Three-body matrix elements with harmonic-oscillator states

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Collaborators

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4/October/2017

Chiral effective field theory (EFT)

S. Weinberg, Phys. A **96**, 327 (1979).
R. Machleidt and D. Entem, Physics Reports **503**, 1 (2011).

Degrees of freedom and symmetry

Nucleons and pions
Chiral symmetry

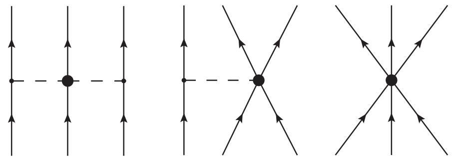
→ Soft scale Q
Hard scale Λ_χ

Perturbative expansion of Lagrangian

$(Q/\Lambda_\chi)^n$ Power counting
Theoretical error

Many-body forces on an equal footing

At N²LO ($n = 3$),
3-nucleon force (3NF) appears.



5 low-energy constants (LECs)
(2 of them appear for the first time)

S. Weinberg, Phys. Lett. B **295**, 114 (1992).
U. van Kolck, Phys. Rev. C **49**, 2932 (1994).

Regularization

Theory valid in the scale $Q \ll \Lambda_\chi$,

$$V_{3N} \longmapsto u_\nu(q,\Lambda)\, V_{3N}\, u_\nu(q',\Lambda),$$

with the regulator u_ν of the cutoff Λ.

→ **Discussed later**.

Out of our scope

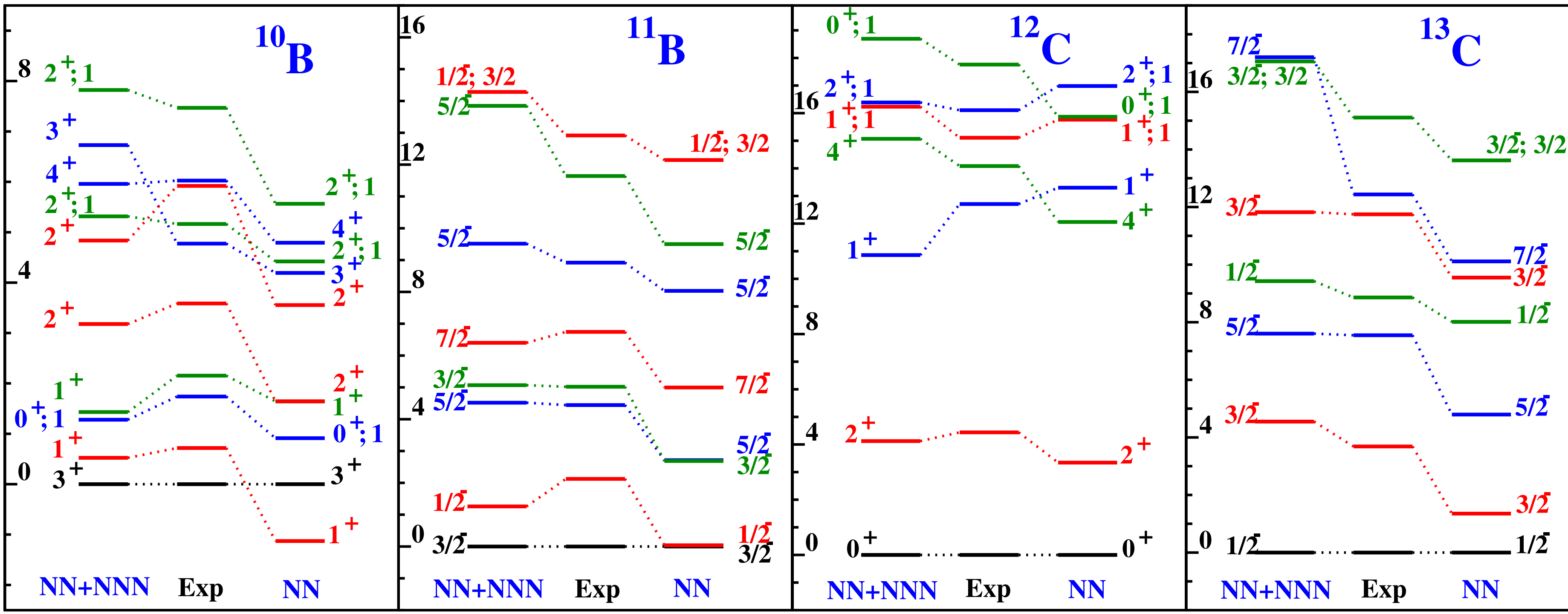
Fujita-Miyazawa, Tucson-Melbourne, Ulbana, etc.

J. Fujita and H. Miyazawa, Prog. Theor. Phys. **17**, 360 (1957).
S. A. Coon *et al*., Nucl. Phys. **A317**, 242 (1979).
J. Carlson *et al*., Nucl. Phys. **A401**, 59 (1983).

p-shell nuclei

ab initio no-core shell model

P. Navrátil *et al.*, Phys. Rev. Lett. **99**, 042501 (2007).

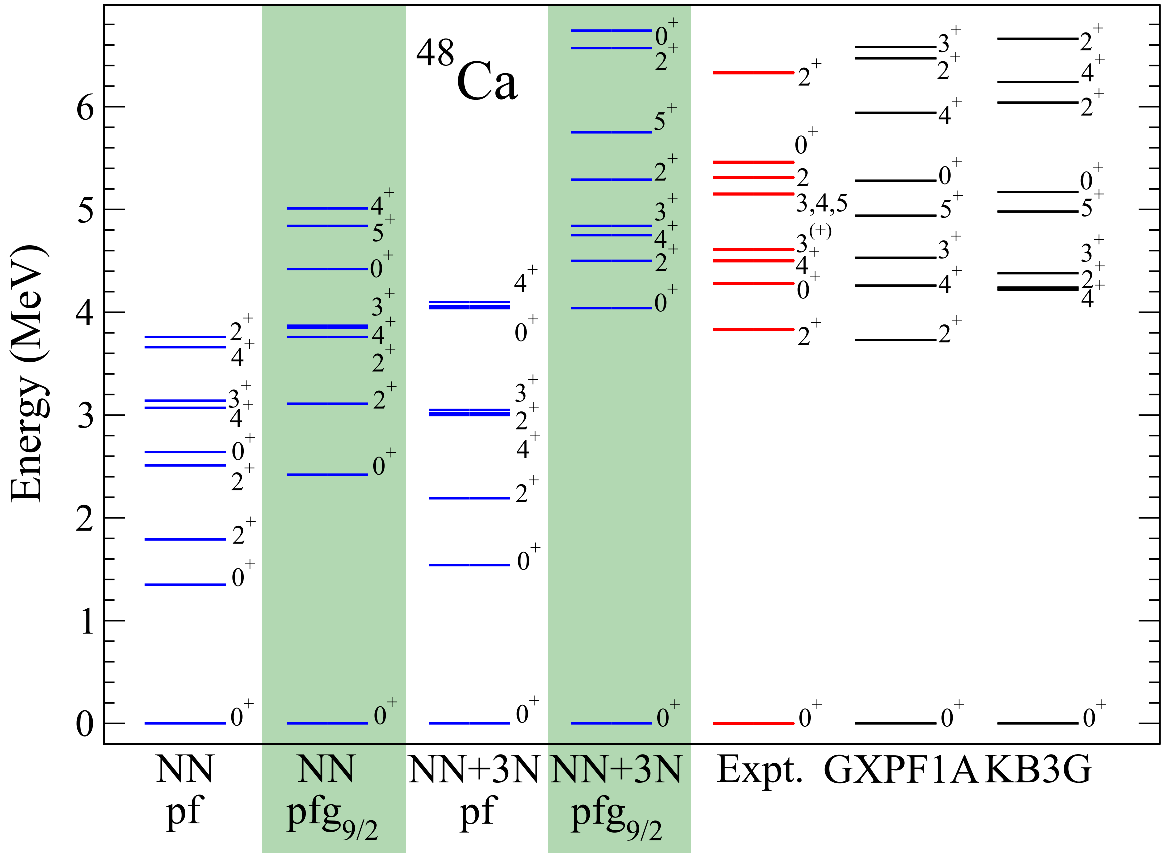


- Inclusion of 3NF improves drastically the **order** (**qualitative**) of excited states, **absolute value** (**quantitative**) as well, compared to the experimental data.

fp-shell nuclei

Shell model with ^{40}Ca core

J. D. Holt *et al.*, Phys. Rev. C **90**, 024312 (2014).

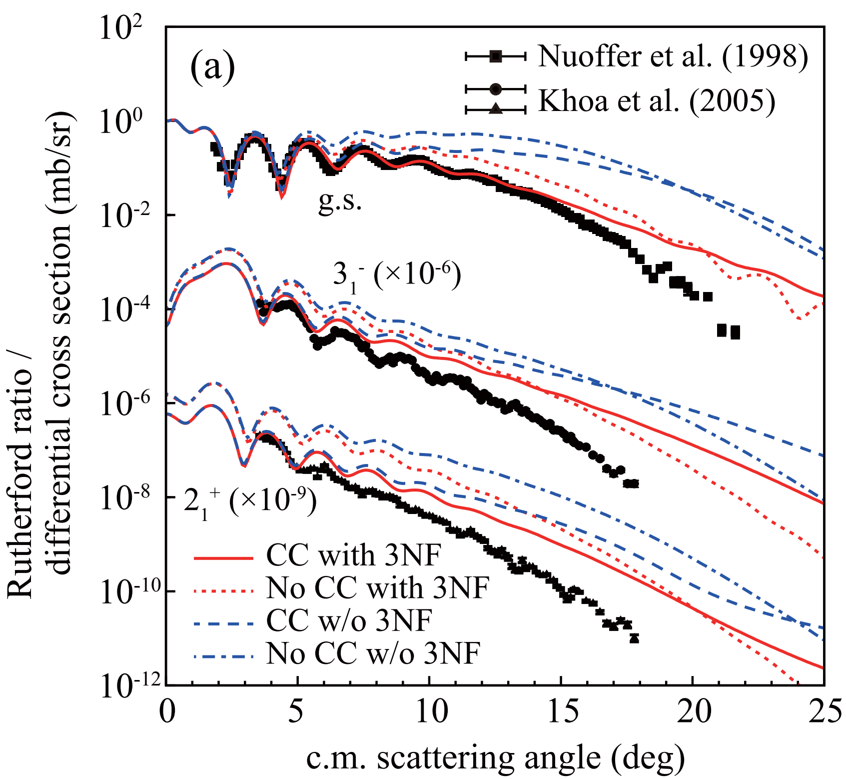


- The 3NF effect with $g_{9/2}$ is significant.

Nucleus-nucleus scattering

Elastic and inelastic ^{16}O-^{16}O scattering

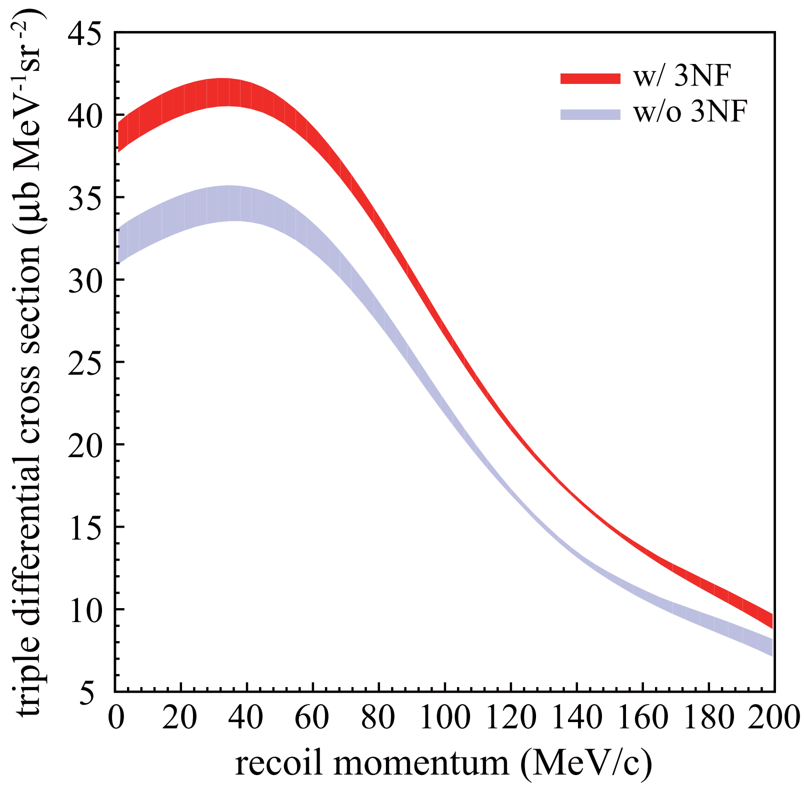
K. Minomo *et al.*, Phys. Rev. C **93**, 014607 (2016).



- Backward angle → high density
- Similar effect on ^{12}C-^{12}C scattering.

Knock-out reaction $^{40}Ca(p, 2p)^{39}K$

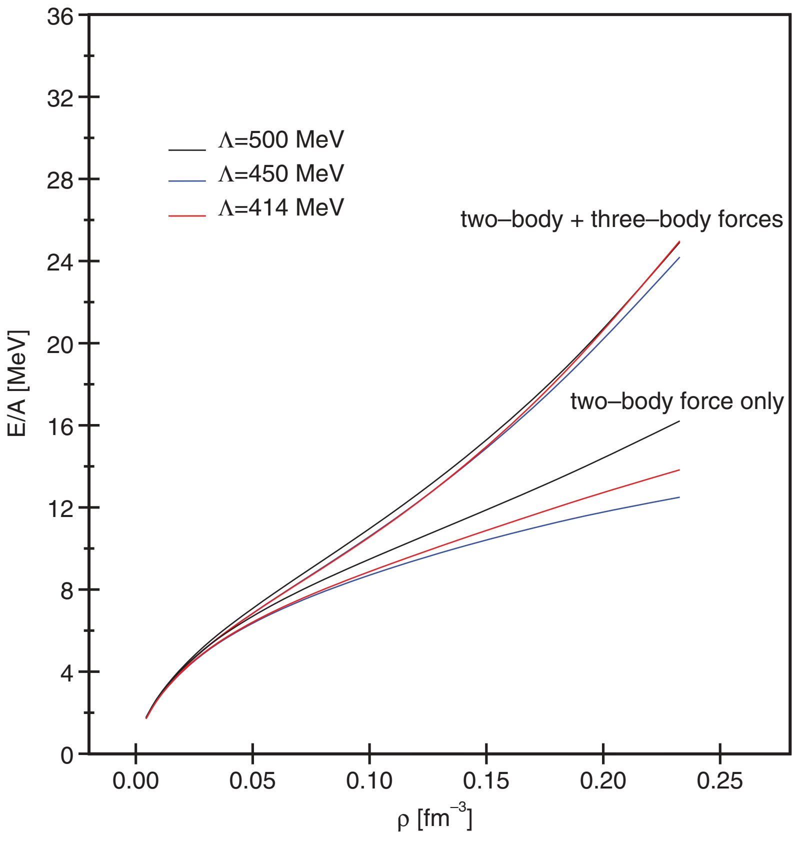
K. Minomo *et al.*, Phys. Rev. C **96**, 024609 (2017).



- Specific kinematical-condition.

Pure neutron matter

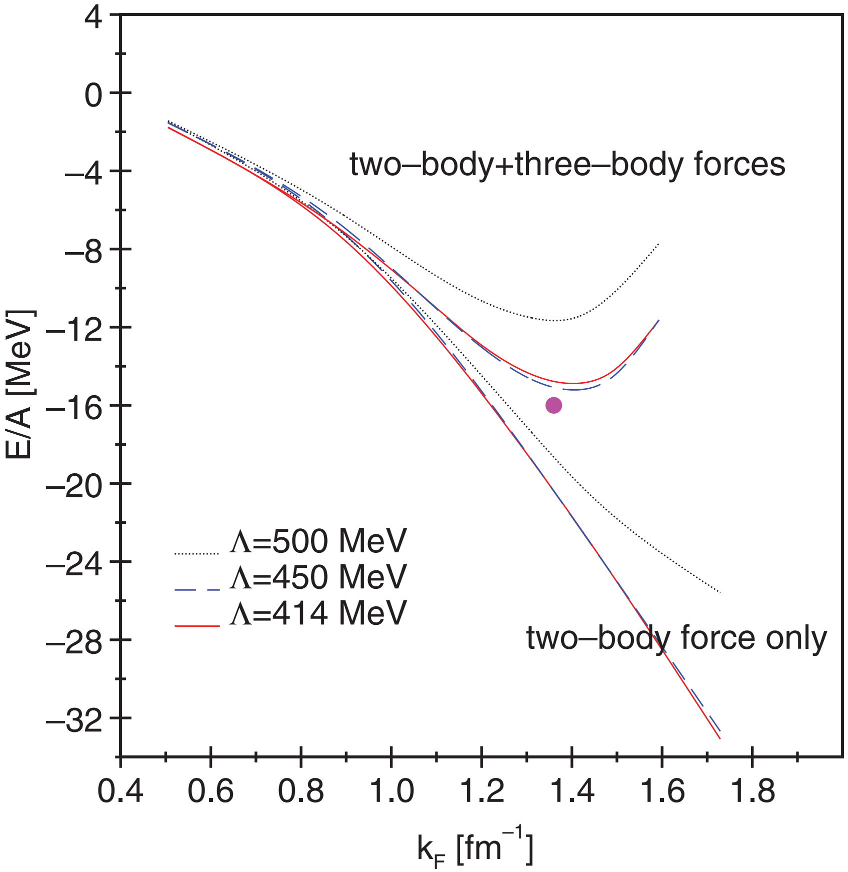
L. Coraggio *et al.*, Phys. Rev. C **87**, 014322 (2013).



- Only the 2-pion exchange term contributes.

Symmetric nuclear matter

L. Coraggio *et al.*, Phys. Rev. C **89**, 044321 (2014).



- Crucial 3NF effect for saturation.

Purpose

Motivation

- Including the **3NF based on the chiral EFT** in **shell model** calculations by means of the harmonic-oscillator (HO) basis-functions.
- Investigating 3NF effect with elucidating **cutoff dependence**, **LEC dependence**, **model-space (nuclides or single-particle orbits) dependence**, etc.

  → It is necessary to develop **our own code** for the 3-body matrix elements (MEs).

This presentation

- Formulation of the 3-body MEs is given simply.
- No observable is shown but only the MEs of the contact term (due to limited time to develop our code).
- Cutoff dependence with a few types of the regulator is investigated.

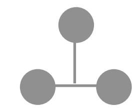
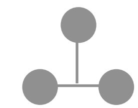
  → Picking up only the contact term breaks consistency of chiral EFT, but this framework can be easily extended to other two long-range terms.

Antisymmetrized 3-body ME

$${}_A\left\langle \left[[\bullet\bullet]\bullet \right]_{JT} \middle| V_{3N} \middle| \left[[\bullet\bullet]\bullet \right]_{JT} \right\rangle_A$$

JT-coupled ME

CM separation
Antisymm.
→

${}_A\langle$  $| V_{3N} |$  $\rangle_A$

Jacobi-HO ME

Separation of CM motion

$$\left| \left[[\bullet\bullet]\bullet \right]_{JT} \right\rangle = \sum (\text{coeff.}) \left\{ 9j \right\} \left\{ 9j \right\}$$

***jj* coupling → *LS* coupling**

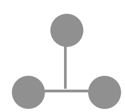
$$\times \left\{ 6j \right\} \langle\langle \text{ HOB } \rangle\rangle \langle\langle \text{ HOB } \rangle\rangle$$

Talmi transformations

I. Talmi, Helv. Phys. Acta **25**, 185 (1952).

$$\times \left\{ 6j \right\} \left\{ 6j \right\} \left\{ 9j \right\}$$

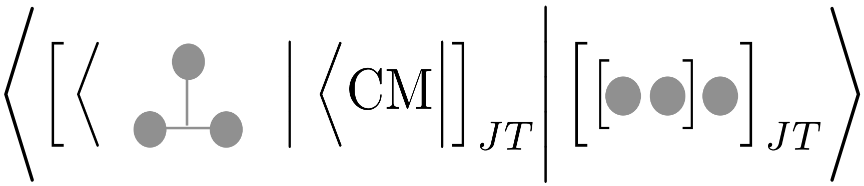
Recoupling for antisymmetrization

$\times \big| \big[\big|$  $\big\rangle \, \big| \text{CM} \big\rangle \big]_{JT} \big\rangle$

※ Harmonic oscillator bracket (HOB)

Explicit expression

21 variables + **7 summations**



$$\equiv T^{n_{12}l_{12}S_{12}I_{12}nlI\mathcal{I}\mathcal{N}\mathcal{L}}_{n_a l_a j_a n_b l_b j_b n_c l_c j_c J_{12} J}$$

$$= \sum_{L_{12}LS\mathcal{J}} \sum_{\mathcal{N}_{12}\mathcal{L}_{12}} \sum_{\omega} (-)^{l_c+l_{12}+J+L_{12}+L+S+\mathcal{J}} \hat{j}_a\hat{j}_b\hat{j}_c\hat{J}_{12}\hat{S}_{12}\hat{I}_{12}\hat{I}\hat{\mathcal{I}}\hat{L}_{12}^2\hat{L}^2\hat{S}^2\hat{\mathcal{J}}^2\hat{\omega}^2$$

$$\times \langle\langle \mathcal{N}_{12}\mathcal{L}_{12}n_{12}l_{12}, L_{12} \,|\, n_a l_a n_b l_b, L_{12}\rangle\rangle_{d_1} \langle\langle \mathcal{N}\mathcal{L}nl, \mathcal{J} \,|\, \mathcal{N}_{12}\mathcal{L}_{12}n_c l_c, \mathcal{J}\rangle\rangle_{d_2}$$

$$\times \begin{Bmatrix} l_{12} & \mathcal{L}_{12} & L_{12} \\ l_c & L & \mathcal{J} \end{Bmatrix} \begin{Bmatrix} \mathcal{L} & l & \mathcal{J} \\ l_{12} & L & \omega \end{Bmatrix} \begin{Bmatrix} \mathcal{L} & \omega & L \\ S & J & \mathcal{I} \end{Bmatrix}$$

$$\times \begin{Bmatrix} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L_{12} & S_{12} & J_{12} \end{Bmatrix} \begin{Bmatrix} L_{12} & S_{12} & J_{12} \\ l_c & \frac{1}{2} & j_c \\ L & S & J \end{Bmatrix} \begin{Bmatrix} l_{12} & l & \omega \\ S_{12} & \frac{1}{2} & S \\ I_{12} & I & \mathcal{I} \end{Bmatrix}$$

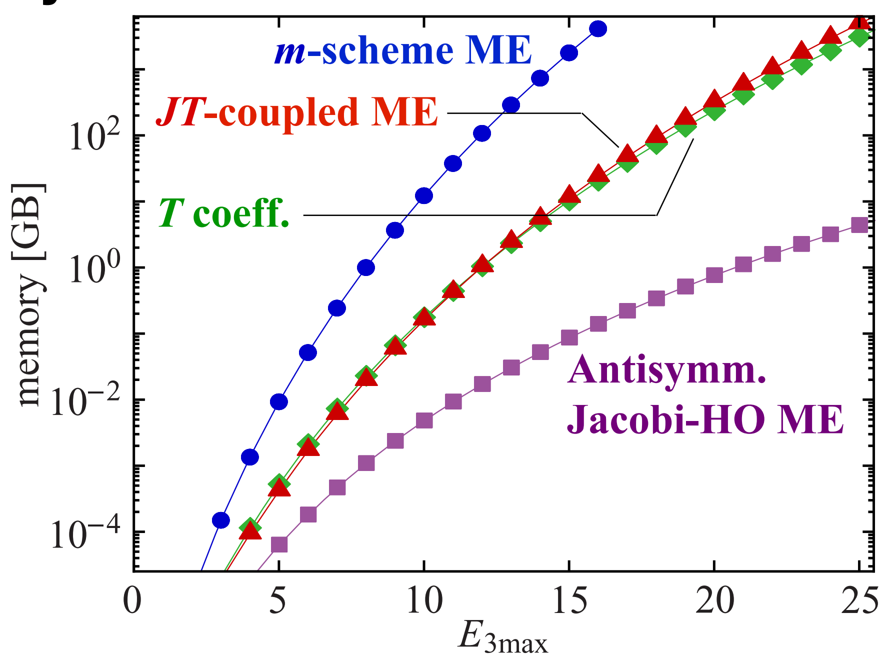
Explicit expression

21 variables + **7 summations**

Calculating the coefficient requires

- **CPU time** occupying ~ 97% of a whole calculation.
  e.g.) *fp*-shell (normal-ordered) ~3 days/thread.

- **Memory** R. Roth *et al*, Phys. Rev. C **90**, 024325 (2014).



3-body ME with HO | Computational challenge

- The computing of the 3-body MEs will be implemented in a hybrid Open-MP-MPI code to take full advantage of the HPC facilities of the Italian supercomputing centre (CINECA).

GALILEO

MARCONI

3-body ME with HO | Antisymmetrization

Numerical way (diagonalization of antisymmetrizer)

P. Navrátil *et al*., Phys. Rev. C **61**, 044001 (2000).

JT-coupled state → Jacobi-HO state

$$\left|\left[[\bullet\bullet]\bullet\right]_{JT}\right\rangle_A = \sqrt{6}\hat{\mathcal{A}}_3\left|\left[[\bullet\bullet]\bullet\right]_{JT}\right\rangle = (\mathrm{coeff.})\left|\mathrm{CM}\right\rangle\sqrt{6}\hat{\mathcal{A}}_3\left|\quad\right\rangle = (\mathrm{coeff.})\left|\mathrm{CM}\right\rangle\left|\quad\right\rangle_A$$

$$\hat{\mathcal{A}}_3 = \frac{1}{3!}\left[\mathbb{1} - \hat{\mathcal{P}}_{ab} - \hat{\mathcal{P}}_{bc} - \hat{\mathcal{P}}_{ca} + \hat{\mathcal{P}}_{ab}\hat{\mathcal{P}}_{bc} + \hat{\mathcal{P}}_{ab}\hat{\mathcal{P}}_{ca}\right]$$

Spectral decomposition

$$\hat{\mathcal{A}}_3 = \sum_\nu \epsilon_\nu \left|\nu\right\rangle\left\langle\nu\right|$$

$$\epsilon_\nu = \begin{cases} 1 & \text{(physical states)} \\ 0 & \text{(spurious states)} \end{cases}$$

P. Navrátil *et al*., Phys. Rev. C **59**, 611 (1999).

$$\hat{\mathcal{A}}_3\left|i;\quad\right\rangle = \sum_{j\nu} C^i_\nu C^j_\nu \left|j;\quad\right\rangle$$

$$C^i_\nu = \left\langle\nu\middle|i;\quad\right\rangle$$

Coefficients obtained numerically.

Numerical way (diagonalization of antisymmetrizer)

P. Navrátil *et al.*, Phys. Rev. C **61**, 044001 (2000).

Eigenvalue equation

$$\left(\mathcal{A}_{ij} \right) \left(C_\nu^j \right) = \epsilon_\nu \left(C_\nu^i \right)$$

Constrain

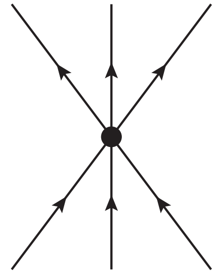
$$\hat{\mathcal{P}}_{ab} \left| i; \quad \right\rangle = - \left| i; \quad \right\rangle$$

Partially antisymmetrized

$$\mathcal{A}_{ij} = \left\langle i; \quad \middle| \hat{\mathcal{A}}_3 \middle| j; \quad \right\rangle$$
$$= \frac{1}{3} \left[\delta_{ij} - (\text{const.}) \left\langle i; \quad \middle| j; \quad \right\rangle \right]$$
$$= \frac{1}{3} \left[\delta_{ij} - (\text{const.}) \langle\langle \text{ HOB } \rangle\rangle \right]$$

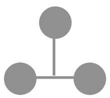
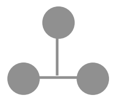
- This approach is general to perform the antisymmetrization for *A*-body system.

Contact term



E. Epelbaum *et al.*, Phys. Rev. C **66**, 064001 (2002).
P. Navrátil, Few-Body Syst. **41**, 117 (2007).

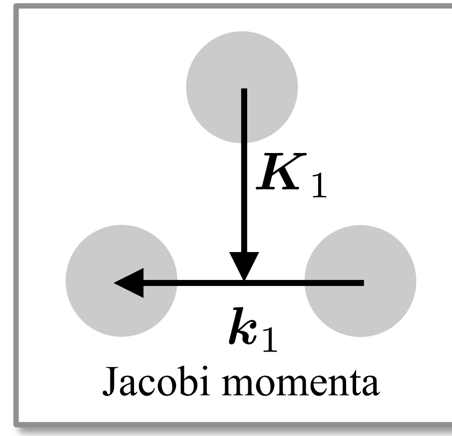
Final form

$\Big\langle$  $\Big| \bar{w}_{3N}^{(\mathrm{ct})} \Big|$  $\Big\rangle$

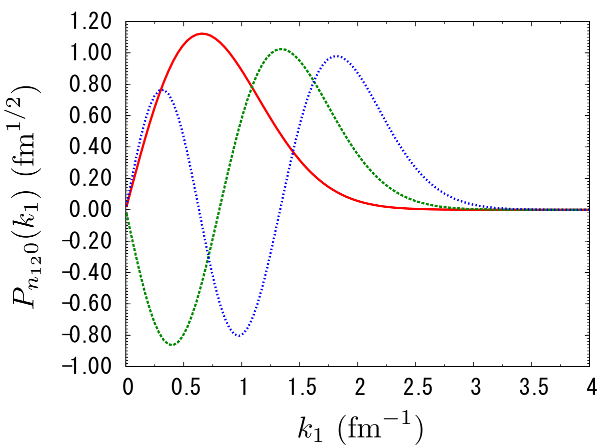
$$= (\mathrm{coeff.}) \ni \textbf{LEC } c_E$$

$$\times \iint dk_1 dK_1 k_1 K_1 P_{n_{12}0}(k_1) P_{n0}(K_1) u_\nu(k_1, K_1, \Lambda)$$

$$\times \iint dk'_1 dK'_1 k'_1 K'_1 P_{n'_{12}0}(k'_1) P_{n'0}(K'_1) u_\nu(k'_1, K'_1, \Lambda)$$

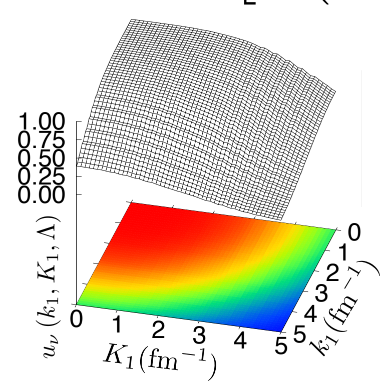


Momentum-space HO **Regulator**



Only *s*-wave due to our regulator.

$$u_\nu(k_1, K_1, \Lambda) = \exp\left[-\left(\frac{k_1^2 + K_1^2}{4\Lambda^2}\right)^\nu\right]$$



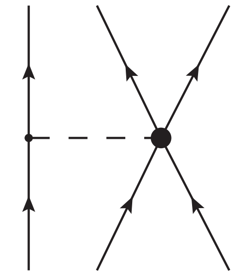
One-pion exchange + contact term

E. Epelbaum *et al.*, Phys. Rev. C **66**, 064001 (2002).
P. Navrátil, Few-Body Syst. **41**, 117 (2007).

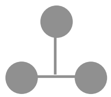
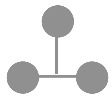
Irreducible-tensor expression

$$\frac{\boldsymbol{\sigma}_c \cdot \boldsymbol{q}_c}{q_c^2 + m_\pi^2} \boldsymbol{\sigma}_b \cdot \boldsymbol{q}_c = \sum_{\lambda_0 \lambda_1 \lambda_2} \sum_{\mathcal{K}_1 \mathcal{K}_2} (\text{coeff.}) f_{\lambda_2}^{(\lambda_0)}(K_1, K_1') \times \left[[\sigma_1(c) \otimes \sigma_1(b)]_{\lambda_0} \otimes \left[Y_{\mathcal{K}_1}\left(\hat{\boldsymbol{K}}_1\right) \otimes Y_{\mathcal{K}_2}\left(\hat{\boldsymbol{K}}_1'\right)\right]_{\lambda_0} \right]_{00}$$

From propagator

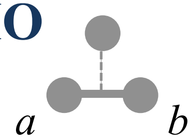


Final form

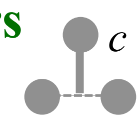
$$\left\langle \right.$$  $$\left| \bar{w}_{3N}^{(1\pi)} \right|$$  $$\left. \right\rangle$$ $\ni$ **LEC c_D**

$$= \sum_{\lambda_0 \lambda_1 \lambda_2} (\text{coeff.}) \iiiint dk_1 dk_1' dK_1 dK_1' k_1 k_1' K_1^{\lambda_0 - \lambda_1 + 1} K_1'^{\lambda_1 + 1} f_{\lambda_2}^{(\lambda_0)}(K_1, K_1') \times P_{n_{12}0}(k_1) P_{n_{12}'0}(k_1') P_{nl}(K_1) P_{n'l'}(K_1') u_\nu(k_1, K_1, \Lambda) u_\nu(k_1', K_1', \Lambda)$$

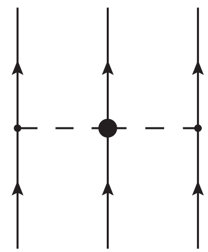
Only *s*-wave HO in *a*-*b* motion



Non *s*-wave appears in (*ab*)-*c* motion



Two-pion exchange term



$$w_{3N}^{(2\pi)} = w_{3N}^{(2\pi;c_1)} + w_{3N}^{(2\pi;c_3)} + w_{3N}^{(2\pi;c_4)}$$

LEC c_1 **LEC c_3** **LEC c_4**

Dividing two propagators using complete set

D. Hüber *et al.*, Few-Body Syst. **22**, 107 (1997).

- c_1 term (for simplicity ignore the regulator at the moment).

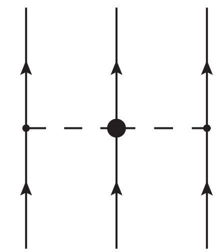
$$w_{3N}^{(2\pi;c_1)} \equiv -\frac{g_A^2 c_1 m_\pi^2}{f_\pi^4} \frac{(\boldsymbol{\sigma}_b \cdot \boldsymbol{q}_b)(\boldsymbol{\sigma}_c \cdot \boldsymbol{q}_c)}{(q_b^2 + m_\pi^2)(q_c^2 + m_\pi^2)} \boldsymbol{\tau}_b \cdot \boldsymbol{\tau}_c$$

$$\left\langle i; \quad \middle| w_{3N}^{(2\pi;c_1)} \middle| j; \quad \right\rangle = -\frac{g_A^2 c_1 m_\pi^2}{f_\pi^4} \langle \boldsymbol{\tau}_b \cdot \boldsymbol{\tau}_c \rangle \left\langle i; \quad \middle| \frac{(\boldsymbol{\sigma}_b \cdot \boldsymbol{q}_b)(\boldsymbol{\sigma}_c \cdot \boldsymbol{q}_c)}{(q_b^2 + m_\pi^2)(q_c^2 + m_\pi^2)} \middle| j; \quad \right\rangle$$

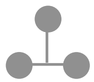
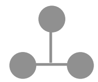
$$\left\langle i; \quad \middle| \frac{(\boldsymbol{\sigma}_b \cdot \boldsymbol{q}_b)(\boldsymbol{\sigma}_c \cdot \boldsymbol{q}_c)}{(q_b^2 + m_\pi^2)(q_c^2 + m_\pi^2)} \middle| j; \quad \right\rangle = \sum_h \left\langle i; \quad \middle| \frac{\boldsymbol{\sigma}_c \cdot \boldsymbol{q}_c}{q_c^2 + m_\pi^2} \middle| h; \quad \right\rangle \left\langle h; \quad \middle| \frac{\boldsymbol{\sigma}_b \cdot \boldsymbol{q}_b}{q_b^2 + m_\pi^2} \middle| j; \quad \right\rangle$$

Quasi one-pion exchange

Two-pion exchange term



- Irreducible-tensor expression and regularization

$\Big\langle$  $\Big| \bar{w}_{3N}^{(2\pi;c_1)} \Big|$  $\Big\rangle$

$$= \sum_{n''_{12}n''l''} (\text{coeff.}) \iiiint dk_1 dk'_1 dK_1 dK'_1 k_1 k'_1 K_1 K'_1 \left[\frac{K_1}{\hat{l}'^2} f_{l'}(K_1, K'_1) - \frac{K'_1}{\hat{l}''^2} f_{l''}(K_1, K'_1) \right]$$

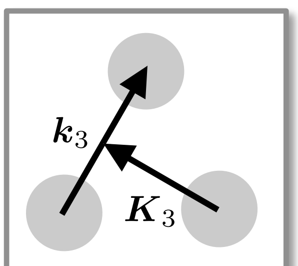
$$\times P_{n''_{12}0}(k_1) P_{n'_{12}0}(k'_1) P_{n''l''}(K_1) P_{n'l'}(K'_1) u_\nu(k_1, K_1, \Lambda) u_\nu(k'_1, K'_1, \Lambda)$$

$$\times \sum_{\lambda\sigma} \sum_{\substack{\tilde{n}_{12}\tilde{n} \\ \tilde{n}''_{12}\tilde{n}''}} (\text{coeff.}) \int dk_3 k_3 P_{\tilde{n}_{12}0}(k_3) \int dk'_3 k'_3 P_{\tilde{n}''_{12}0}(k'_3)$$

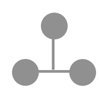
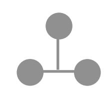
$$\times \iint dK_3 dK'_3 K_3 K'_3 P_{\tilde{n}\lambda}(K_3) P_{\tilde{n}''l''}(K'_3) \left[\frac{K_3}{\hat{l}''^2} f_{l''}(K_3, K'_3) - \frac{K'_3}{\hat{\lambda}^2} f_\lambda(K_3, K'_3) \right].$$

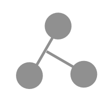
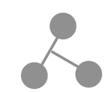
States h

First part



Second part (necessary to perform Talmi transformation)

$\Big\langle h;$  $\Big| \frac{\sigma_b \cdot q_b}{q_b^2 + m_\pi^2} \Big| j;$  $\Big\rangle$

$= \sum_{j'h'} (\text{coeff.}) \Big\langle h';$  $\Big| \frac{\sigma_b \cdot q_b}{q_b^2 + m_\pi^2} \Big| j';$  $\Big\rangle$

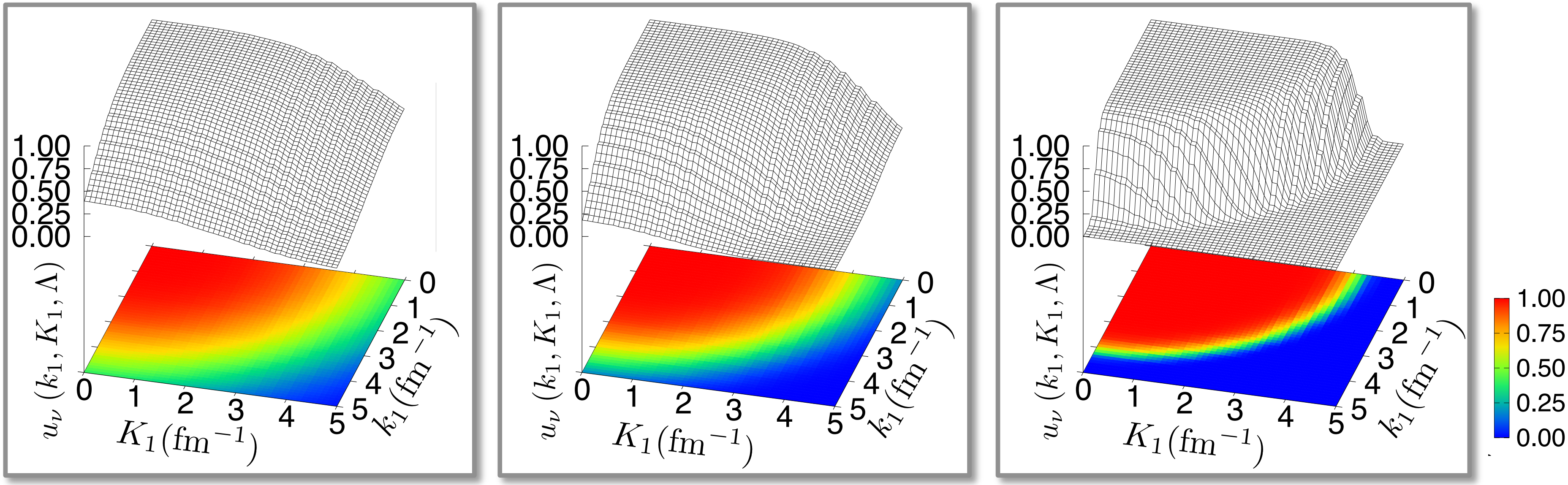
- Same procedure is applicable for c_3 and c_4 terms.

Three sets of the regulator and LECs

L. Coraggio *et al.*, Phys. Rev. C **89**, 044321 (2014).

$$u_\nu\left(k_1, K_1, \Lambda\right) = \exp\left[-\left(\frac{k_1^2 + K_1^2}{4\Lambda^2}\right)^\nu\right]$$

$\Lambda = 500\ \mathrm{MeV}, \nu = 2$ | $\Lambda = 450\ \mathrm{MeV}, \nu = 3$ | $\Lambda = 414\ \mathrm{MeV}, \nu = 10$



$c_E = -0.18$
R. Machleidt and D.R. Entem, Phys. Rep. **503** 1 (2011).

$c_E = -0.11$
L. Coraggio *et al.*, Phys. Rev. C **87**, 014322 (2013).

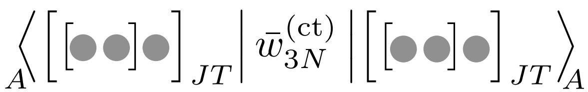
$c_E = -0.07$
L. Coraggio *et al.*, Phys. Rev. C **75**, 024311 (2007).

- The value of the LEC c_E is determined from, together with c_D, the **^{3}H and ^{3}He binding energy** and their **Gamow-Teller MEs**.

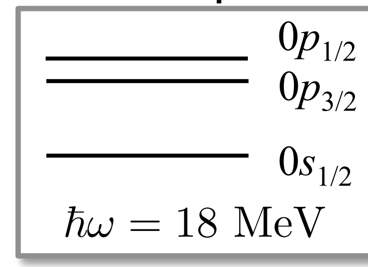
Result | Correlation plot of MEs of contact term

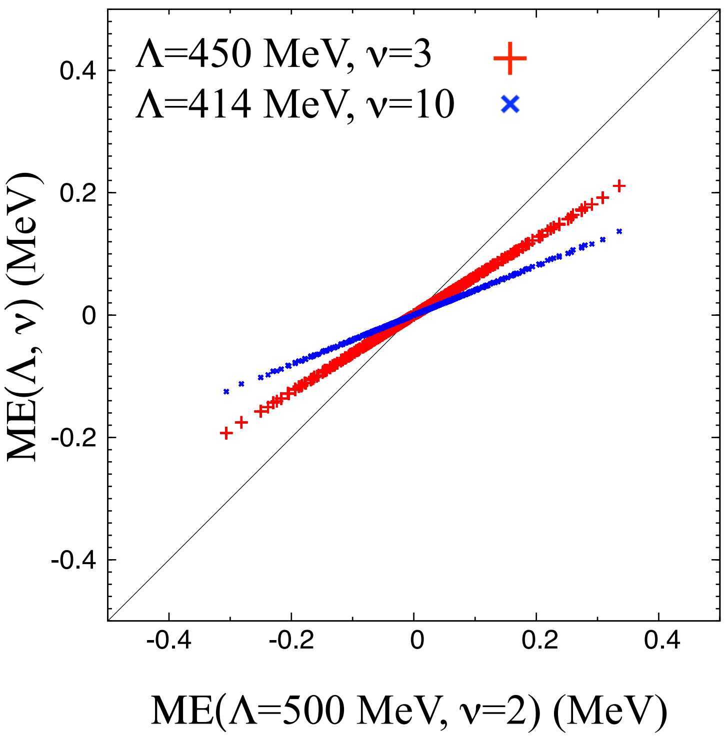
***p*-shell (no-core)**

JT-coupled ME

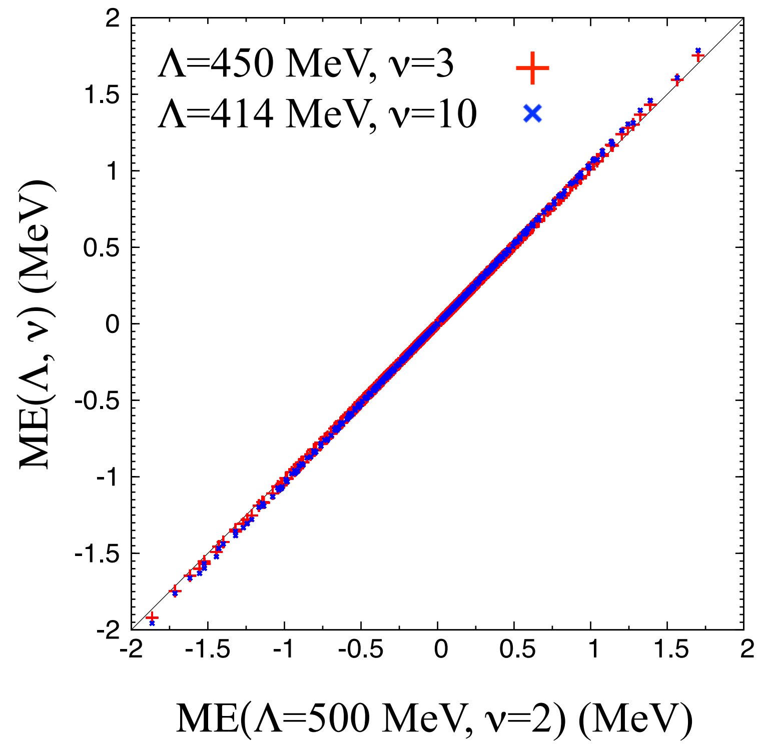


Model space





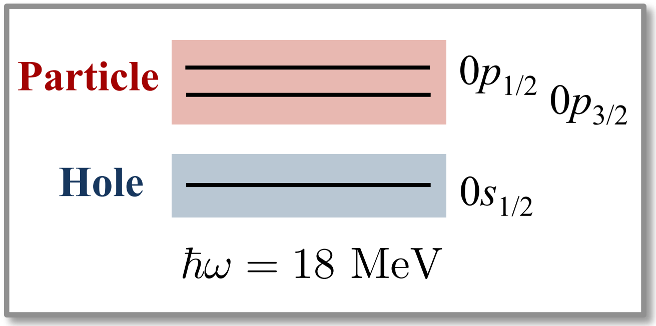
$c_E \longmapsto 1$



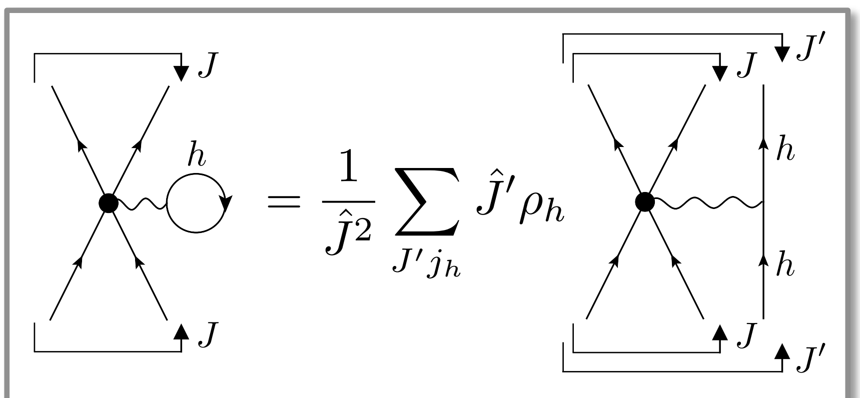
- The difference originates from LEC.

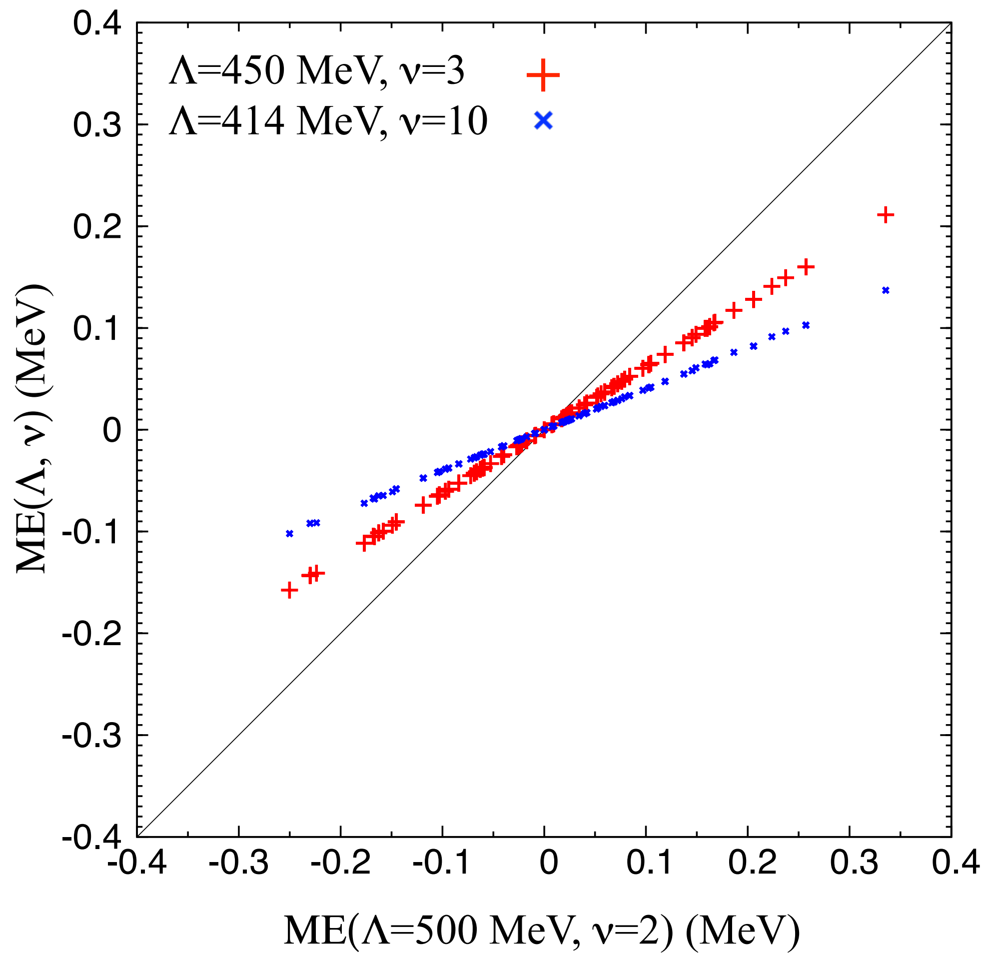
p-shell (*s*-core)

Model space



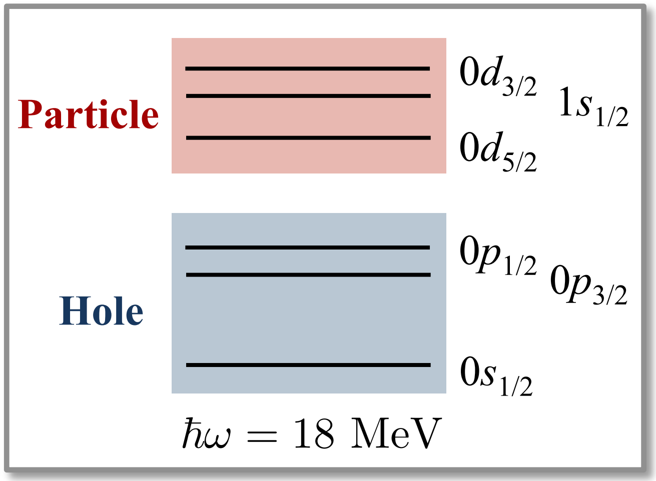
Normal-ordered ME (1st order)



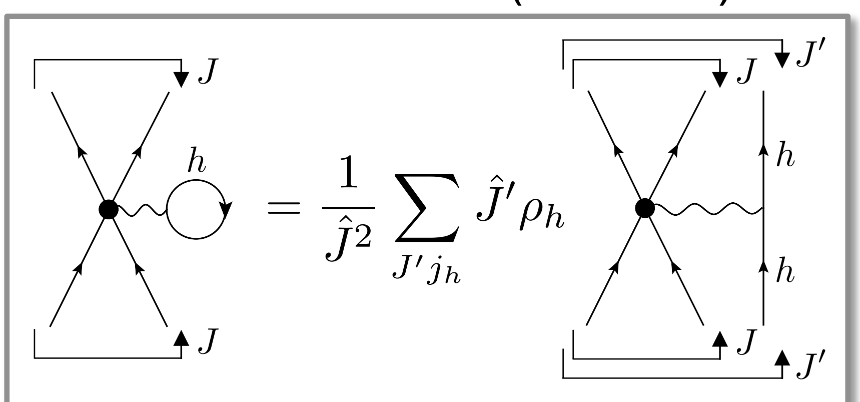


sd-shell (*sp*-core)

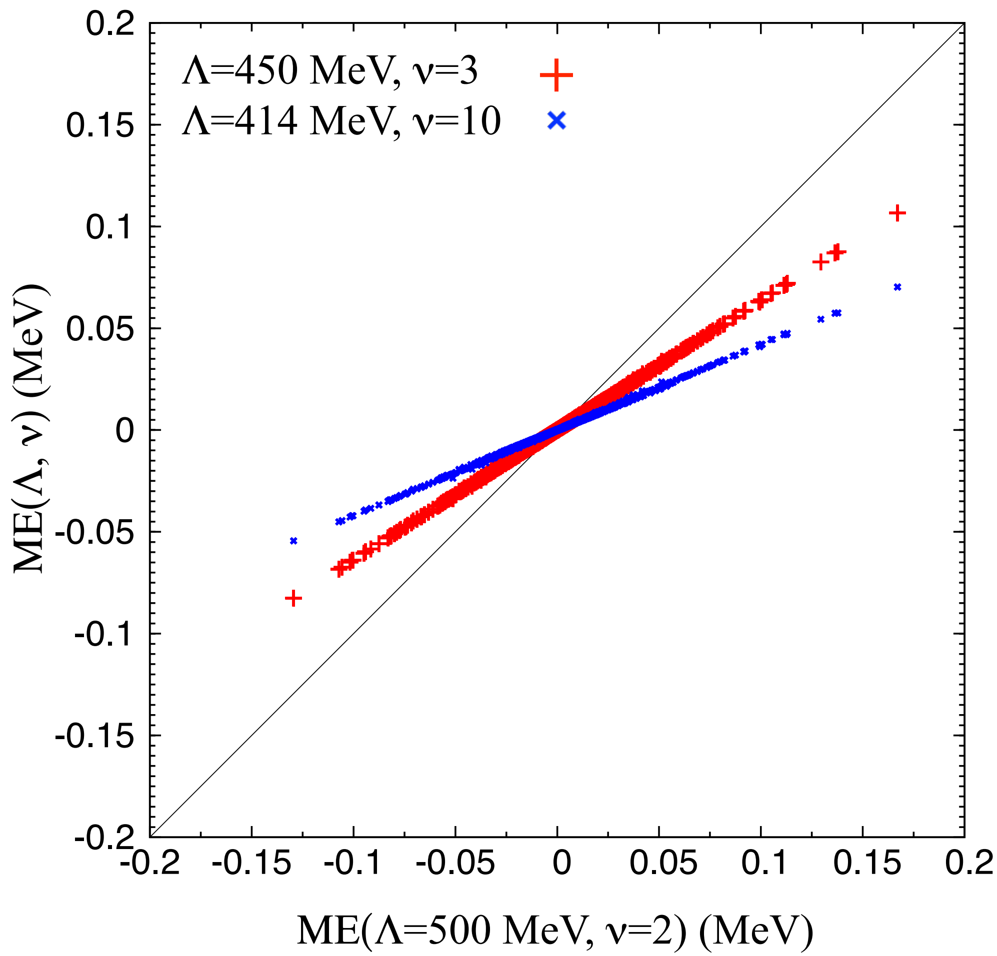
Model space



Normal-ordered ME (1st order)

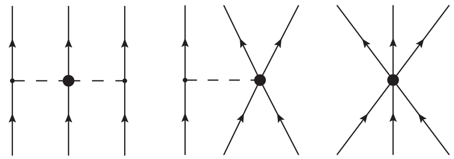


- An almost universal slope compared to the *p*-shell results.



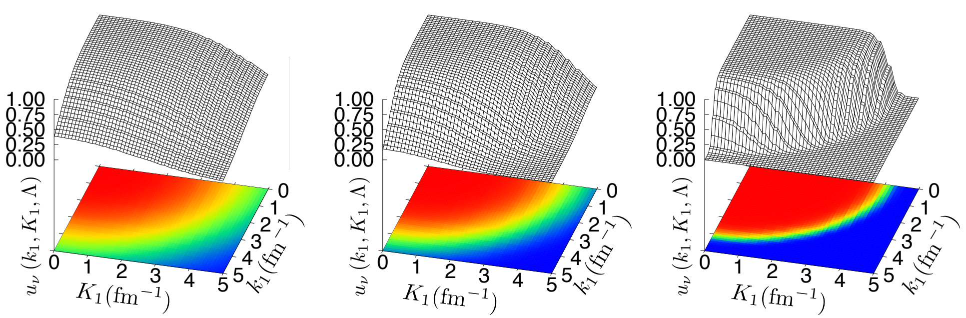
Summary

3NF of chiral N²LO

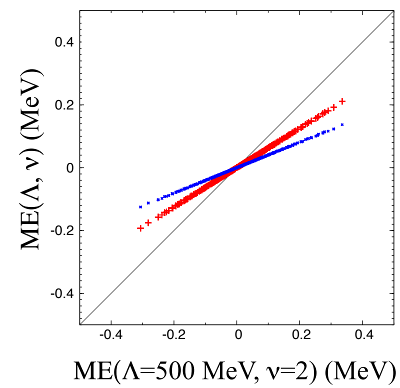


JT-coupled ME → Jacobi-HO ME

Cutoff and LEC dependence



Correlation plot



Future plan

- The **long-range terms** (2-pion exchange and 1-pion exchange + contact)
- **Observables** (Spectroscopy, etc.)
  → Benchmark for *p*-shell nuclei.