 3NF at $N^3LO$, which is under construction.

R. Machleidt, arXiv:nucl-th/07040807
*Nuclear forces from chiral effective field theory*

**Overall, the nature of the ‘real’ and ‘effective’ three-body forces  remains quite complicated and elusive.**

Fayache, Vary, Barrett, Navratil, Aroua, nucl-th/0112066

*An initio No-Core Shell Model with Many-Body Forces*

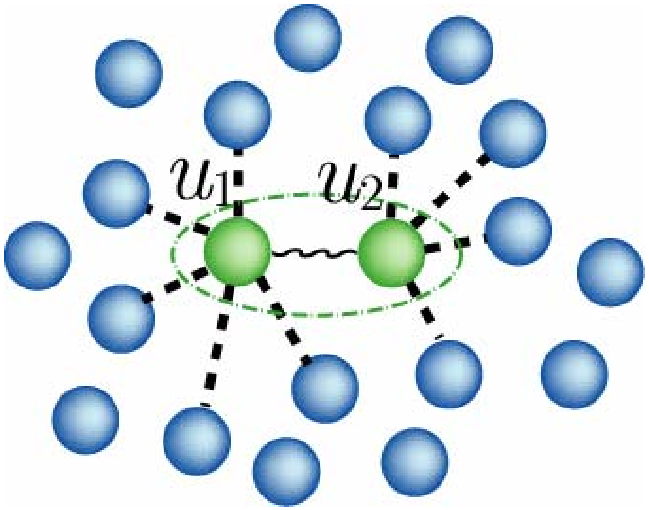
**Need of careful treatment of**

**the ‘real’ and ‘effective’ three-body forces**

# Correlation problems in UMOA

Solving of *subsystem* equations
in an entire many-body system

*Systematically and consistently*




With employing 2NF

n=2

With employing 2NF+3NF

n=2, 3

# 2. Short Review of UMOA with 2NF

**Hamiltonian of a many nucleon system**

**interacting via a nucleon-nucleon interaction**

$$H = \sum_i t_i + \sum_{i<j} v_{ij} = \sum_i (t_i + u_i) + \left[ \sum_{i<j} v_{ij} - \sum_i u_i \right]$$

$$= \sum_i h_i + \left[ \sum_{i<j} v_{ij} - \sum_i u_i \right]; \quad h_i \equiv t_i + u_i$$

$v_{ij}$ : realistic NN int. $\Leftarrow$ AV8, AV18, CD-Bonn, Nijmegen, NLO, $\cdots$

Coulomb int.

**Medium effect**

***$u_i$*: auxiliary, but self-consistently determined potential**

**Anti-hermitian *two-body* correlation operator**

$$S^{(2)} = \sum_{i<j} S_{ij}, \; [S^{(2)\dagger} = -S^{(2)}]$$

**To treat short-range correlation of NN force**

Second quantization form

$$S^{(2)} = \left(\frac{1}{2!}\right)^2 \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | S_{12} | \gamma\delta \rangle \, c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma$$

# Description of correlations in similarity transformation

## Schroedinger eq. for a many-body system

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

$|\Psi_0\rangle$ correlated ground state

$|\Phi_0\rangle$ reference state (uncorrelated state)

**Exponential ansatz**

$$|\Psi_0\rangle = \mathrm{e}^{S^{(2)}}|\Phi_0\rangle \qquad \mathrm{e}^{S^{(2)}} : \text{unitary} \rightarrow S^{(2)\dagger} = -S^{(2)}$$

$$\Rightarrow \mathrm{e}^{-S^{(2)}} H \,\mathrm{e}^{S^{(2)}} \mathrm{e}^{-S^{(2)}} |\Psi_0\rangle = E_0\, \mathrm{e}^{-S^{(2)}} |\Psi_0\rangle$$

$$\Rightarrow [\mathrm{e}^{-S^{(2)}} H \mathrm{e}^{S^{(2)}}]|\Phi_0\rangle = E_0|\Phi_0\rangle$$

# Unitary transformation of Hamiltonian and its cluster expansion

$$\widetilde{H} \equiv e^{-S^{(2)}} H e^{S^{(2)}} \qquad (S^{(2)\dagger} = -S^{(2)})$$

$$= \widetilde{H}^{(1)} + \widetilde{H}^{(2)} + \widetilde{H}^{(3)} + \cdots$$

**Second quantization form**

$$\widetilde{H}^{(1)} \equiv \sum_{\alpha\beta} \langle \alpha | h_1 | \beta \rangle c_\alpha^\dagger c_\beta ,$$

$$\widetilde{H}^{(2)} \equiv \left(\frac{1}{2!}\right)^2 \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \tilde{v}_{12} | \gamma\delta \rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma - \sum_{\alpha\beta} \langle \alpha | u_1 | \beta \rangle c_\alpha^\dagger c_\beta ,$$

$$\widetilde{H}^{(3)} \equiv \left(\frac{1}{3!}\right)^2 \sum_{\alpha\beta\gamma\lambda\mu\nu} \langle \alpha\beta\gamma | \tilde{v}_{123}^{(2)} | \lambda\mu\nu \rangle c_\alpha^\dagger c_\beta^\dagger c_\gamma^\dagger c_\nu c_\mu c_\lambda - \left(\frac{1}{2!}\right)^2 \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \tilde{u}_{12} | \gamma\delta \rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma ,$$

$\cdots\cdots\cdots\cdots\cdots\cdots$ **Non-perturbative, but Correlation expansion**

⟺ Commutator expansion $\widetilde{H} = H + \left[H, S^{(2)}\right] + \frac{1}{2}\left[[H, S^{(2)}], S^{(2)}\right] + \cdots$

# *Two-body* cluster terms

$$\tilde{v}_{12} \equiv \mathrm{e}^{-S_{12}}(h_1 + h_2 + v_{12})\mathrm{e}^{S_{12}} - (h_1 + h_2)$$

or $\mathrm{e}^{-S_{12}} H_{12}\, \mathrm{e}^{S_{12}} = (h_1 + h_2) + \tilde{v}_{12}$

$$H_{12} \equiv h_1 + h_2 + v_{12}$$

Two-body subsystem Hamiltonian

$$\tilde{u}_{12} \equiv \mathrm{e}^{-S_{12}}(u_1 + u_2)\mathrm{e}^{S_{12}} - (u_1 + u_2)$$

**Three-body cluster terms** *induced by the two-body correlations*

$$\tilde{v}_{123}^{(2NF)} \equiv \mathrm{e}^{-S_{123}^{(2)}}(h_1 + h_2 + h_3 + v_{12} + v_{23} + v_{31})\mathrm{e}^{S_{123}^{(2)}} - (h_1 + h_2 + h_3 + \tilde{v}_{12} + \tilde{v}_{23} + \tilde{v}_{31});$$

$$\left[\tilde{v}_{123}^{(2NF)} \to 0 \text{ as } S_{123}^{(2)} \to 0\right]$$

$$S_{123}^{(2)} \equiv S_{12} + S_{23} + S_{31}$$

# Evaluation of Three-body cluster terms

$$\tilde{v}_{123}^{(2NF)} \cong \tilde{v}_{123}^{(v)} + \tilde{v}_{123}^{(h)},$$

$$\tilde{v}_{123}^{(v)} \cong \sum_{(123)} \left\{ [\tilde{v}_{12}, S_{23} + S_{13}] - \tfrac{1}{2}[\tilde{v}_{12}, [S_{12}, S_{23} + S_{13}]] + \tfrac{1}{2}[[\tilde{v}_{12}, S_{23} + S_{13}], S_{23} + S_{13}] \right\} + \cdots$$

$$\tilde{v}_{123}^{(h)} \cong \sum_{(123)} \left\{ \begin{array}{l} -\tfrac{1}{2}[[h_1 + h_2, S_{12}], S_{23} + S_{13}] + \tfrac{1}{6}[[[h_1 + h_2, S_{12}], S_{12}], S_{23} + S_{13}] \\ -\tfrac{1}{3}[[[h_1 + h_2, S_{12}], S_{23} + S_{13}], S_{123}^{(2)}] \end{array} \right\} + \cdots,$$

K. Suzuki and R. Okamoto, Prog. Theor. Phys.**76**, 127(1986)

**Similarly we can evaluate four-body cluster terms.**

# Particle-hole transformation of transformed Hamiltonian

$$\tilde{H} \approx E_0$$

**Ground-state energy**

$$+\sum_{\alpha\beta}\langle\alpha|\tilde{h}|\beta\rangle a^\dagger_\alpha a_\beta - \sum_{\alpha'\beta'}\langle\alpha'|\tilde{h}|\beta'\rangle s'_{\overline{\alpha'}} s'_{\overline{\beta'}} b^\dagger_{\alpha'} b_{\beta'}$$

$$+\sum_{\alpha\beta'}\langle\alpha|\tilde{h}|\beta'\rangle s'_{\overline{\beta'}} a^\dagger_\alpha b^\dagger_{\beta'} + \sum_{\alpha'\beta}\langle\alpha'|\tilde{h}|\beta\rangle s'_{\overline{\alpha'}} b_{\alpha'} a_\beta$$

**Effective one-body Hamiltonian**

$$+\left(\tfrac{1}{2!}\right)^2 \sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\tilde{V}^{(2)}_p|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta$$

$$+\left(\tfrac{1}{2!}\right)^2 \sum_{\alpha'\beta'\gamma'\delta'}\langle\alpha'\beta'|\tilde{V}^{(2)}_h|\gamma'\delta'\rangle s'_{\overline{\alpha'}} s'_{\overline{\beta'}} s'_{\overline{\gamma'}} s'_{\overline{\delta'}} b^\dagger_{\alpha'} b^\dagger_{\beta'} b_{\gamma'} b_{\delta'}$$

$$+\sum_{\alpha\beta'\gamma\delta'}\langle\alpha\beta'|\tilde{V}^{(2)}_{ph}|\gamma'\delta\rangle s'_{\overline{\beta'}} s'_{\overline{\delta'}} a^\dagger_\alpha b^\dagger_{\beta'} b_{\delta'} a_\gamma + \cdots$$

**Effective two-body Hamiltonian**

$$+\left(\tfrac{1}{3!}\right)^2 \sum_{\alpha\beta\gamma\delta}\langle\alpha_1\alpha_2\alpha_3|\tilde{V}^{(3)}_p|\beta_1\beta_2\beta_3\rangle a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} a^\dagger_{\alpha_3} a_{\beta_3} a_{\beta_2} a_{\beta_1}$$

$$+\cdots$$

**Effective three-body Hamiltonian**

# Contributions to Ground-state energy and effective one-, two-, three-body Hamiltonians

## Ground-state energy

$$E_0 = \sum_{\lambda \le \rho_F} \langle \lambda | \tilde{h}_1 | \lambda \rangle - \frac{1}{2!} \sum_{\lambda\mu \le \rho_F} \langle \lambda\mu | \tilde{v}_{12} | \lambda\mu \rangle + \frac{1}{3!} \sum_{\lambda\mu\nu \le \rho_F} \langle \lambda\mu\nu | \tilde{v}_{123} | \lambda\mu\nu \rangle$$

$$- \frac{1}{4!} \sum_{\lambda\mu\nu\phi \le \rho_F} \langle \lambda\mu\nu\phi | \tilde{v}_{1234} | \lambda\mu\nu\phi \rangle \pm \cdots$$

## *Effective* one-body Hamiltonian

$$\langle \alpha | \tilde{h}^{(1)} | \beta \rangle \equiv \langle \alpha | h_1 | \beta \rangle - \sum_{\lambda \le \rho_F} \langle \alpha\lambda | \tilde{v}_{12} | \beta\lambda \rangle + \frac{1}{2!} \sum_{\lambda\mu \le \rho_F} \langle \alpha\lambda\mu | \tilde{v}_{123} | \beta\lambda\mu \rangle$$

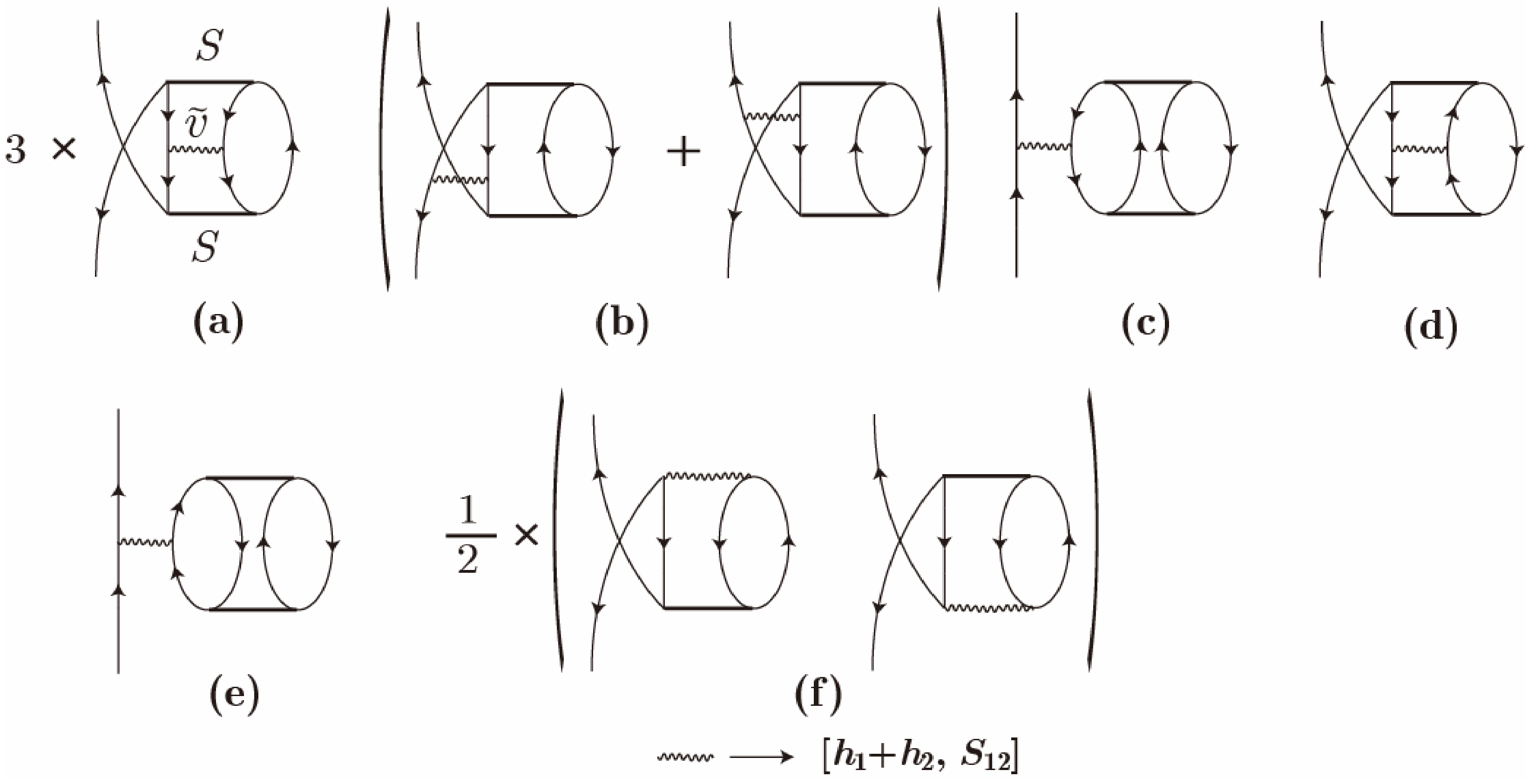
$$- \frac{1}{3!} \sum_{\lambda\mu\nu \le \rho_F} \langle \alpha\lambda\mu\nu | \tilde{v}_{1234} | \beta\lambda\mu\nu \rangle \pm \cdots$$

## *Effective* two-body interaction

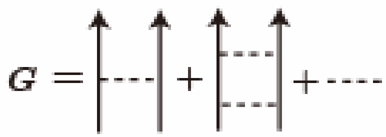
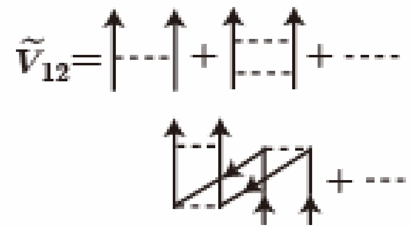
$$\langle \alpha\beta | \widetilde{V}^{(2)} | \gamma\delta \rangle \equiv \langle \alpha\beta | \tilde{v}_{12} | \gamma\delta \rangle - \frac{1}{2!} \sum_{\lambda \le \rho_F} \langle \alpha\beta\lambda | \tilde{v}_{123} | \gamma\delta\lambda \rangle$$

$$+ \frac{1}{3!} \sum_{\lambda\mu \le \rho_F} \langle \alpha\beta\lambda\mu | \tilde{v}_{1234} | \gamma\delta\lambda\mu \rangle \mp \cdots$$

# Contributions of 3-,4-body cluster terms to single particle(hole) Hamiltonian

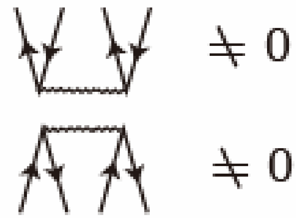
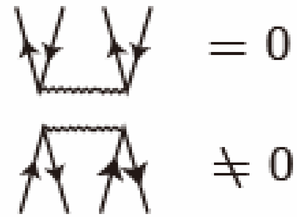
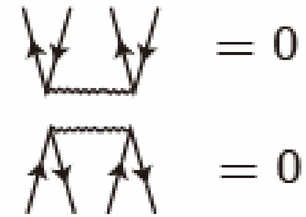
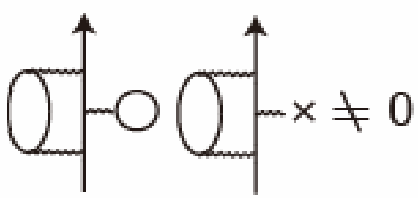
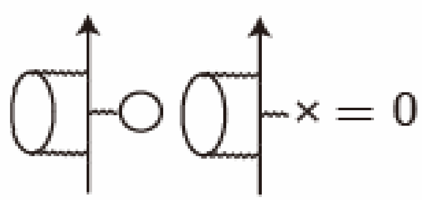
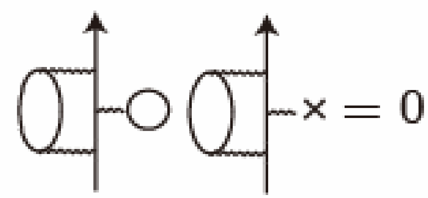
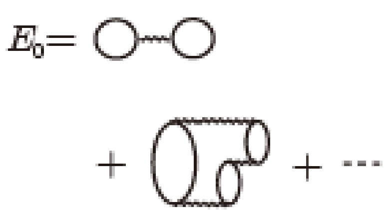
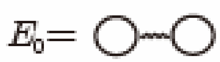
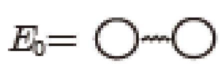


# Comparison of G-matrix, CCM and UMOA (1)

| | $G$-matrix theory | CCM | UMOA |
|---|---|---|---|
| Basic Element | <br>=Sum of Ladders | <br>$=G+G_1G+G_2GG+\cdots$<br>$=G+$Folded diagrams | $W_{12}=G+1/2(G_1G+GG_1)$<br>$+\cdots$<br>=Herimitian counter part of $\tilde{V}_{12}$. |
| Hermitisity | Non-Hermitian (Hermitian if the starting energies are all degenerate) | Non-Herimitian | Herimitian |
| $E$-dependence | $E$-dependent | $E$-independent | $E$-independent |

$$G_n \equiv \frac{1}{n!}\frac{d^nG(\varepsilon)}{d\varepsilon^n}$$

# Comparison of G-matrix, CCM and  UMOA (2)

| | $G$-matrix theory | CCM | UMOA |
|---|---|---|---|
| Decoupling Property | Non-decoupled<br> | Half-decoupled<br> | Decoupled<br> |
| Self-consistency | Generally impossible<br> | Possible<br> | Possible<br> |
| Ground-state energy (Potential energy of a Closed-Shell Core) |  | <br>(No other contributions) | <br>+(Contributions from three-or-more -body Cluster trems) |

# Relation between
# Non-unitary and unitary transformation

$$\widetilde{H} = e^{-\omega} H e^{\omega},\; e^{\omega};\ \text{non-unitary}$$

$$\widetilde{H} = e^{-S^{(2)}} H e^{S^{(2)}},\; e^{S^{(2)}};\ \text{unitary}$$

**Relation between wave operator and correlation operator**

$$S^{(2)} = \operatorname{arctanh}(\omega^{(2)} - \omega^{(2)\dagger})$$


I. Shavitt, L.T. Redman, J. Chem. Phys. **73**(1980), 5711

P. Westhouse, J. Quantum Chem.20(1981), 1243.

K. Suzuki, Prog.Theor.Phys.**68**(1982),246

# Decoupling equation and its general solution

$$\left|\psi_k\right\rangle = \mathrm{e}^{\omega}\left|\phi_k\right\rangle, k = 1, 2, \cdots, d$$

$$\omega = Q\omega P \rightarrow \omega^2 = 0$$

$$Q \cdot \mathrm{e}^{-\omega} H \mathrm{e}^{\omega} \cdot P = 0,\ H = H_0 + V, H_0 = PH_0P + QH_0Q$$

$$\rightarrow QVP + QHQ\omega - \varpi PHP - \omega PVQ\omega = 0$$

$$\omega = \sum_{k=1}^{d} Q\left|\psi_k\right\rangle\left\langle\tilde{\phi}_k\right|P$$

# Matrix elements of $U \equiv \mathrm{e}^S$

$$U = (1+\omega-\omega^\dagger)(1+\omega\omega^\dagger+\omega^\dagger\omega)^{-1/2}$$

$$\omega^\dagger\omega\left|\alpha_k\right\rangle = \mu_k^2\left|\alpha_k\right\rangle, \left|\nu_k\right\rangle \equiv \frac{1}{\mu_k}\omega\left|\alpha_k\right\rangle; k=1,2,\cdots,d$$

For $\left|p\right\rangle \in \mathrm{P}, \left|q\right\rangle \in \mathrm{Q}$

$$\left\langle p'|U|p\right\rangle = \sum_{k=1}^{d}(1+\mu_k^2)^{-1/2}\left\langle p'|\alpha_k\right\rangle\left\langle\alpha_k|p\right\rangle,$$

$$\left\langle q|U|p\right\rangle = \sum_{k=1}^{d}(1+\mu_k^2)^{-1/2}\mu_k\left\langle q|\nu_k\right\rangle\left\langle\alpha_k|p\right\rangle,$$

$$\left\langle p|U|q\right\rangle = -\sum_{k=1}^{d}(1+\mu_k^2)^{-1/2}\mu_k\left\langle p|\alpha_k\right\rangle\left\langle\nu_k|q\right\rangle,$$

$$\left\langle q'|U|q\right\rangle = \sum_{k=1}^{d}\left\{(1+\mu_k^2)^{-1/2}-1\right\}\left\langle q'|\nu_k\right\rangle\left\langle\nu_k|q\right\rangle + \delta_{q'q}.$$

# Determination of two-body correlation operator

**Projection operators in two-body state space**

$$P^{(2)}+Q^{(2)}=1,\ {P^{(2)}}^2=P^{(2)},{Q^{(2)}}^2=Q^{(2)},P^{(2)}Q^{(2)}=Q^{(2)}P^{(2)}=0$$

**Eigen value equation for the two-body sub-system in an entire many-body system**

$$H_{12}\equiv h_1+h_2+v_{12},$$

$$H_{12}\left|\psi_k^{(2)}\right\rangle=E_k^{(2)}\left|\psi_k^{(2)}\right\rangle,\quad (k=1,2,\cdots,d,d+1,\cdots,n)$$

$$\left|\psi_k^{(2)}\right\rangle=\left(P^{(2)}+Q^{(2)}\right)\left|\psi_k^{(2)}\right\rangle=\left|\phi_k^{(2)}\right\rangle+\omega^{(2)}\left|\phi_k^{(2)}\right\rangle,(k=1,2,\cdots,d)$$

$$\left|\phi_k^{(2)}\right\rangle\equiv P^{(2)}\left|\psi_k^{(2)}\right\rangle,\ Q^{(2)}\left|\psi_k^{(2)}\right\rangle=\omega^{(2)}\left|\phi_k^{(2)}\right\rangle$$

**General solution for the wave operator**

$$\left\langle\psi_k^{(2)}\,|\,\psi_{k'}^{(2)}\right\rangle=\delta_{kk'}$$

$$\omega^{(2)}=\sum_{k=1}^{d}Q^{(2)}\left|\psi_k^{(2)}\right\rangle\left\langle\tilde{\phi}_k^{(2)}\right|P^{(2)}$$

$$\because\left\langle\tilde{\phi}_k^{(2)}\middle|\phi_{k'}^{(2)}\right\rangle=\delta_{kk'},\left|\tilde{\phi}_k^{(2)}\right\rangle:\text{bi-orthogonal state}$$

# Decoupling equation in two-body subsystem

**Decoupling equation** for transformed Hamiltonian of two-body subsystem

$$Q^{(2)} e^{-S_{12}} H_{12} e^{S_{12}} P^{(2)} = 0$$

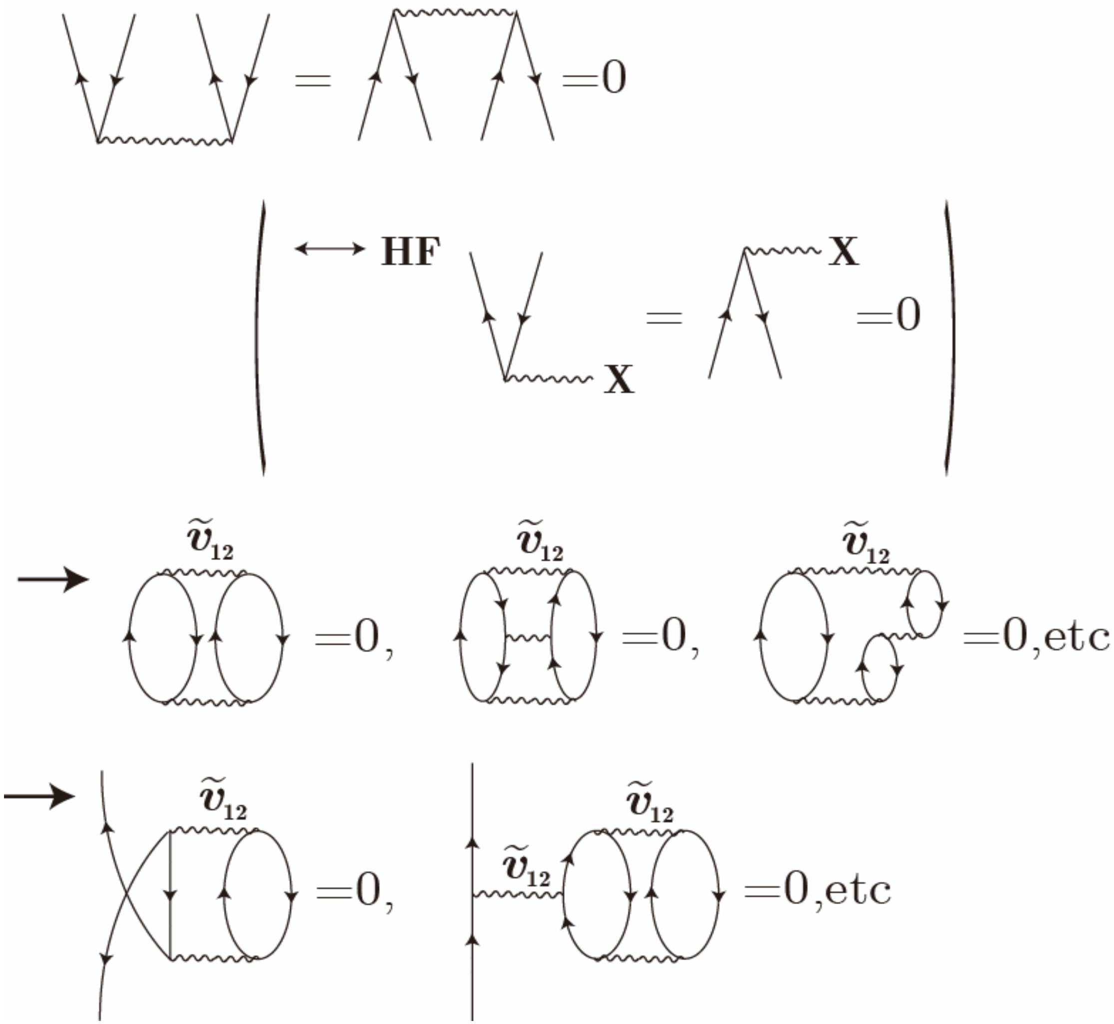
$$\rightarrow Q^{(2)} (h_1 + h_2 + \tilde{v}_{12}) P^{(2)} = 0$$

$$\text{if } Q^{(2)} (h_1 + h_2) P^{(2)} = 0, \quad \text{then}$$

$$Q^{(2)} \tilde{v}_{12} P^{(2)} = 0$$

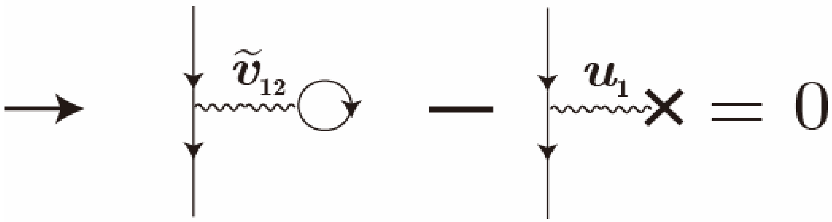
# Decoupling property of “effective two-body” interaction

$$Q\tilde{v}_{12}P = P\tilde{v}_{12}Q = 0$$

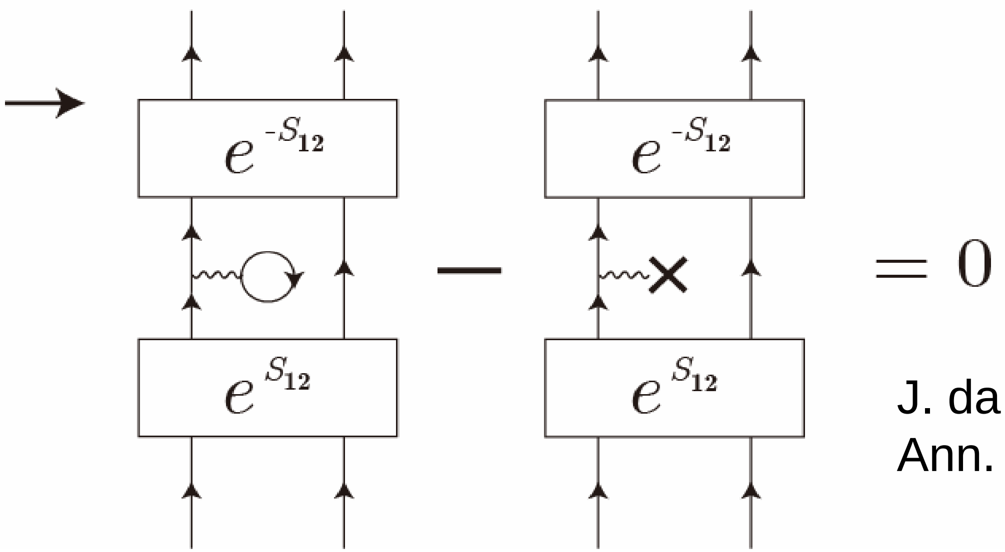


# Self-consistency between single-particle potential and "two-body effective interaction"(two-body cluster terms)

$$\langle \alpha | u_1 | \beta \rangle = \sum_{\lambda \leqq \rho_F} \langle \alpha\lambda | \tilde{v}_{12} | \beta\lambda \rangle$$




cancellation of one-body and bubble-diagram contribution




J. da Providencia and C. M. Shakin, Ann. Phys.**30**(1964), 95.

# How to choose *P* and *Q* spaces?

The one-body hamiltonian $h_i$ contains self-consistent potential $u_i$,

and determination of $Q(u_1+u_2)Q$ has been considered

to be very difficult, because there is

**no prescription for calculating matrix elements of $u_i$**

**between states with very high momentum**.

⇓

**We should choose *P* and *Q* as spaces**

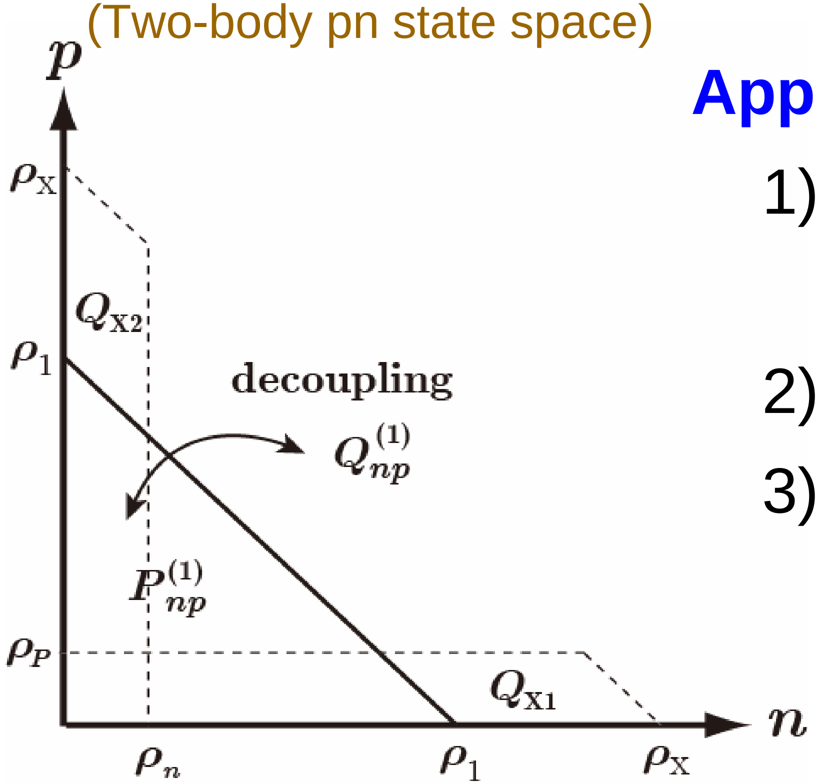
**which are well separated in energy**

**in order to make the mixing between P and Q spaces**

**small as long as possible.**

# **Two-step** determination of the "effective interactions"

## First-step decoupling




$$P^{(\mathrm{I})} \equiv P_{pn}^{(1)}, Q^{(\mathrm{I})} \equiv Q_{pn}^{(1)}, \tilde{v}_{12}^{(\mathrm{I})} \equiv \tilde{v}_{12}^{(1)}$$

$$\rho = 2n_a + \ell_a + 2n_b + \ell_b$$

$$\rho_1 = 16, 18$$

**Efficient calculation of effects of high-momentum states**

**Approximate decoupling** ;

1) average over $j_a, L_{\mathrm{CM}}$ in two-body relative-CM system
2) diagonal in CM q.n.
3) $u_1$= 0 for Q $^{(\mathrm{I})}$ space

$$\langle \alpha | u_1^{(\mathrm{I})} | \beta \rangle \to 0 \text{ for when } 2n_\alpha + \ell_\alpha + 2n_\lambda + \ell_\lambda > \rho_1$$

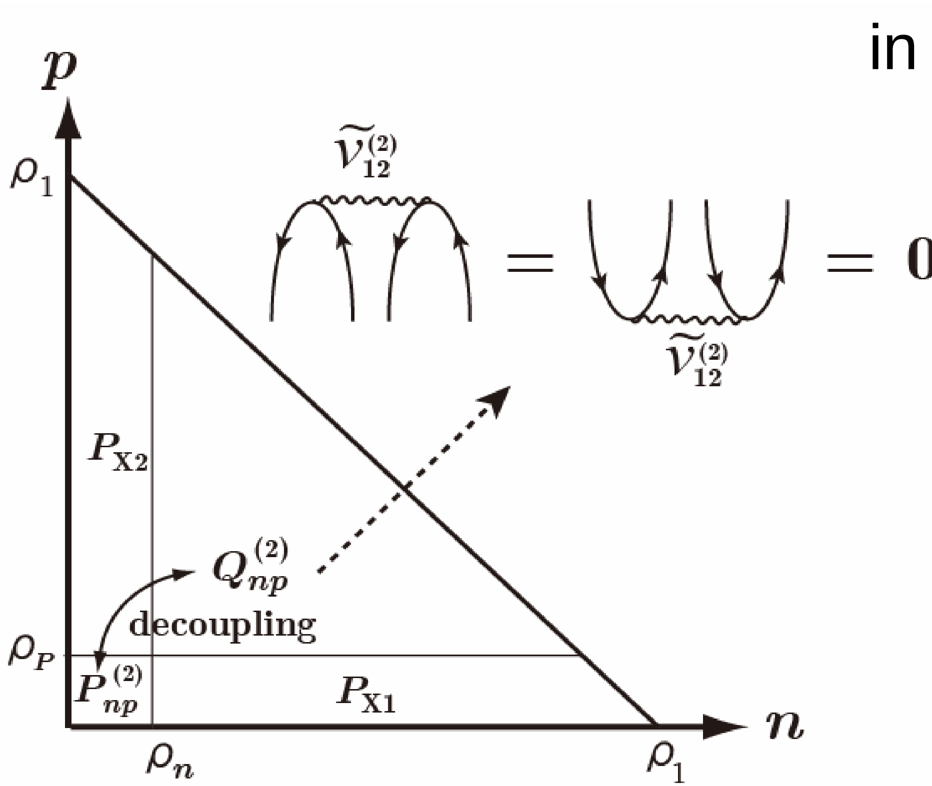
$$\text{or} \quad 2n_\beta + \ell_\beta + 2n_\lambda + \ell_\lambda > \rho_1$$

$$H_{12}^{(\mathrm{I})} = t_1 + (u_1^{(\mathrm{I})}) + t_2 + (u_2^{(\mathrm{I})}) + v_{12}$$

$$\to S^{(\mathrm{I})} \to \tilde{v}_{12}^{(\mathrm{I})}$$

$$\widetilde{H}^{(\mathrm{I})} \equiv e^{-S^{(\mathrm{I})}} H e^{S^{(\mathrm{I})}}$$

# Second-step decoupling




$$P^{(II)} \equiv P_{pn}^{(2)}, Q^{(II)} \equiv Q_{pn}^{(2)}, \tilde{v}_{12}^{(II)} \equiv \tilde{v}_{12}^{(2)}$$

## Exact decoupling

in two-body shell-model basis

$$H_{12}^{(II)} = t_1 + u_1^{(II)} + t_2 + u_2^{(II)} + \tilde{v}_{12}^{(I)}$$

$$\rightarrow S^{(II)} \rightarrow \tilde{v}_{12}^{(II)}$$

$$\widetilde{H}^{(II)} \equiv e^{-S^{(II)}} \widetilde{H}^{(I)} e^{S^{(II)}}$$

# Procedure of selfconsistent calculation

$$\langle \alpha \mid u_1^{(n)} \mid \beta \rangle = \sum_{\lambda \le \rho_F} \langle \alpha\lambda \mid \tilde{v}_{12}^{(n-1)} \mid \beta\lambda \rangle$$

$$H_{12}^{(n)} = t_1 + u_1^{(n)} + t_2 + u_2^{(n)} + v_{12}$$

$$S_{12}^{(n)} \rightarrow \tilde{v}_{12}^{(n)} \rightarrow \langle \alpha \mid u_1^{(n+1)} \mid \beta \rangle = \sum_{\lambda \le \rho_F} \langle \alpha\lambda \mid \tilde{v}_{12}^{(n)} \mid \beta\lambda \rangle$$

$$H_{12}^{(n+1)} = t_1 + u_1^{(n+1)} + t_2 + u_2^{(n+1)} + v_{12}$$

**Generate selfconfining pot. $u_1$**

# Effects of the three-body cluster terms

Sizable contribution to the ground-state energy
Convergence of cluster expansion

**In theory, unitarily transformation does not terminate in its expansion series.**

**In the actual calculations, however,**

$$E_0 = E_0^{(2BC)} + \Delta E_0^{(3BC)} + \cdots;$$

$$\rightarrow \left| \frac{\Delta E_0^{(3BC)}}{E_0^{(2BC)}} \right| \times 100 \approx 1.5\,(\%)$$

***almost converges***

Not always so for relative single particle energies

**Reducing of the dependence of the calculated results on $\hbar\omega$ of employed s.p. H.O. basis**

**A significant effect in reproducing the correct nuclear size**

K.Suzuki, R. Okamoto, Prog. Theor. Phys.76(1986),127-142.

For calculated results

see Dr. Fujii' s talk ,

Thursday, September 27, 2007

http://www.int.washington.edu/talks/WorkShops/int_07_3/

# 3.Formulation of UMOA with 2NF and 3NF

Brief description was given in
K. Suzuki, Prog. Theor. Phys.79 (1998), 330.

## Hamiltonian with 2NF and 3NF

$$H = \sum_i t_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk} = \sum_i (t_i + u_i) + \left[ \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk} - \sum_i u_i \right]$$

$$= \sum_i h_i + \left[ \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk} - \sum_i u_i \right]; \quad h_i \equiv t_i + u_i$$

$$\left( v_{ij}, v_{ijk} \right)$$ ⟸ **Chiral Nuclear Force**

↑

**Genuine three-nucleon force(3NF)**

**Three-body sub-system Hamiltonian**

$$H_{123} \equiv (h_1 + h_2 + h_3) + (v_{12} + v_{23} + v_{31}) + v_{123},$$

**Three-body subsystem Hamiltonian *dressed with two-body correlations***

**in an entire many-body system**

$$\widetilde{H}_{123} \equiv \mathrm{e}^{-S_{123}^{(2)}} H_{123}\, \mathrm{e}^{S_{123}^{(2)}}$$

$$= (h_1 + h_2 + h_3) + (\tilde{v}_{12} + \tilde{v}_{23} + \tilde{v}_{31}) + \tilde{v}_{123}^{(2)},$$

$$\tilde{v}_{123}^{(2)} \equiv \mathrm{e}^{-S_{123}^{(2)}} (h_1 + h_2 + h_3 + v_{12} + v_{23} + v_{31} + v_{123}) \mathrm{e}^{S_{123}^{(2)}}$$

$$- (h_1 + h_2 + h_3 + \tilde{v}_{12} + \tilde{v}_{23} + \tilde{v}_{31});$$

$$\Rightarrow \tilde{v}_{123}^{(2)} = \tilde{v}_{123}^{(2NF)} + \mathrm{e}^{-S_{123}^{(2)}} v_{123} \mathrm{e}^{S_{123}^{(2)}}; \quad S_{123}^{(2)} \equiv S_{12} + S_{23} + S_{31}$$

$$\left[ \tilde{v}_{123}^{(2)} \rightarrow v_{123} \text{ as } S_{123}^{(2)} \rightarrow 0 \right]$$

***three-body interaction induced by the two-body correlations***

**three-body interaction *dressed with the two-body correlations***

# Calculation of three-body correlation operator

**Projection operators in three-body state space**

$$P^{(3)} + Q^{(3)} = 1,\ P^{(3)^2} = P^{(3)},\ Q^{(3)^2} = Q^{(3)},\ P^{(3)}Q^{(3)} = Q^{(3)}P^{(3)} = 0$$

**Solution for the three-body subsystem Hamiltonian**

$$\boxed{\widetilde{H}_{123}\left|\psi_k^{(3)}\right\rangle = E_k^{(3)}\left|\psi_k^{(3)}\right\rangle}, \quad (k = 1, 2, \cdots, d^{(3)}, d^{(3)}+1, \cdots, n^{(3)})$$

$$\left|\psi_k^{(3)}\right\rangle = \left(P^{(3)} + Q^{(3)}\right)\left|\psi_k^{(3)}\right\rangle = \left|\phi_k^{(3)}\right\rangle + \omega^{(3)}\left|\phi_k^{(3)}\right\rangle, \ (k = 1, 2, \cdots, d^{(3)})$$

$$\left|\phi_k^{(3)}\right\rangle \equiv P^{(3)}\left|\psi_k^{(3)}\right\rangle, \ Q^{(3)}\left|\psi_k^{(3)}\right\rangle = \omega^{(3)}\left|\phi_k^{(3)}\right\rangle$$

$$\left\langle \psi_k^{(3)} \mid \psi_{k'}^{(3)}\right\rangle = \delta_{kk'}$$

**General solution for the wave operator**

$$\omega^{(3)} = \sum_{k=1}^{d^{(3)}} Q^{(3)}\left|\psi_k^{(3)}\right\rangle\left\langle\tilde{\phi}_k^{(3)}\right| P^{(3)} \quad \because \left\langle\tilde{\phi}_k^{(3)}\middle|\phi_{k'}^{(3)}\right\rangle = \delta_{kk'}, \left|\tilde{\phi}_k^{(3)}\right\rangle : \text{bi-orthogonal state}$$

**Relation between mapping operator and correlation operator**

$$S^{(3)} = \operatorname{arctanh}(\omega^{(3)} - \omega^{(3)^\dagger})$$

# Transformed Hamiltonian in terms of three-body correlations

$$\widetilde{\widetilde{H}} \equiv e^{-S^{(3)}} \widetilde{H} e^{S^{(3)}} = e^{-S^{(3)}} [e^{-S^{(2)}} H e^{S^{(2)}}] e^{S^{(3)}}$$

If $S^{(2)\dagger} = -S^{(2)}$ and $S^{(3)\dagger} = -S^{(3)\dagger}$, then $\left\{\exp\left[S^{(2)} + S^{(3)}\right]\right\}^{\dagger} = \exp\left[-S^{(2)} - S^{(3)}\right]$,

but

$$\left\{\exp\left[S^{(2)} + S^{(3)}\right]\right\}^{\dagger} \exp\left[S^{(2)} + S^{(3)}\right] = \exp\left[-S^{(2)} - S^{(3)}\right] \exp\left[S^{(2)} + S^{(3)}\right]$$

$$\neq 1 \quad \left(\because [S^{(2)}, S^{(3)}] \neq 0\right)$$

## Anti-hermitian *three-body* correlation operator

$$S^{(3)} = \sum_{i<j<k} S_{ijk} \, , [S^{(3)\dagger} = -S^{(3)}]$$

Second quantization form

$$S^{(3)} = \left(\frac{1}{3!}\right)^2 \sum_{\alpha\beta\gamma\lambda\mu\nu} \langle \alpha\beta\gamma \,|\, S_{123} \,|\, \lambda\mu\nu \rangle \, c_\alpha^\dagger c_\beta^\dagger c_\gamma^\dagger c_\nu c_\mu c_\lambda$$

# Decoupling equation for transformed Hamiltonian of three-body subsystem

$$Q^{(3)} \cdot \mathrm{e}^{-S_{123}} \widetilde{H}_{123} \, \mathrm{e}^{S_{123}} \cdot P^{(3)} = 0$$

$$\rightarrow Q^{(3)} \cdot \mathrm{e}^{-S_{123}} \left[ (h_1 + h_2 + h_3) + (\tilde{v}_{12} + \tilde{v}_{23} + \tilde{v}_{31}) + \tilde{v}_{123}^{(2)} \right] \mathrm{e}^{S_{123}} \cdot P^{(3)} = 0$$

If

$$Q^{(3)}(h_1 + h_2 + h_3)P^{(3)} = Q^{(3)}(\tilde{v}_{12} + \tilde{v}_{23} + \tilde{v}_{31})P^{(3)} = 0,$$

$$Q^{(3)} \tilde{v}_{123}^{(2)} \, P^{(3)} = 0$$

# Three-body cluster terms

***from 2NF and 3NF***

$$\tilde{v}_{123} \equiv e^{-S_{123}} \left[ e^{-S_{123}^{(2)}} (h_1 + h_2 + h_3 + v_{12} + v_{23} + v_{31} + v_{123}) e^{S_{123}^{(2)}} \right] e^{S_{123}}$$

$$- (h_1 + h_2 + h_3 + \tilde{v}_{12} + \tilde{v}_{23} + \tilde{v}_{31})$$

$$= e^{-S_{123}} \left[ \tilde{v}_{123}^{(2)} + (h_1 + h_2 + h_3 + \tilde{v}_{12} + \tilde{v}_{23} + \tilde{v}_{31}) \right] e^{S_{123}}$$

$$- (h_1 + h_2 + h_3 + \tilde{v}_{12} + \tilde{v}_{23} + \tilde{v}_{31})$$

$$\therefore \tilde{v}_{123} = e^{-S_{123}} \left[ \left\{ \tilde{v}_{123}^{(2NF)} + e^{-S_{123}^{(2)}} v_{123} e^{S_{123}^{(2)}} \right\} + (h_1 + h_2 + h_3 + \tilde{v}_{12} + \tilde{v}_{23} + \tilde{v}_{31}) \right] e^{S_{123}}$$

$$- (h_1 + h_2 + h_3 + \tilde{v}_{12} + \tilde{v}_{23} + \tilde{v}_{31}),$$

**three-body cluster terms *induced by the two-body correlations***

$$\left[ \tilde{v}_{123} \to \tilde{v}_{123}^{(2NF)} + e^{-S_{123}^{(2)}} v_{123} e^{S_{123}^{(2)}} \quad \text{as } S_{123} \to 0 \right]$$

**three-body cluster terms induced by three-body correlations, and *dressed with the two-body correlations***

# Effective Two-body interaction matrix element derived from 2NF and 3NF

**2NF** 3NF

$$\left\{ \tilde{V}_{123}^{(2NF)} + e^{-S_{123}^{(2)}} v_{123} e^{S_{123}^{(2)}} \right\}$$

$$\left\langle \alpha\beta \middle| \tilde{V}^{(2)} \middle| \gamma\delta \right\rangle \equiv \left\langle \alpha\beta \middle| \tilde{v}_{12} \middle| \gamma\delta \right\rangle - \frac{1}{2!} \sum_{\lambda \le \rho_F} \left\langle \alpha\beta\lambda \middle| \tilde{v}_{123} \middle| \gamma\delta\lambda \right\rangle$$

???

$\tilde{V}_{123}^{(2NF)}$ **Significant effects in reproducing the correct nuclear size ( in $^{16}O$ )**

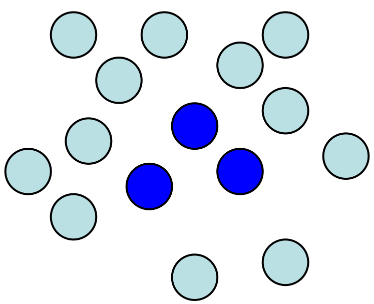
***Microscopic origin* of**

**Effective NN interaction with density dependence**

# 4. Calculation procedure

**Solving of eigenvalue eq. for three-body *subsystem***
**in an finite many-body system**

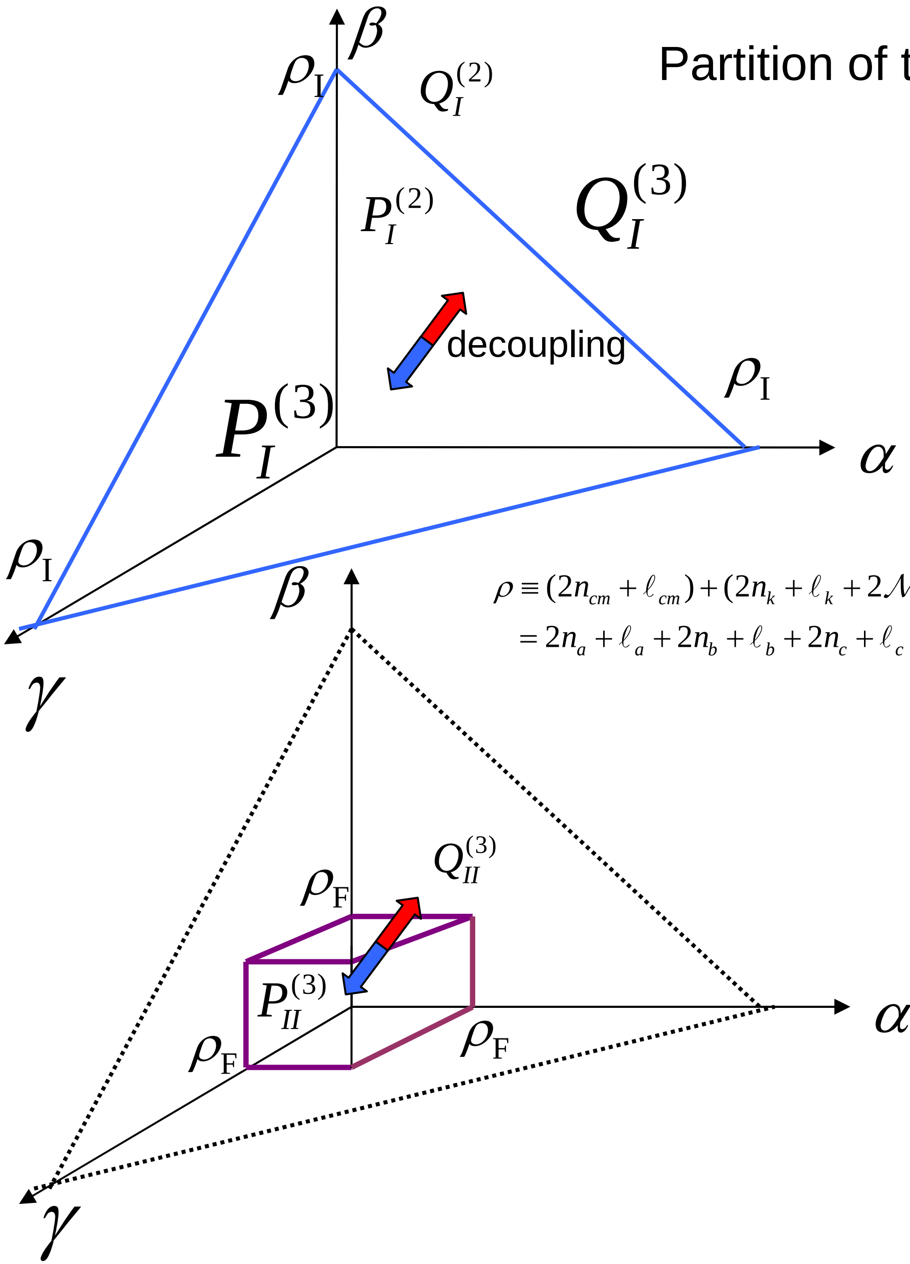
$$\left[(h_1+h_2+h_3)+(\tilde{v}_{12}+\tilde{v}_{23}+\tilde{v}_{31})+\tilde{v}^{(2)}_{123}\right]\left|\psi^{(3)}_{nIMTM_t}\right\rangle = E^{(3)}_{nIT}\left|\psi^{(3)}_{nIMTM_t}\right\rangle$$



$$h_i = t_i + u_i, \quad (i = 1, 2, 3)$$

$\Longleftrightarrow$ Three-nucleon problem in *free space*

# Two-step decoupling calculation




Partition of three-nucleon state space $\{|\alpha\beta\gamma\rangle\}$

$$\rho \equiv (2n_{cm}+\ell_{cm})+(2n_k+\ell_k+2\mathcal{N}_k+\mathcal{L}_k)$$
$$=2n_a+\ell_a+2n_b+\ell_b+2n_c+\ell_c$$

**First-step decoupling**

Approximate decoupling

*cm.-diagonal approximation,…*

**Second-step decoupling**

precise decoupling

in shell-model states

To evaluate Pauli principle effects

precisely as long as possible

# First step decoupling

**Diagonalization of three-body subsytem Hamiltonian**

**in CM-intrinsic basis vector**

↓

**Construction of intrinsic basis vector**
**in terms of Jacobi coordinate basis**
**in Harmonic oscillator**
**and its antisymmetrization**

# Normalized, but *non-antisymmetrized* three-body state in angular momentum coupling for Harmonic oscillator basis

$$|\alpha) \equiv | n_a \ell_a j_a m_\alpha m_\alpha^t), \; a \equiv \{n_a \ell_a j_a m_\alpha^t\}$$

$$|\alpha\beta\gamma) \equiv | n_a \ell_a j_a m_\alpha m_\alpha^t, n_b \ell_b j_b m_\beta m_\beta^t, n_c \ell_c j_c m_\lambda m_\gamma^t)$$

$$|[ab]_{J_{ab}T_{ab}} c)_{IM_I TM^t} \equiv \sum_{m_\alpha, m_\beta, m_\gamma, M_{ab}, \tau_\alpha, \tau_\beta, \tau_\gamma, M_{ab}^t} \langle \alpha\beta | J_{ab} T_{ab} \rangle \langle J_{ab} T_{ab} \gamma | IT \rangle$$

$$\times | n_a \ell_a j_a m_\alpha m_\alpha^t, n_b \ell_b j_b m_\beta m_\beta^t, n_c \ell_c j_c m_\gamma m_\gamma^t)$$

$$= \sum_{m_\alpha, m_\beta, m_\gamma, M_{ab}, \tau_\alpha, \tau_\beta, \tau_\gamma, M_{ab}^t} \langle \alpha\beta | J_{ab} T_{ab} \rangle \langle J_{ab} T_{ab} \gamma | IT \rangle \bullet | \alpha\beta\gamma),$$

$$\rightarrow | \alpha\beta\gamma) = \sum_{J_{ab}, T_{ab}, I} \langle \alpha\beta | J_{ab} T_{ab} \rangle \langle J_{ab} T_{ab} \gamma | IT \rangle \bullet | [ab]_{J_{ab}T_{ab}} c)_{IM_I TM^t},$$

where

$$\langle \alpha\beta | J_{ab} T_{ab} \rangle \langle J_{ab} T_{ab} \gamma | IT \rangle$$

$$\equiv \left\langle j_a m_\alpha j_b m_\beta | J_{ab} M_{ab} \right\rangle \left\langle J_{ab} M_{ab} j_c m_\gamma | IM_I \right\rangle$$

$$\times \left\langle \tfrac{1}{2} m_\alpha^t \, \tfrac{1}{2} m_\beta^t | T_{ab} M_{Tab} \right\rangle \left\langle T_{ab} M_{Tab} \, \tfrac{1}{2} m_\gamma^t | TM^t \right\rangle$$

$$(\alpha\beta\gamma | [ab]_{J_{ab}T_{ab}} c)_{IM_I TM^t} = \left\langle \alpha\beta | J_{ab} T_{ab} \right\rangle \left\langle J_{ab} T_{ab|} \gamma | IM_I TM^t \right\rangle$$

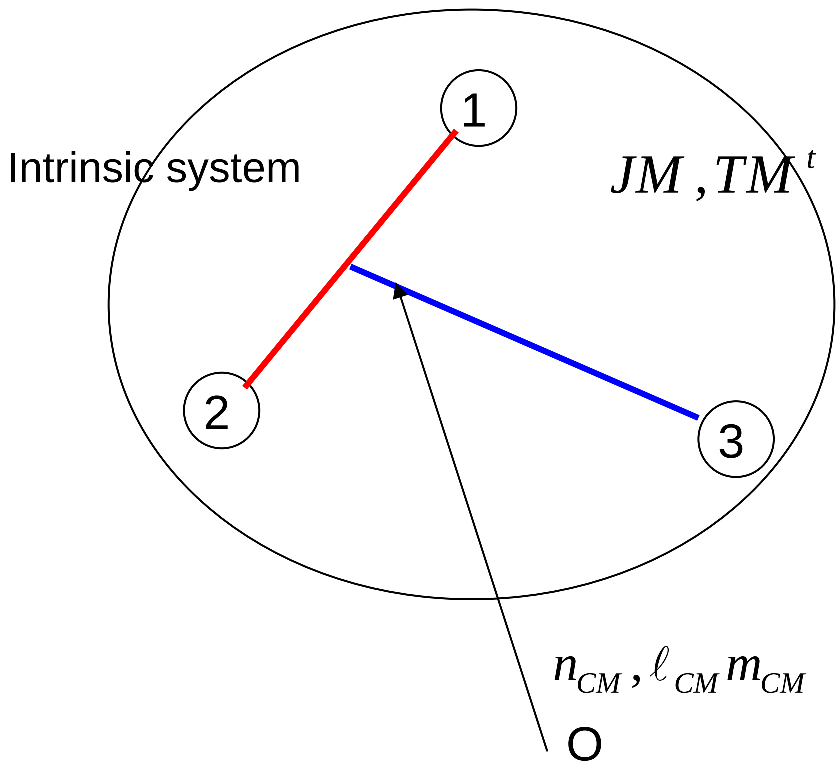
# Three-body state in total system(=CM- and *intrinsic* system) with angular momentum coupling

N; total quantum number *of intrinsic system*

$$\left|abc:[n_{CM}\ell_{CM}][NJTi]IM_I M^t\right\rangle$$

$$=\sum_{m_{CM},M}\left\langle \ell_{CM} m_{CM} JM \mid IM_I\right\rangle \left|abc:[n_{CM}\ell_{CM} m_{CM}]\right\rangle \left|abc:[NJMTi]\right\rangle,$$

$$\left\langle n_{CM}\ell_{CM} m_{CM} \mid n'_{CM}\ell'_{CM} m'_{CM}\right\rangle = \delta(n_{CM} n'_{CM})\,\delta(\ell_{CM}\ell'_{CM})\,\delta(m_{CM}, m'_{CM})$$




Total angular momentum *of the total system*

$$IM_I, TM^t$$

# Jacobi basis for intrinsic system of a three body system

$$|A_{k=3}) \equiv |[n_3\ell_3 j_3 s_3 t_3; \mathcal{N}_3\mathcal{L}_3\mathcal{J}_3]JT);$$

where $|n_3\ell_3 j_3 s_3 t_3\rangle$ is anti-symmetric; $(-)^{\ell_3+s_3+t_3} = -1$

Completeness of the Jacobi bases

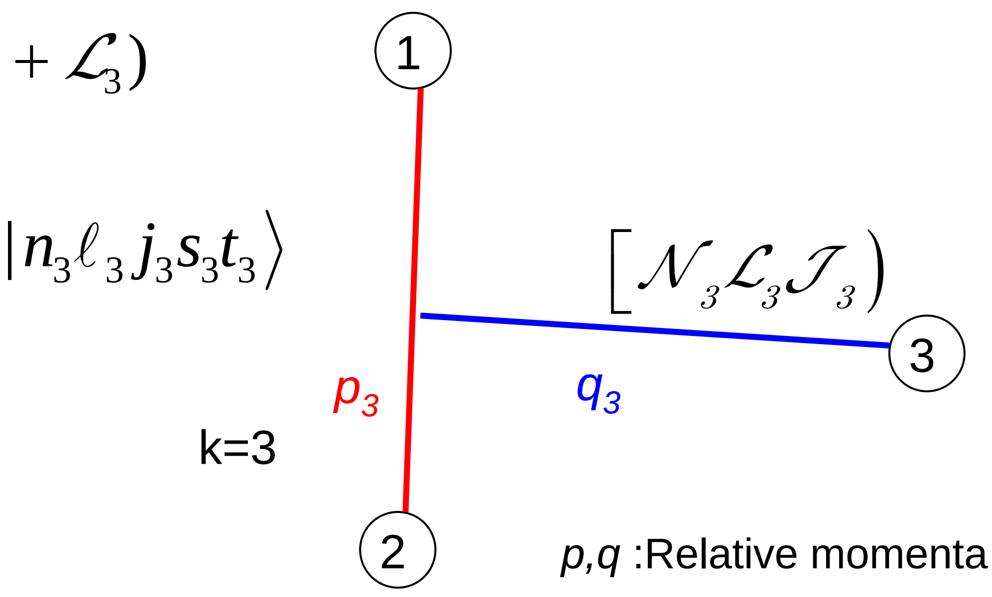
$$\sum_{A_k} |A_k)(A_k| = \hat{1} \quad (k = 1, \text{or}, 2, \text{or}, 3\ )$$

Total angular momentum *for intrinsic system*

Total quantum number *for intrinsic system*

Intrinsic system $N, JM, TM^t$

$$N \equiv (2n_3 + \ell_3) + (2\mathcal{N}_3 + \mathcal{L}_3)$$




*p,q* :Relative momenta

# Construction of an intrinsic state for (totally anti-symmetric) three-body state in terms of Jacobi basis

$$\left| NJMTM^t i \right\rangle = \sum_{A_k} | A_k MM^t)(A_k MM^t \left| NJMTM^t i \right\rangle$$

$$= \sum_{A_k} C_{A_k i} \, | A_k MM^t) = \sum_{A_k} C_{A_k i} \, | A_{k=3} MM^t),$$

$$| A_{k=3}) \equiv | [n_3 \ell_3 j_3 s_3 t_3; \mathcal{N}_3 \mathcal{L}_3 \mathcal{J}_3 ] JT)$$

$$C_{A_k i} \equiv (A_k \left| NJTi \right\rangle ; N \equiv (2n_3 + \ell_3) + (2\mathcal{N}_3 + \mathcal{L}_3)$$

$$k = 3; C_{A_3 i} = (n_3 \ell_3 j_3 s_3 t_3; \mathcal{N}_3 \mathcal{L}_3 \mathcal{J}_3 ]JT \left| NJTi \right\rangle;$$

↑

$(k = 1, \text{or}, 2, \text{or}, 3\ )$

( a kind of) coefficient of fractional parentage

$C_{A_k i}$ is obtained by diagonalizing the anti-symmetrizer in the Jacobi basis |A).

The $i$ labels different intrinsic-system state with the same quantum number set {N,J,T}

# CFP in three-nucleon state in *total system*

The intrinsic motion is augmented by c.m. H.O. basis state, |*ncm,lcm*), which couple to a total angular momentum $I\ M_I$.

$$\left\{ \left| n_{cm} \ell_{cm} \right) \left| NJTi \right\rangle \right\}_{IM_I}$$

Analogously the Jacobi state $|A_k)$ are augmented by C.M. states. Note that the c.f.p.'s are *m*-independent. Therefore the c.f.p.'s are identical in the total and intrinsic basis as

$$C_{A_k i} = \left\{ \left( n_{cm} \ell_{cm} \right| \left\langle A_k \right| \right\}_I \left\{ \left| n_{cm} \ell_{cm} \right) \left| NJTi \right\rangle \right\}_I$$

# Three-body state for total system in *m*-scheme coupling

$$\left|\alpha\beta\gamma\right\rangle = \sum \left\langle \alpha\beta \mid J_{12}t_{12}\right\rangle \left\langle J_{12}t_{12}\gamma \mid IT\right\rangle \left|(ab)J_{12}t_{12},c\right\rangle_{IMTM^t}$$

$$= \sum \left\langle \alpha\beta \mid J_{12}t_{12}\right\rangle \left\langle J_{12}t_{12}\gamma \mid IT\right\rangle \cdot {}_I\left\langle (n_{cm}\ell_{cm})A_k \left|(ab)J_{12}t_{12},c\right\rangle_I \left|(n_{CM}\ell_{CM})A\right\rangle_{IMTM^t}$$

$$= \sum \left\langle \alpha\beta \mid J_{12}t_{12}\right\rangle \left\langle J_{12}t_{12}\gamma \mid IT\right\rangle \left\langle \ell_{cm}m_{cm}JM_J \mid IM\right\rangle$$

$$\times {}_I\left\langle (n_{cm}\ell_{cm} \mid \left\langle A_k \right|(ab)J_{12}t_{12},c\right\rangle_I \cdot \left|n_{cm}\ell_{cm}m_{cm}\right\rangle \times C_{A_k i} \cdot \left|NJM_J TM^t i\right\rangle$$

$$= \sum \left\langle \alpha\beta \mid J_{12}t_{12}\right\rangle \left\langle J_{12}t_{12}\gamma \mid IT\right\rangle \left\langle \ell_{cm}m_{cm}JM_J \mid IM\right\rangle$$

$$\times {}_I\left\langle (n_{cm}\ell_{cm} \mid \left\langle A_k \right|(ab)J_{12}t_{12},c\right\rangle_I \times C_{A_k i} \cdot \left|n_{cm}\ell_{cm}m_{cm}\right\rangle \left|NJM_J TM^t i\right\rangle$$

$$\therefore \left|\alpha\beta\gamma\right\rangle = \sum \left\langle \alpha\beta \mid J_{12}t_{12}\right\rangle \left\langle J_{12}t_{12}\gamma \mid IT\right\rangle \left\langle \ell_{cm}m_{cm}JM_J \mid IM_I\right\rangle$$

$$\times \underbrace{{}_I\left\langle (n_{cm}\ell_{cm} \mid \left\langle A_k \right|(ab)J_{12}t_{12},c\right\rangle_I}_{\text{Transition matrix element}} \times \underbrace{C_{A_k i}}_{\text{c.f.p}} \cdot \underbrace{\left|n_{cm}\ell_{cm}m_{cm}\right\rangle}_{\text{c.m. state}} \underbrace{\left|NJM_J TM^t i\right\rangle}_{\text{intrinsic state}},$$

$$N_{\text{total}} \equiv N_{cm} + N$$

$$= (2n_{cm} + \ell_{cm}) + (2n_k + \ell_k + 2\mathcal{N}_k + \mathcal{L}_k)$$

$$= 2n_a + \ell_a + 2n_b + \ell_b + 2n_c + \ell_c$$

k=1,or, 2, or, 3

# Matrix element of three-nucleon force for total system of three-body in *m*-scheme coupling

$$\langle \alpha\beta\gamma | V^{(3NF)} | \alpha'\beta'\gamma' \rangle$$

$$= \sum \langle \alpha\beta | J_{12} t_{12} \rangle \langle J_{12} t_{12} \gamma | IT \rangle$$

$$\times \langle \alpha'\beta' | J'_{12} t'_{12} \rangle \langle J'_{12} t'_{12} \gamma' | IT \rangle$$

$$\times [(ab|_{J_{12}} (c|]_I [| n_{cm} \ell_{cm}) | A_k)]_I$$

$$\times C_{A_k i} C_{A'_k i'} \cdot \langle NJTi | V^{(3NF)} | NJTi' \rangle$$

$$\times [{}_I (n'_{cm} \ell'_{cm} | (A'_{k'}][| a'b')_{J'_{12}} | c')]_I$$

Given in

A. Nogga, P. Navratil, B. R. Barrett, J. P. Vary, Phys. Rev. **C73**, 064002(2006),

, but not in the same authors with the same title of nucl-th/0511082v1

## Transition matrix elements

$$T \equiv {}_{IM}\left\langle \left[\left\langle n_{CM}\ell_{CM};\right|\left\langle A\right|\right] \middle| (ab)_{J_{12}T_{12}}\, c \right\rangle_{IM_I} = T_{spin-orbit}\cdot T_{isospin}$$

## Spin-orbital part of the transformation coefficient

$$T_{spin-orbit} \equiv \sum_{\lambda_{12},S_3,L_3,L,\Lambda} \sqrt{\hat{j}_{12}\hat{j}_3\hat{L}_3\hat{S}_3} \begin{Bmatrix} \ell_{12} & \ell_3 & L_3 \\ s_{12} & 1/2 & S_3 \\ j_{12} & j_3 & J \end{Bmatrix} (-)^{L_3+S_3+\ell_{CM}+I} \sqrt{\hat{L}\hat{J}} \begin{Bmatrix} \ell_{CM} & L_3 & L \\ S_3 & I & J \end{Bmatrix}$$

$$\times \sqrt{\hat{L}_{12}\hat{s}_{12}\hat{j}_a\hat{j}_b} \begin{Bmatrix} \ell_a & \ell_b & L_{12} \\ 1/2 & 1/2 & s_{12} \\ j_a & j_b & J_{12} \end{Bmatrix} \sqrt{\hat{J}_{12}\hat{j}_c\hat{L}\hat{S}_3} \begin{Bmatrix} L_{12} & s_{12} & J_{12} \\ \ell_c & 1/2 & j_c \\ L & S_3 & I \end{Bmatrix}$$

$$\times (-)^{\ell_{12}+\ell_3-L_3} (-)^{\ell_{CM}+\ell_3+\ell_{12}+L} \sqrt{\hat{\Lambda}\hat{L}_3} \begin{Bmatrix} \ell_{CM} & \ell_3 & \Lambda \\ \ell_{12} & L & L_3 \end{Bmatrix}$$

$$\times (-)^{\lambda_{12}+\ell_c-\Lambda} (-)^{\ell_c+L_{12}-L} (-)^{\ell_c+\ell_{12}+\lambda_{12}+L} \sqrt{\hat{\Lambda}\hat{L}_{12}} \begin{Bmatrix} \ell_c & \lambda_{12} & \Lambda \\ \ell_{12} & L & L_{12} \end{Bmatrix}$$

$$\times [n_{CM}, \ell_{CM}, n_3\ell_3; \Lambda \,\|\, N_{12}\lambda_{12}, n_c\ell_c; \Lambda]_d \bullet [N_{12}, \lambda_{12}, n_{12}\ell_{12}; L_{12} \,\|\, n_a\ell_a, n_b\ell_b; L_{12}]_{d'}$$

$$d = 2, d' = 1$$

# Isospin part of the transformation coefficient

$$T_{isospin} \equiv \left\langle \tfrac{1}{2}\tau_\alpha \, \tfrac{1}{2}\tau_\beta \,|\, t_{12} \; \tau_\alpha + \tau_\beta \right\rangle \left\langle t_{12} \; \tau_\alpha + \tau_\beta \; \tfrac{1}{2}\tau_\beta \,|\, T \; \tau_\alpha + \tau_\beta + \tau_\gamma \right\rangle$$

## Calculation of m.e. of $(t_1+t_2+t_3)$ between three-body cm-,intrinsic states

$$\langle n_{cm}\ell_{cm}, NJTi|(t_1+t_2+t_3)|n'_{cm}\ell'_{cm}, N'J'T'i'\rangle$$
$$\approx \delta(n_{cm}n'_{cm})\delta(\ell_{cm}\ell'_{cm})\langle n_{cm}\ell_{cm}, NJTi|(t_1+t_2+t_3)|n_{cm}\ell_{cm}, N'J'T'i'\rangle$$

$$(t_1+t_2+t_3) = -\frac{\hbar^2}{2(3m)}(\vec{\nabla}_3)^2 - \frac{\hbar^2}{2(\frac{1}{2}m)}(\vec{\nabla}_1)^2 - \frac{\hbar^2}{2(\frac{2}{3}m)}(\vec{\nabla}_2)^2$$

c.m.-part Intrinsic-part

$$\langle n_{cm}\ell_{cm}, NJTi|(t_1+t_2+t_3)|n_{cm}\ell_{cm}, N'J'T'i'\rangle$$
$$= \langle n_{cm}\ell_{cm}, NJTi|(t_1+t_2+t_3)|n_{cm}\ell_{cm}, N'JTi'\rangle \delta_{JJ'}\delta_{JT'}$$
$$= \sum_{A_k, A_{k'}} C_{A_k, NJTi} C_{A_{k'}, N'JTi'} \langle n_{cm}\ell_{cm}, n_k\ell_k j_k s_k t_k; \mathcal{N}_k\mathcal{L}_k\mathcal{J}_k|(t_1+t_2+t_3)|n_{cm}\ell_{cm}, n_{k'}\ell_{k'} j_{k'} s_{k'} t_{k'}; \mathcal{N}_{k'}\mathcal{L}_{k'}\mathcal{J}_{k'}\rangle$$

$$\langle n_{cm}\ell_{cm}, n_k\ell_k j_k s_k t_k; \mathcal{N}_k\mathcal{L}_k\mathcal{J}_k|(t_1+t_2+t_3)|n_{cm}\ell_{cm}, n_{k'}\ell_{k'} j_{k'} s_{k'} t_{k'}; \mathcal{N}_{k'}\mathcal{L}_{k'}\mathcal{J}_{k'}\rangle$$
$$= \frac{\hbar\omega}{2}(2n_{cm}+\ell_{cm}+\tfrac{3}{2}) + \delta_{\ell_k\ell_{k'}}\frac{\hbar\omega}{2}\begin{Bmatrix} \sqrt{(n_k+1)(n_k+\ell_k+\frac{3}{2})}\,\delta_{n_{k'},n_k+1} \\ +(2n_k+\ell_k+\frac{3}{2})\delta_{n_{k'},n_k} \\ +\sqrt{n_k(n_k+\ell_k+\frac{1}{2})}\,\delta_{n_{k'},n_k-1} \end{Bmatrix}$$
$$+\delta_{\mathcal{L}_k\mathcal{L}_{k'}}\frac{\hbar\omega}{2}\begin{Bmatrix} \sqrt{(\mathcal{N}_k+1)(\mathcal{N}_k+\mathcal{L}_k+\frac{3}{2})}\,\delta_{\mathcal{N}_{k'},\mathcal{N}_k+1} \\ +(2\mathcal{N}_k+\mathcal{L}_k+\frac{3}{2})\delta_{\mathcal{N}_{k'},\mathcal{N}_k} \\ +\sqrt{\mathcal{N}_k(\mathcal{N}_k+\mathcal{L}_k+\frac{1}{2})}\,\delta_{\mathcal{N}_{k'},\mathcal{N}_k-1} \end{Bmatrix}$$

# Second step decoupling

**Diagonalization of three-body subsytem Hamiltonian**

**in shell-model basis vector**

**Construction of intrinsic basis vector**
**in terms of Harmonic oscillator shell model**
**and its antisymmetrization**

# Construction of independent antisymmetric and orthonormalized three-body basis vectors

**Antisymmetrization operator of three-body system**

$$P(\alpha_1\alpha_2\alpha_3 \mid \beta_1\beta_2\beta_3) = \frac{1}{3!}\sum_{\wp(\beta_1\beta_2\beta_3)} \delta p \cdot \wp(\delta_{\alpha_1\beta_1}\delta_{\alpha_2\beta_2}\delta_{\alpha_3\beta_3})$$

The summation over all the permutation with respect to ($\beta$1, $\beta$2, $\beta$3) and $\delta$ p takes the value +1(-1) for even (odd) parmutation.

satisfies the relation of projection operator

$$\sum_{\gamma_1\gamma_2\gamma_3} P(\alpha_1\alpha_2\alpha_3 \mid \gamma_1\gamma_2\gamma_3) P(\gamma_1\gamma_2\gamma_3 \mid \beta_1\beta_2\beta_3) = P(\alpha_1\alpha_2\alpha_3 \mid \beta_1\beta_2\beta_3)$$

$$\hat{P}_I^2 = \hat{P}_I$$

## The Antisymmetrization operator in coupled-angular momentum representation

$$P_I(a_1a_2(J_{a_1a_2})a_3\,|\,b_1b_2(J_{b_1b_2})b_3)$$

$$= \sum_{m_{\alpha_1}m_{\alpha_2}m_{\alpha_3}} \sum_{m_{\beta_1}m_{\beta_2}m_{\beta_3}} \sum_{M_{a_1a_2}M_{b_1b_2}} \left(\frac{1}{2I+1}\right) \sum_{M}$$

$$\left\langle j_{a_1}m_{\alpha_1} j_{a_2}m_{\alpha_2}\,|\,J_{a_1a_2}M_{a_1a_2}\right\rangle \left\langle J_{a_1a_2}M_{a_1a_2} j_{a_3}m_{\alpha_3}\,|\,IM\right\rangle$$

$$\times \left\langle j_{b_1}m_{\beta_1} j_{b_2}m_{\beta_2}\,|\,J_{b_1b_2}M_{b_1b_2}\right\rangle \left\langle J_{b_1b_2}M_{b_1b_2} j_{b_3}m_{\beta_3}\,|\,IM\right\rangle$$

$$\times P_I(\alpha_1\alpha_2\alpha_3\,|\,\beta_1\beta_2\beta_3)$$

$$= \frac{1}{3!}(1+P_{a_1a_2J_{a_1a_2}}) \left[ \begin{array}{l} \delta_{a_1b_1}\delta_{a_2b_2}\delta_{a_3b_3}\delta_{J_{a_1a_2}J_{b_1b_2}} \\ +\hat{J}_{a_1a_2}\hat{J}_{b_1b_2} \begin{Bmatrix} j_{a_3} & j_{a_2} & J_{b_1b_2} \\ j_{a_1} & I & J_{a_1a_2} \end{Bmatrix} (1+P_{a_2a_3J_{b_1b_2}})\delta_{a_1b_3}\delta_{a_2b_2}\delta_{a_3b_1} \end{array} \right],$$

$$P_{a_1a_2J_{a_1a_2}}\, f(a_1a_2J_{a_1a_2}) \equiv -(-)^{j_{a_1}+j_{a_2}+J_{a_1a_2}}\, f(a_2a_1J_{a_1a_2})$$


A. Kuriyama, T. Marumori, K. Matsuyanagi, R.O., Prog.Theor.Phys.Suppl. No.58(1975), 32, 103.

# Orthonormal basis vectors

Diagonalization of $\hat{P}_I$

C.f.p. for three-body system

$$\hat{U}_I \hat{P}_I \hat{U}_I^{-1} = \begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \rightarrow \hat{U}_I = (\mathbf{U}_I(1), \mathbf{U}_I(2), \cdots)$$

Column vectors

$$\left| \Phi_{jI}[a_1, a_2, a_3] \right\rangle \equiv \mathbf{U}_I(j) \left| \phi_I[a_1, a_2, a_3] \right\rangle$$

$$= \sum_{P(a_1,a_2,a_3),J_{a_1a_2}} D_{jI,[a_1a_2(J_{a_1a_2})a_3]} \left| [a_1 a_2 (J_{a_1a_2}) a_3] I \right\rangle$$

$$\equiv \sum_{k=1,2,3} \sum_{B_k} D_{jI,B_k} \left| B_k \right\rangle,$$

$$B_{k=3} \equiv \{ [a_1 a_2 (J_{a_1a_2}) a_3] I \},$$

$$B_{k=2} \equiv \{ [a_3 a_1 (J_{a_3a_1}) a_2] I \},$$

$$B_{k=1} \equiv \{ [a_2 a_3 (J_{a_2a_3}) a_1] I \},$$

# 5. Summary

**1) UMOA with 2NF and 3NF can be formulated systematically.**

**2) Explicit expression for 3NF, m-scheme matrix elements are known in coordinate Harmonic oscillator representation;**

**Thanks for**

**A. Nogga, P. Navratil, B. R. Barrett, J. P. Vary, Phys. Rev. C73, 064002(2006)**

**3) Considering of approximation methods and efficient algorithms are on-going.**

**Some supercomputers (@ RCNP, RIKEN) could be open !!**

# Discussions

**Use of Symplectic shell-model basis might be promising**

as *effective* (or *optimal*) s.p. basis

**→efficient truncation of s.p. basis ?**

**→reducing the magnitude of three-or-more-body cluster terms effects ?**

**→ check of the reliability of the usual removal of C.M. motion effect**

**→description of cluster-like excitation ?**

**Great thanks to David Rowe, Jerry Draayer**

# Collaborators

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