

A comparative analysis of three-nucleon potentials in nuclear matter



Alessandro Lovato



In collaboration with Omar Benhar, Stefano Fantoni and K. E. Schmidt

Outline

- Ab initio many body method
- Nuclear Hamiltonian: 2- and 3- body potentials
- Chiral NNN potential and its local form
- Local Chiral NNN contact term cutoff dependence
- Comparative study of local three-body potential in nuclear matter
- Conclusions

Ab initio many body method

Our aim is to perform *ab initio* calculations in nuclear matter

The interaction must not to be affected by uncertainties involved in many body techniques

Ab initio many body calculations

- Fully predictive
- Their approximations can be estimated
- Provide a test for the interaction itself

A “Realistic” nuclear hamiltonian

The non relativistic Hamiltonian describing nuclear matter is

$$H = \sum_{i=1}^A \frac{\mathbf{p}_i^2}{2m} + \sum_{j>i=1}^A v_{ij} + \dots$$

(Some) **Realistic** nucleon-nucleon (NN) potentials

■ Argonne v_{18} , v_8

- Mainly phenomenological
- Local in coordinate space

■ CD-BONN

- Meson-exchange based
- Nonlocal

■ Chiral N³LO

- From Chiral Lagrangians
- Nonlocal

Parameters of these potentials obtained

Fitting the ~ 4300 nn and np Nijmegen scattering data below 350 MeV with $\chi^2 \approx 1$.

Fitting the binding energy of the deuteron

No many-body method involved in the fit

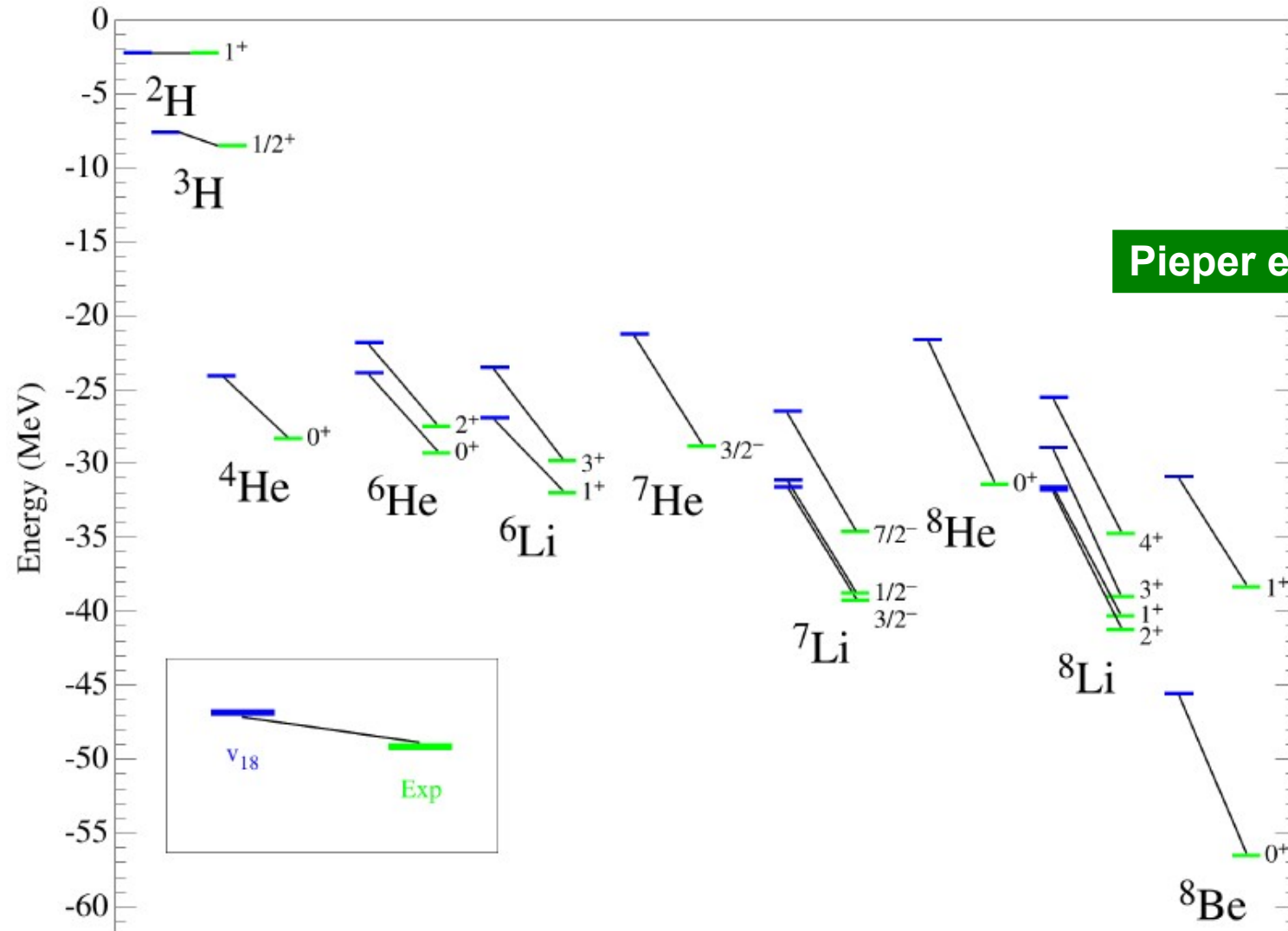


Potentials with high predictive power, suitable for “ab initio” calculations.

NN potential is not enough

When two body potential only is considered:

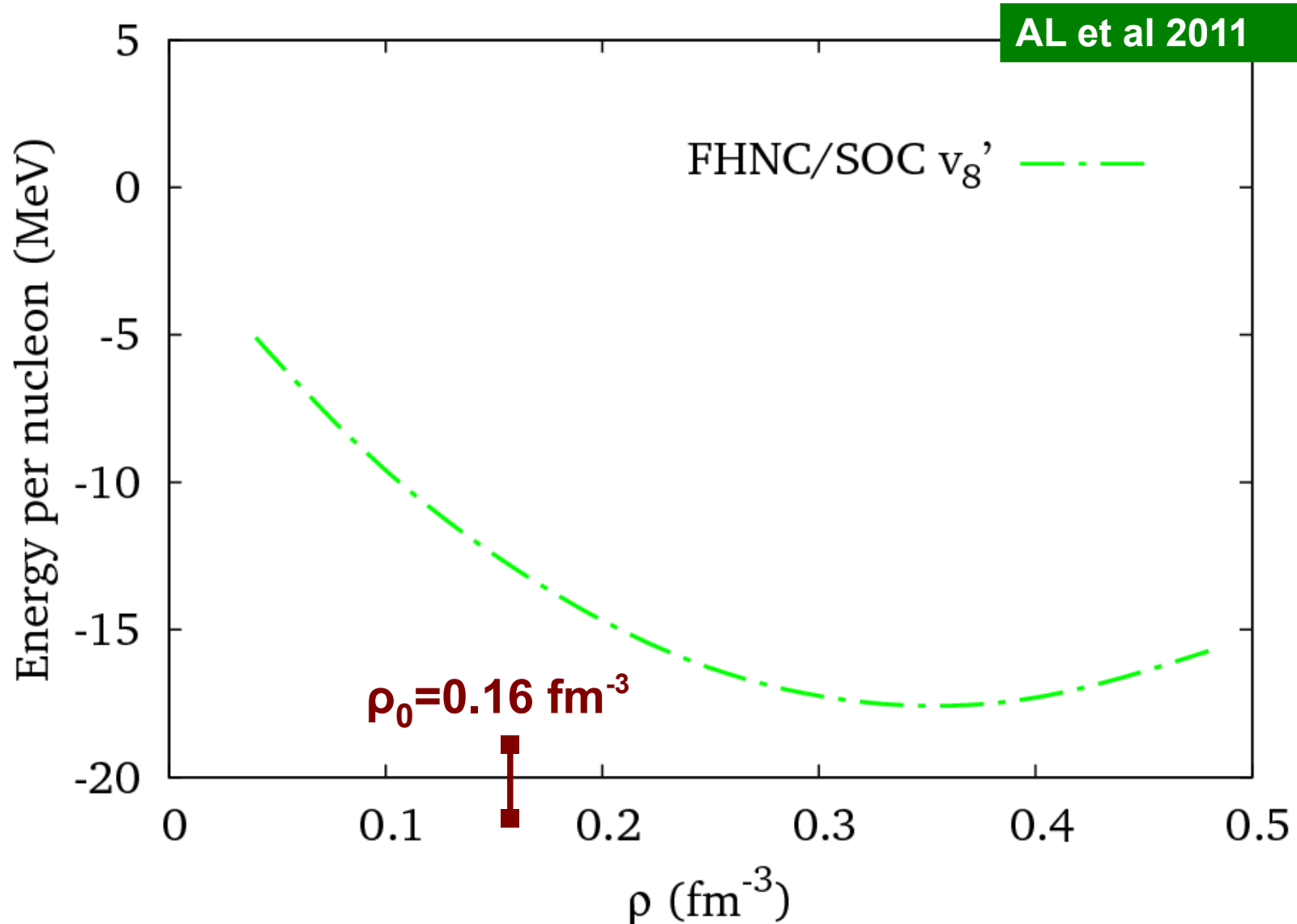
- Bad description of three and more nuclei bound and scattering states.



NN potential is not enough

When two body potential only is considered:

- Equilibrium density of symmetric nuclear matter overestimated.



NNN potential

Originates from the fact that nucleons are not elementary particles.

Three-body force is **NOT** an iteration of the two-body force

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Two-body force



Bogner's idea

NNN potential

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Two-body force



Three-body force

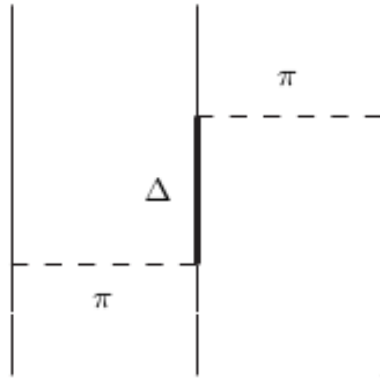


Bogner's idea

Urbana IX three body potential

UIX potential consists of **two contributions**

$V^{2\pi}$ – Fujita Myiazawa



Cyclic sum of three permutations

$$V^{2\pi} = A^{2\pi} (O_{123}^{2\pi} + O_{231}^{2\pi} + O_{312}^{2\pi})$$

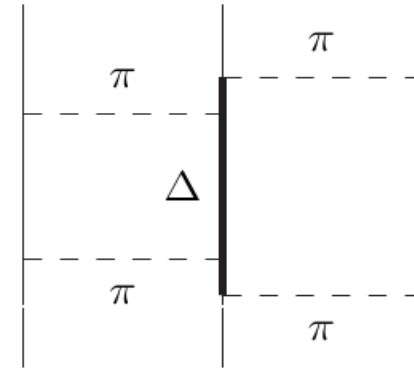
$$O_{123}^{2\pi} = \left(\{\hat{X}_{12}, \hat{X}_{23}\} \{\tau_{12}, \tau_{13}\} + \frac{1}{4} [\hat{X}_{12}, \hat{X}_{23}] [\tau_{12}, \tau_{23}] \right)$$

$$\hat{X}_{ij} = Y(m_\pi r) \sigma_{ij} + T(m_\pi r) S_{ij}$$



Cutoff functions of OPE

V^R – scalar repulsive term



Cyclic sum of three permutations

$$V^R = U_0 \sum_{cycl} T^2(m_\pi r_{12}) T^2(m_\pi r_{23})$$



Cutoff functions of OPE

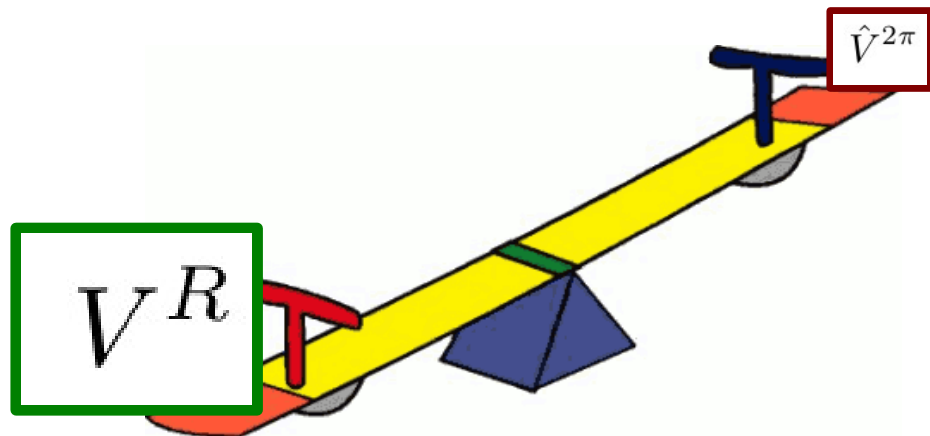
Urbana IX three body potential

UIX potential has two parameters

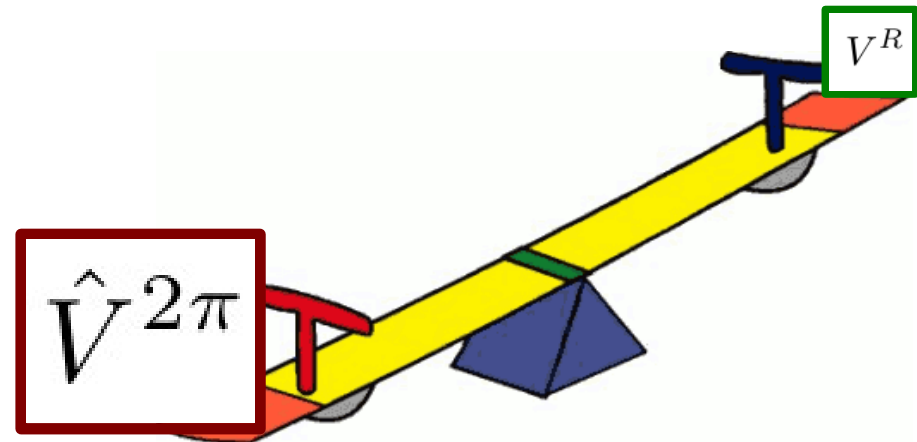
- $A^{2\pi}$ adjusted to reproduce the observed binding energies of ${}^3\text{H}$.
- U_0 tuned for FHNC/SOC calculations to reproduce the empirical equilibrium density of SNM

Lagaris and Pandharipande argued that, because of correlations, the relative weight of the contribution depends upon the density of the system:

High density

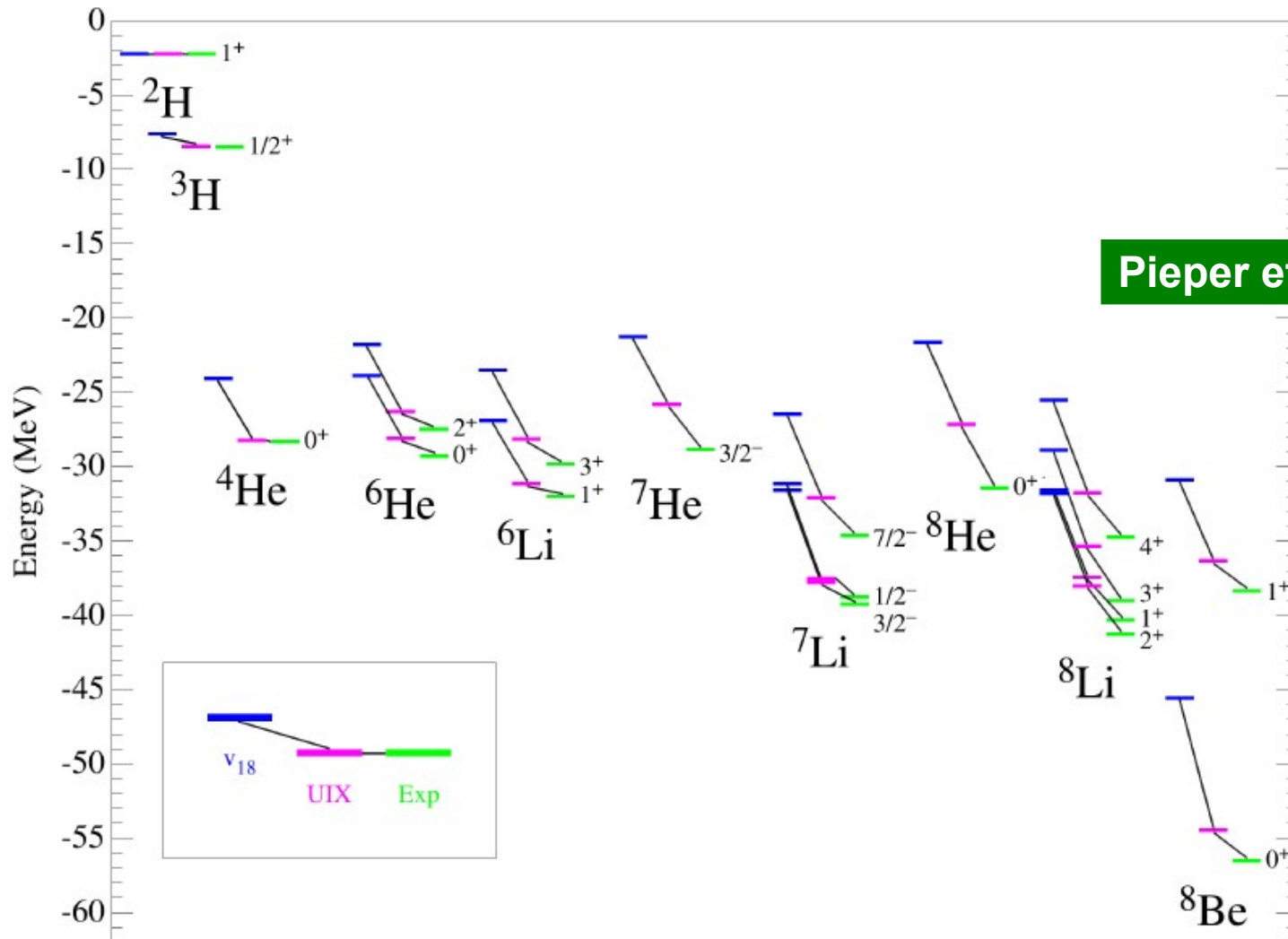


Low density



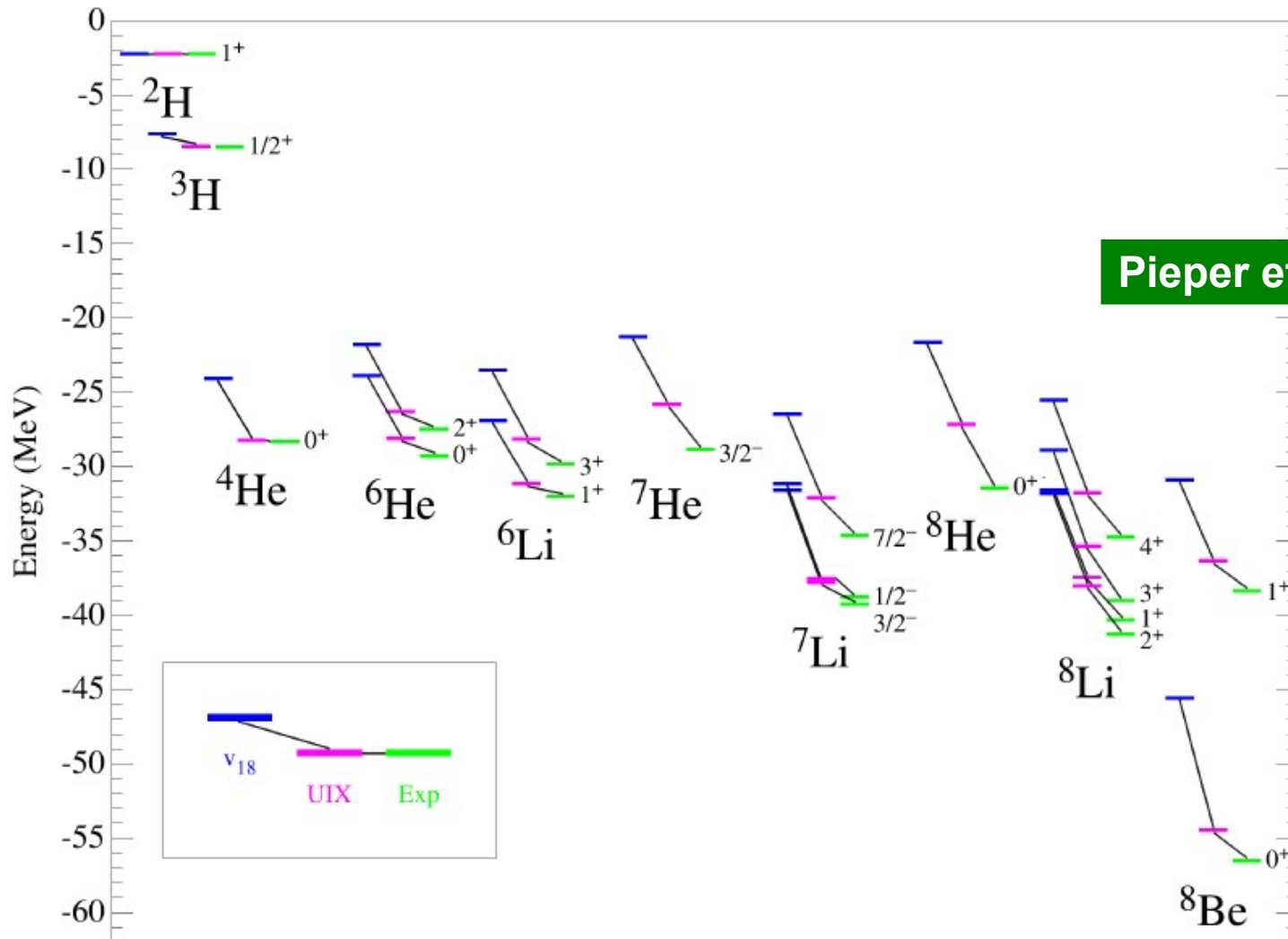
Urbana IX three body potential

Improved description of energy levels of light nuclei



Urbana IX three body potential

Improved description of energy levels of light nuclei



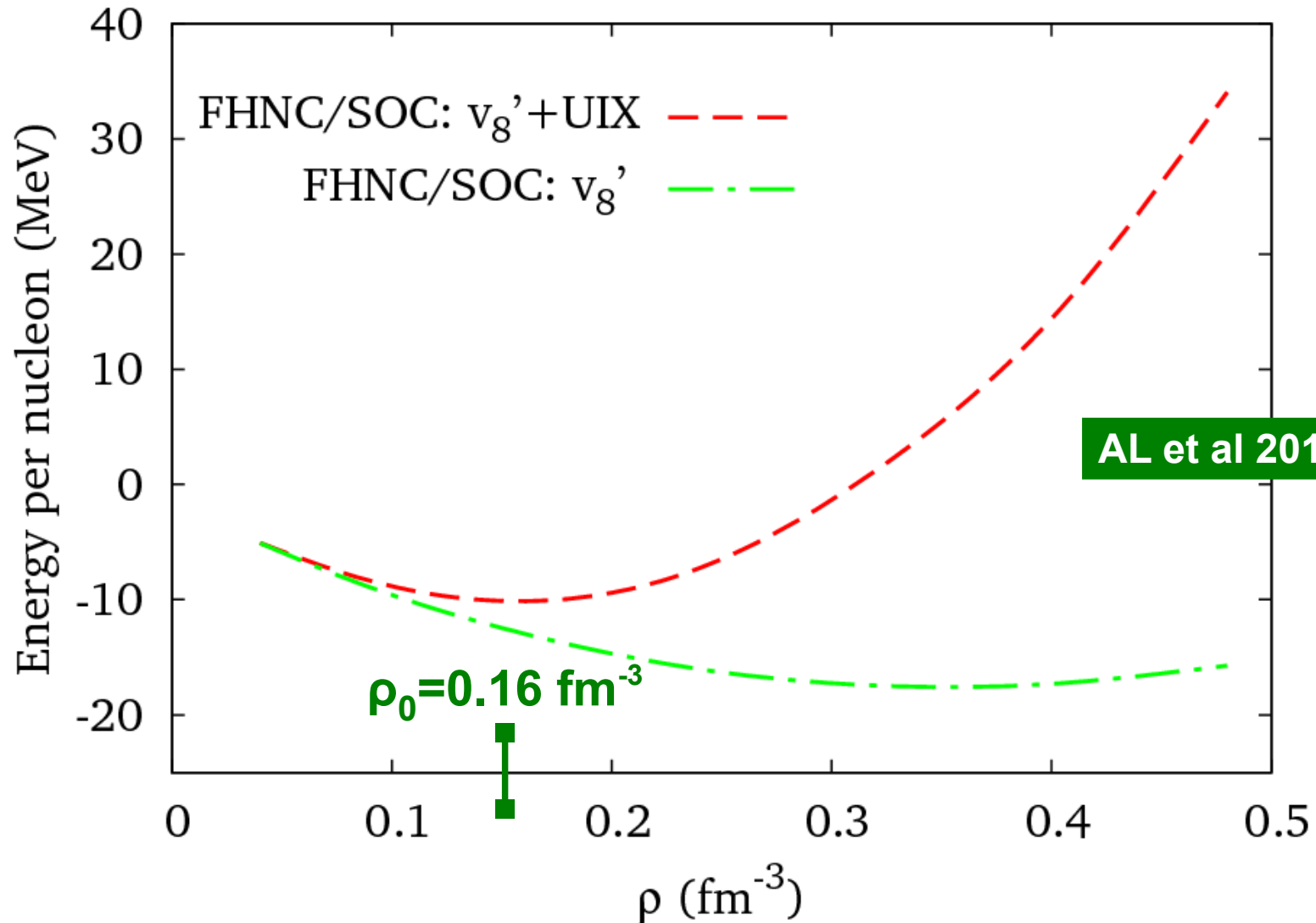
Pieper et al 2001



Still some discrepancies with experimental data!

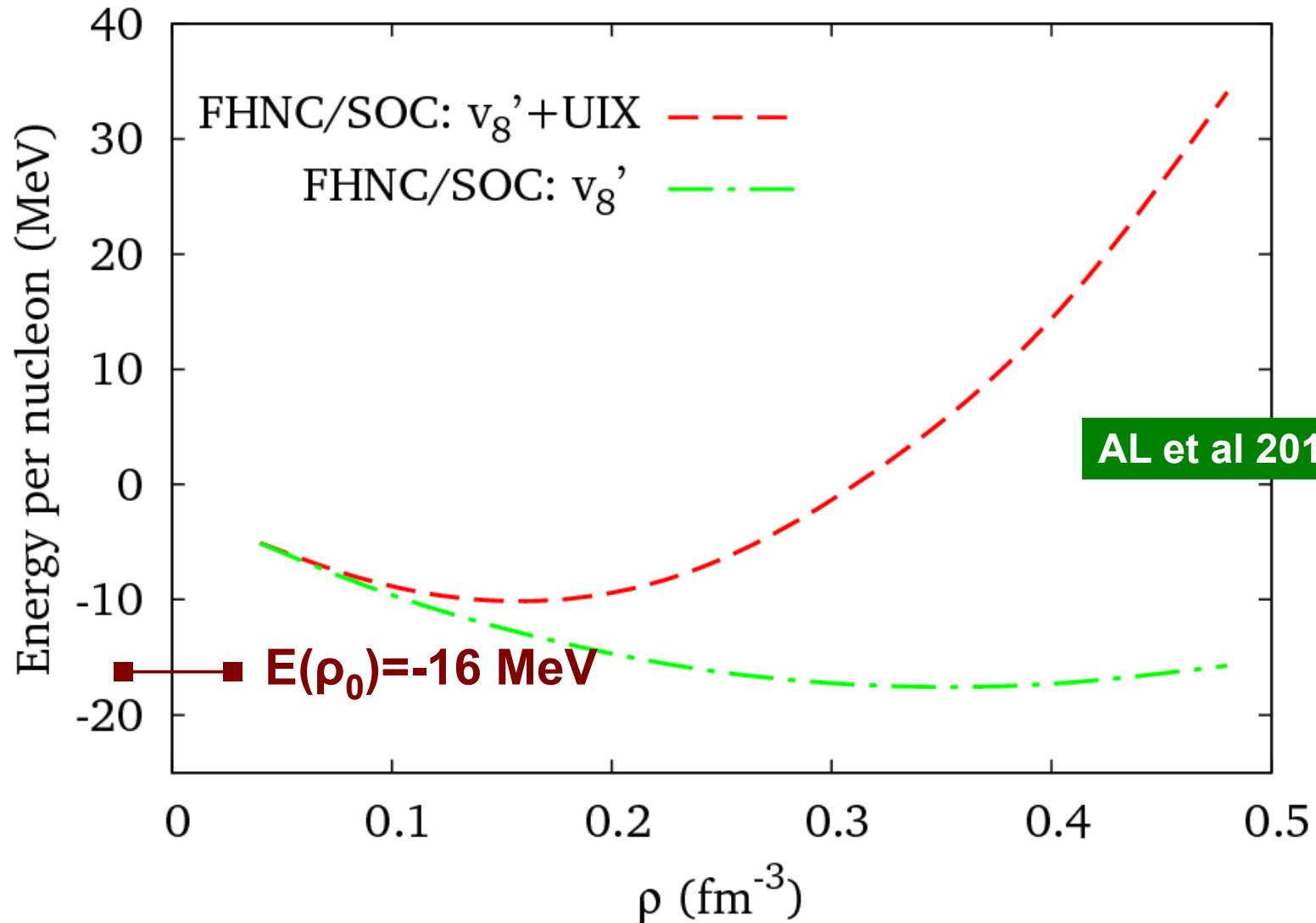
Urbana IX three body potential

SNM saturation density is well reproduced



Urbana IX three body potential

SNM saturation density is well reproduced



AL et al 2011

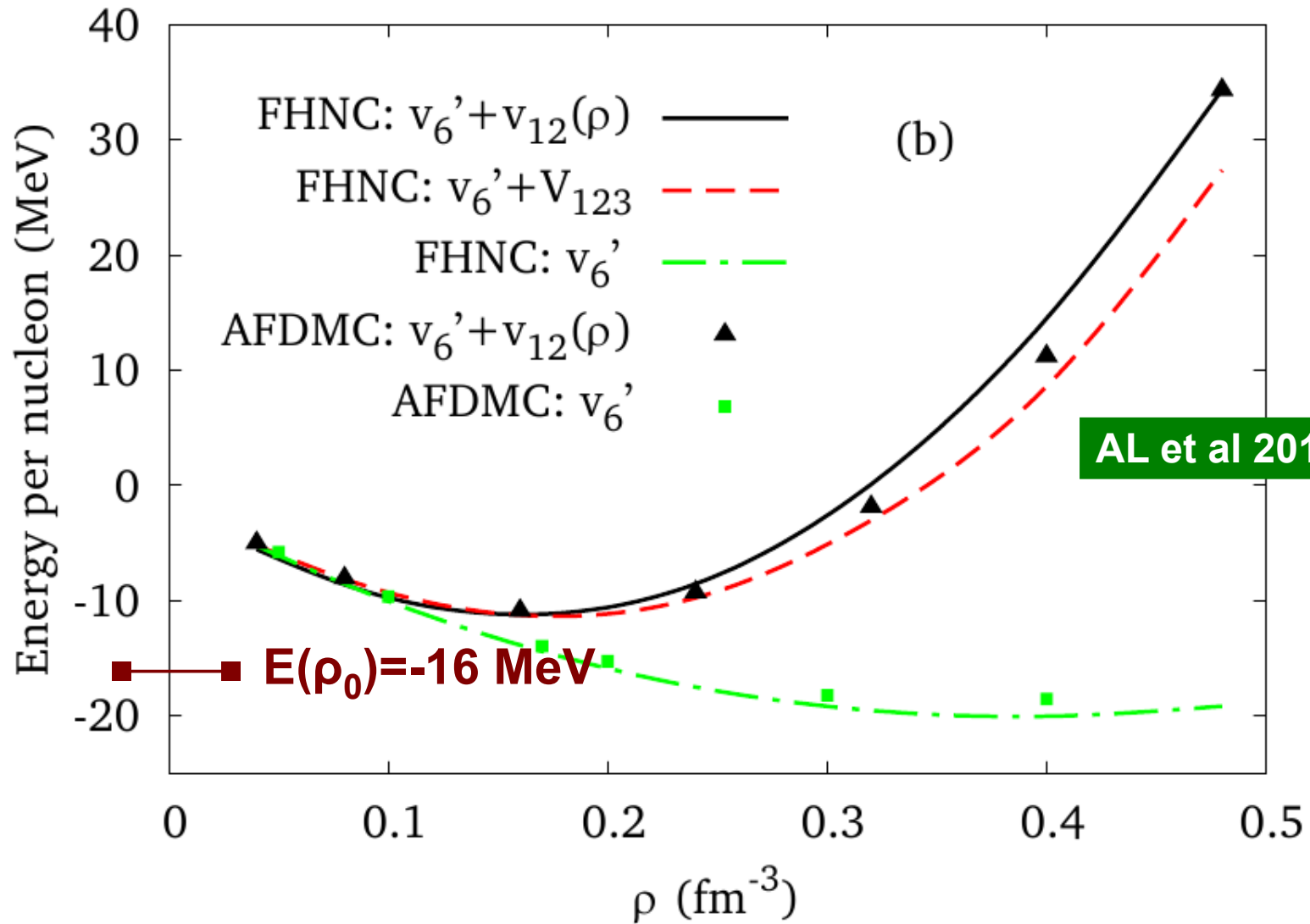
$E(\rho_0) = -16 \text{ MeV}$

SNM is underbound



Urbana IX three body potential

SNM saturation density is well reproduced



SNM is underbound



Urbana IX three body potential

The value of the n-d scattering length obtained with Argonne $v_{18} + UIX$ is not compatible with experimental data

	$v_{18} + UIX$	Exp.
$^2a_{nd}$ (fm)	0.578	$0.645 \pm 0.003 \pm 0.007$

Kievsky et al 2010

Theoretical problems



$V^{2\pi}$: no a priori reasons to stop at the first order in the perturbative expansion in the coupling constant $g_0 \sim 10$.



Adjusting U_0 to reproduce the correct value of ρ_0 , calculated within the FHNC/SOC framework, makes the potential affected by the uncertainties of the many-body technique. “**ab initio**”?

We need to go
beyond the UNIX
potential!



How to go beyond Urbana IX ?

Same strategy used for NN potential?

Decomposition of NN potential in spin-isospin structures respecting the symmetry of the interaction

Argonne v_{18} , or v_8 '

$$\hat{V}_{12} = \sum_{p=1}^n v^p(r_{12}) \hat{O}_{12}^p$$

Fitting the **huge amount**
of nn and pn data



Shape of the radial
functions $v^p(r)$

Following the same strategy adopted for the NN potential seems not to be feasible without an additional theoretical guidance.

- Large variety of different possible structures in the three-nucleon force
- Difficulties in extracting information of three nucleon force from NNN data

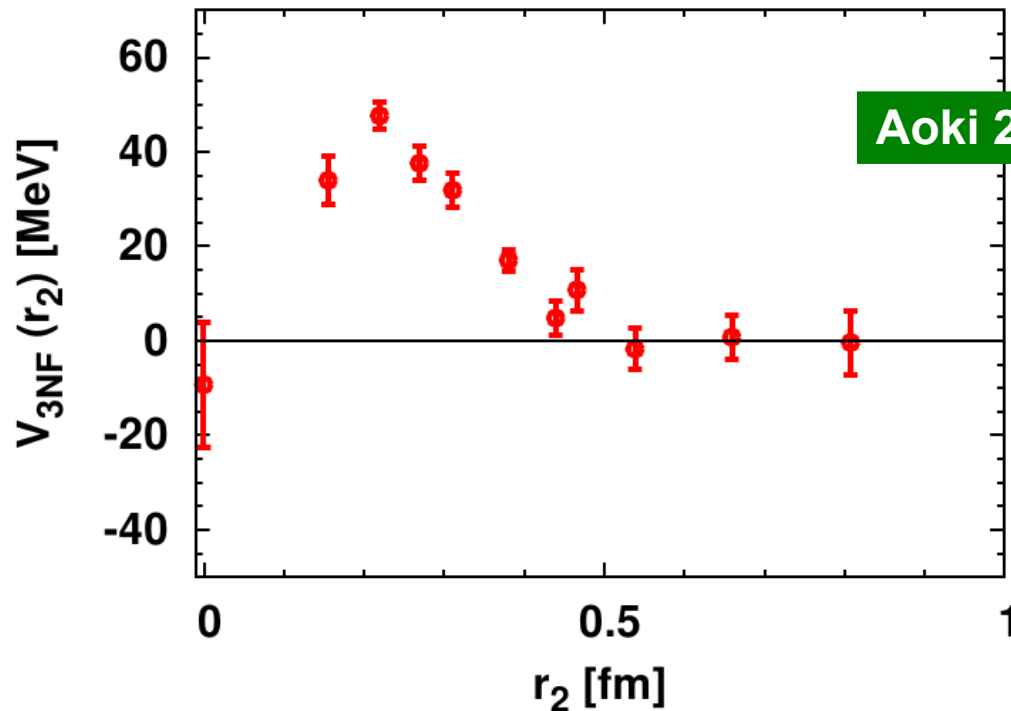
Describing interacting nucleons

THE SYSTEM

- Pions with external momentum of the order of m_π
- Non-relativistic nucleons with spatial-momentum of the order of m_π .

QCD is NOT perturbative at this scale

Lattice QCD



Effective theories
describing phenomena
which occur at a chosen
length (or energy) range.

ChPT

Chiral Perturbation Theory

If u and d quarks are massless, QCD is invariant under the **chiral symmetry group**

$$G = SU(2)_R \times SU(2)_L$$

For the hadronic spectrum to be represented, **G is spontaneously broken**

$$G = SU(2)_R \times SU(2)_L \longrightarrow H = SU(2)_I$$

Goldstone theorem

- Three massless pseudoscalar bosons appear.
- Goldstone bosons decouple in small momentum limit.

Pions!

Expansion
in powers of
 q/Λ



Chiral Perturbation Theory (ChPT)

- Quarks u and d **do have mass**, pions are pseudogoldstone bosons and have small masses, vanishing in the chiral limit
- The interactions of Goldstone bosons vanish at zero momentum transfer

Chiral Perturbation Theory

Effective Lagrangian and physical amplitudes are expanded in powers of

Soft scale m_π



$$\frac{Q}{\Lambda_\chi}$$



Hard scale $\Lambda_\chi \approx m_\rho$

The order of the **chiral nuclear potential** is related with the power of Q/Λ

LO	NLO	NNLO	NNNLO
↕	↕	↕	↕
1	$(Q/\Lambda_\chi)^2$	$(Q/\Lambda)^3$	$(Q/\Lambda)^4$

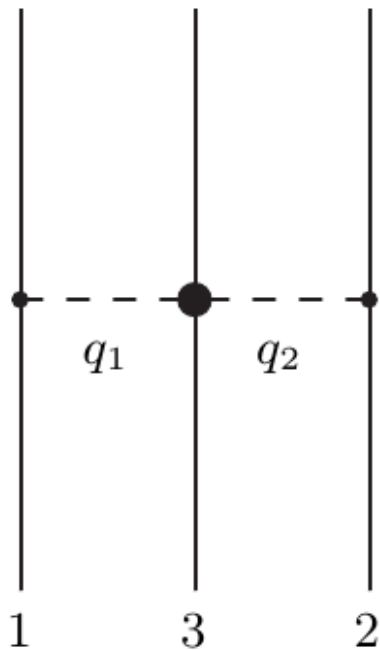
Higher order in ChPT involve more Feynman diagrams.
Weinberg scheme!

Chiral 3-body potential at NNLO

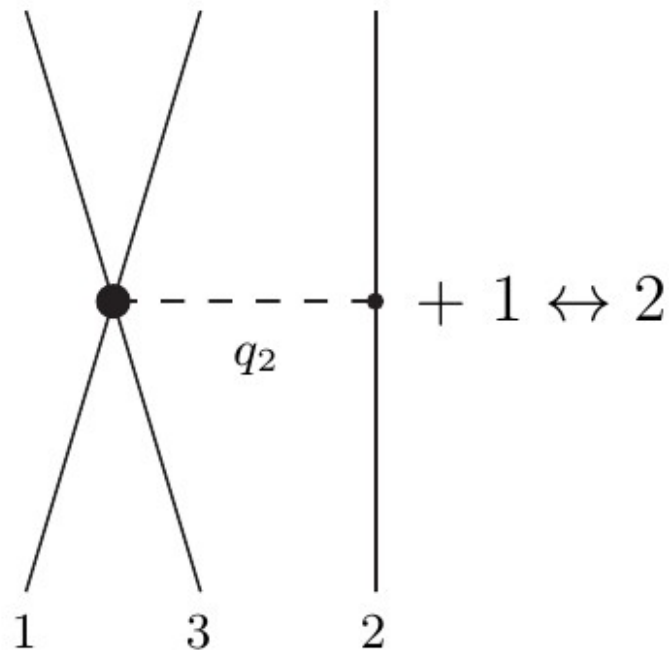
In a theory without explicit Δ degrees of freedom, the first contribution to the chiral 3NF appears at $N^2\text{LO}$ in the Weinberg counting scheme.

The interaction is described by three different physical mechanisms

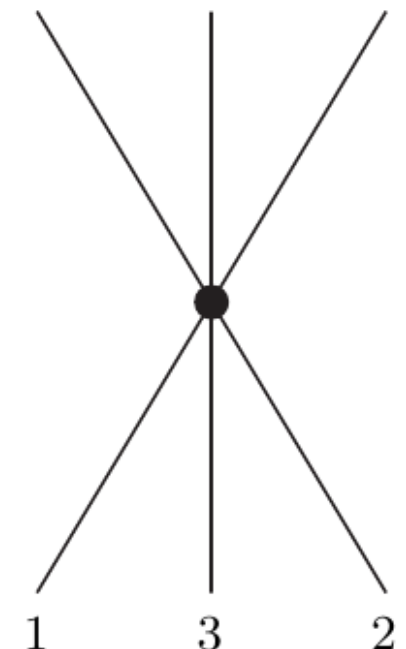
Two-pion exchange
(TPE)



One-pion exchange
(OPE)



Contact term



Cyclic sum

$$V^x(1, 2, 3) = V^x(1 : 2, 3) + V^x(2 : 1, 3) + V^x(3 : 1, 2)$$

Chiral 3-body NNLO potential

Fourier transforming the Chiral NNLO 3-body potential, originally derived in momentum space, yields a local expression in coordinate space:

NNLO potential

$$V^x(3 : 12) = \int \frac{d^3 q_1}{(2\pi)^3} \frac{d^3 q_2}{(2\pi)^3} \tilde{V}^x(3 : 12) \underbrace{F_\Lambda(q_1^2) F_\Lambda(q_2^2)}_{\text{Navratil 2007}} e^{i\mathbf{q}_1 \cdot \mathbf{r}_{13}} e^{i\mathbf{q}_2 \cdot \mathbf{r}_{23}}$$

Navratil 2007

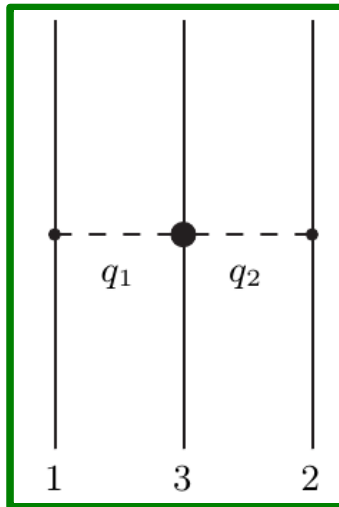
$$F_\Lambda(q_i^2) = \exp\left(-\frac{q_i^4}{\Lambda^4}\right)$$

- Depends on transferred momenta
- Generates powers of q/Λ beyond NNLO

Radial functions appearing in the coordinate space version of the chiral NNLO potential:

$$\begin{aligned} z_n(r) &= \frac{4\pi}{m_\pi^3} \int \frac{d^3 q}{(2\pi)^3} \frac{F_\Lambda(q^2)}{(q^2 + m_\pi^2)^n} e^{i\mathbf{q} \cdot \mathbf{r}} \\ &= \frac{2}{\pi m_\pi^3} \int dq q^2 \frac{F_\Lambda(q^2)}{(q^2 + m_\pi^2)^n} j_0(qr) \end{aligned}$$

TPE term



$$= c_1 V_1(3 : 12) + c_3 V_3(3 : 12) + c_4 V_4(3 : 12)$$

Tucson Melbourne potential has **the same spin-isospin structure** of the chiral NNLOL potential TPE term.

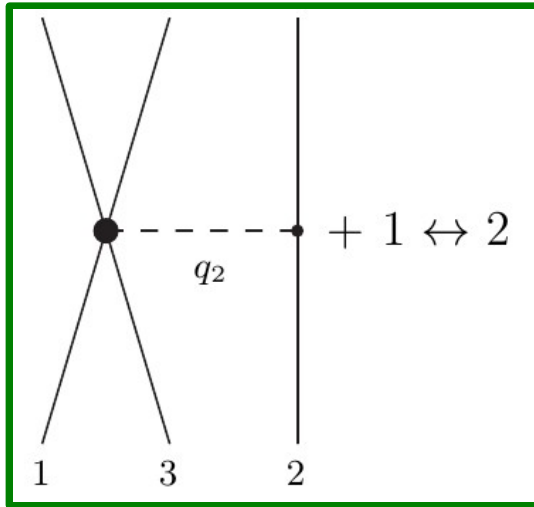
$$c_1 = \frac{a}{m_\pi^2} \quad , \quad c_3 = 2b \quad , \quad c_4 = -4d \quad , \quad F_\Lambda(q^2) = \left(\frac{\Lambda^2 - m_\pi^2}{\Lambda^2 + q^2} \right)^2 .$$

UIX potential: the anticommutator and the commutator terms in $V^{2\pi}$ correspond to V_3 and V_4

$$c_3 W_0 = 4A_{2\pi} \quad , \quad c_4 W_0 = 4C_{2\pi}$$

V_1 term **is not present** in UIX.

OPE term



From the chiral Lagrangian

$$= -c_D V_0^D \frac{(\boldsymbol{\sigma}_2 \cdot \mathbf{q}_2)}{(q_2^2 + m_\pi^2)} \left[\alpha_1 (\boldsymbol{\sigma}_1 \cdot \mathbf{q}_2) \tau_{12} + \alpha_2 (\boldsymbol{\sigma}_1 \cdot \mathbf{q}_2) \tau_{13} + \alpha_3 \mathbf{q}_2 (\boldsymbol{\sigma}_1 \times \boldsymbol{\sigma}_3) \vec{\tau}_2 \cdot (\vec{\tau}_1 \times \vec{\tau}_3) + 1 \leftrightarrow 2 \right]$$

When applied to an antisymmetric wavefunction

Epelbaum et al. (2002)

$$V^{OPE}(3 : 12) \mathcal{A}_{12} |\Psi\rangle \quad \mathcal{A}_{12} = 1 - \frac{(1 + \sigma_{12})}{2} \frac{(1 + \tau_{12})}{2}$$

All structures lead to the same expression, it is convenient to consider only one

$$V^{OPE}(3 : 12) = -c_D V_0^D \frac{(\boldsymbol{\sigma}_2 \cdot \mathbf{q}_2)}{(q_2^2 + m_\pi^2)} \left[\alpha_1 (\boldsymbol{\sigma}_1 \cdot \mathbf{q}_2) \tau_{12} + 1 \leftrightarrow 2 \right]$$

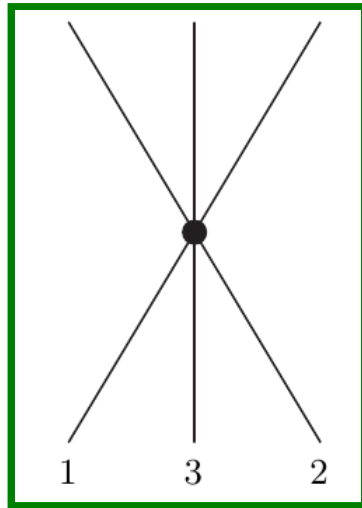
Regulator dependence on the transferred momentum \mathbf{q}_2



The antisymmetrization operator also exchanges **the positions of nucleons**

In principle all the different terms need to be considered.

Contact term



$$= c_E W_0^E \tau_{12}$$

Because of \mathcal{A}_{123} all terms coming from the Lagrangian give the same contribution

Regulator dependence on the transferred momentum \mathbf{q}_2

In principle all the different terms need to be considered.

- **TM'** potential has a repulsive three-nucleon contact term without isospin dependence

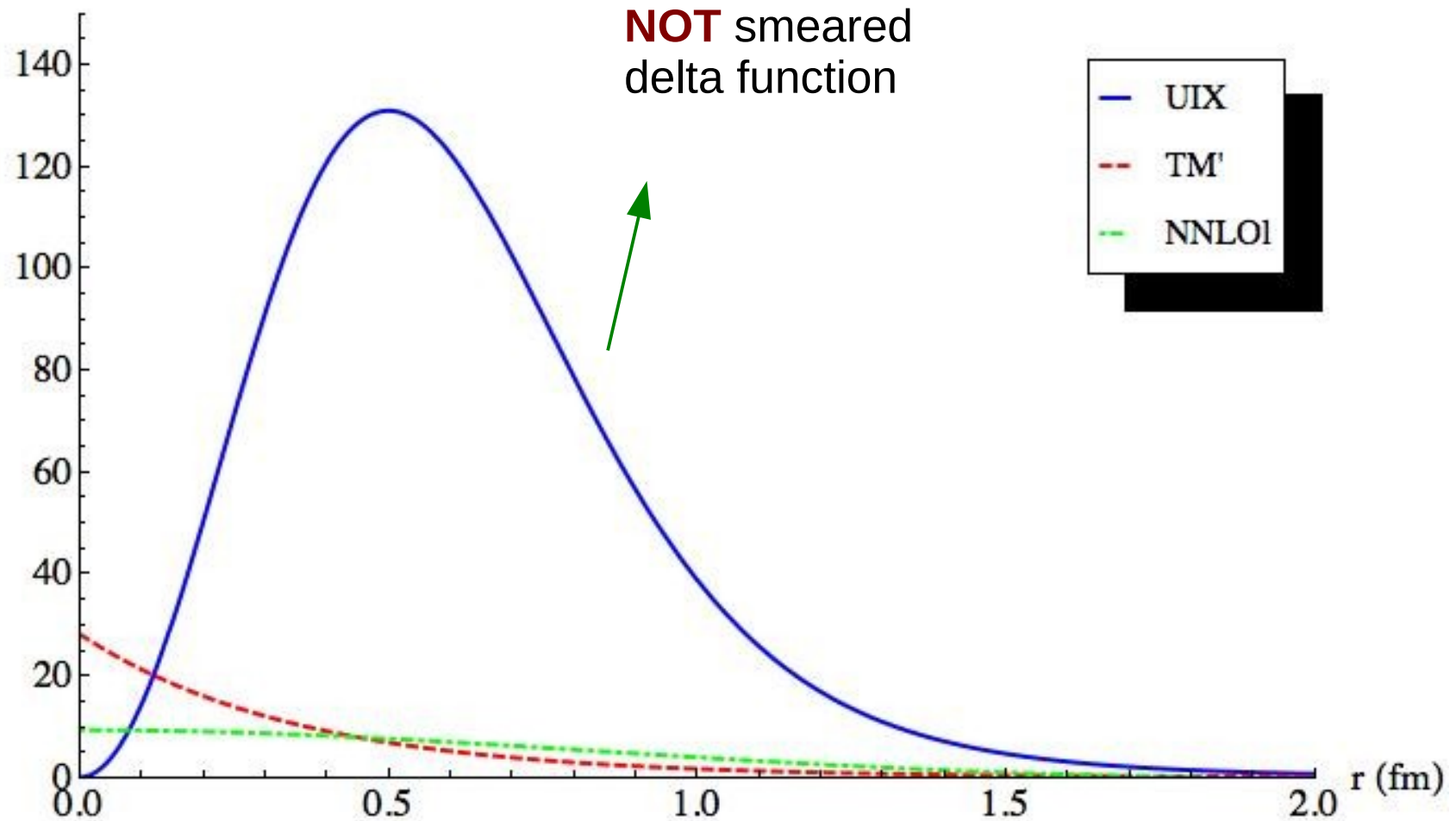
$$V_E(3 : 12) = c_E W_0^E$$

- **UIX**: V^R although is not a contact term, has the same structure of the contact term of NNLO

$$U_0 \longleftrightarrow c_E W_0^E$$

Contact term

Repulsive term radial functions are different



NNLO contact term issue in nuclear matter

Full momentum space expression of NNLO contact term

$$V^{cont}(3 : 12) = c_E(\beta_1 + \beta_2\sigma_{12} + \beta_3\tau_{12} + \beta_4\sigma_{12}\tau_{12} + \beta_5\sigma_{12}\tau_{23} \\ + \beta_6(\vec{\sigma}_1 \times \vec{\sigma}_2) \cdot \vec{\sigma}_3 + (\vec{\tau}_1 \times \vec{\tau}_2) \cdot \vec{\tau}_3 + 1 \leftrightarrow 2)$$

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Fourier transform of the isospin and scalar term yields

$$V_E^\tau(3 : 12) = c_E^\tau W_0^E \tau_{12} z_0(r_{13}) z_0(r_{23})$$

$$V_E^I(3 : 12) = c_E^I W_0^E z_0(r_{13}) z_0(r_{23})$$

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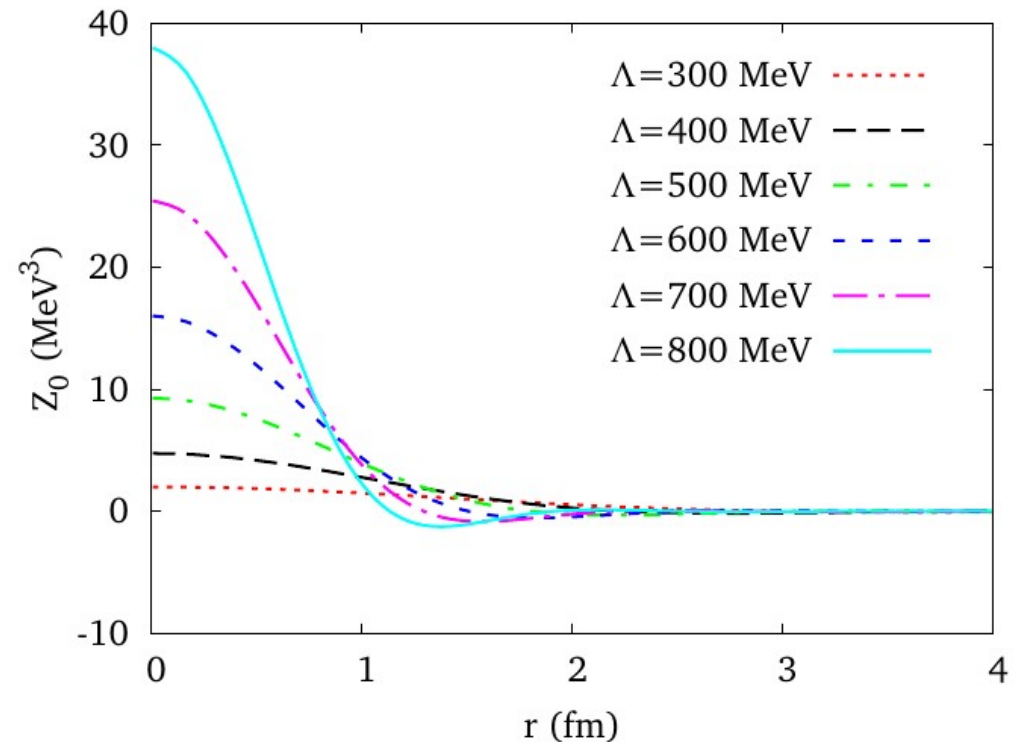
$$V_E^\tau(3 : 12) = c_E^\tau W_0^E \tau_{12} z_0(r_{13}) z_0(r_{23})$$

$$V_E^I(3 : 12) = c_E^I W_0^E z_0(r_{13}) z_0(r_{23})$$

Convenient normalization for the radial function

$$Z_0(r) = \frac{(4\pi)}{m_\pi^3} z_0(r)$$

$$\lim_{\Lambda \rightarrow \infty} Z_0(r) = \delta(r)$$



NNLO contact term issue in nuclear matter

In the limit of infinite cutoff

$$\sum_{cycl} V_0^E \delta(\mathbf{r}_{13}) \delta(\mathbf{r}_{23}) \tau_{12} \mathcal{A}_{123} = - \sum_{cycl} V_0^E \delta(\mathbf{r}_{13}) \delta(\mathbf{r}_{23}) \mathcal{A}_{123}$$

The terms are **equivalent!**

Crucial for the equivalence

The exchange of particles lying in the same position is the identity!

$$e^{i\mathbf{k}_{ij} \cdot \mathbf{r}_{ij}} \delta(\mathbf{r}_{ij}) = \delta(\mathbf{r}_{ij})$$

At finite values of the cutoff this is not true anymore.

Not considering all the terms lead to ambiguities in both
PNM and SNM

NNLOL contact term issue in nuclear matter

Assume that reproducing the binding energies of light nuclei and $2a_{\text{nd}}$ and requires a repulsive V_E

$$\Rightarrow \begin{cases} c_E^T < 0 \\ c_E^I > 0 \end{cases}$$

Pure Neutron Matter (PNM)

For Pauli principle, in PNM the expectation value of a three-body contact term is zero.

WHILE...

$$\langle V_E^{I,\tau} \rangle_{PNM} = \mathcal{O}\left(\frac{q^4}{\Lambda^4}\right)$$

Λ (MeV)	$\langle V_E^{I,\tau_{12}} \rangle_{PNM}^{FG} / A$ (MeV)
300	9.15
400	5.95
500	3.60
600	2.15
700	1.30
800	0.81
∞	0

Furthermore

$$\langle \tau_{12} \rangle_{PNM} = 1 \Rightarrow \begin{cases} \langle V_E^I \rangle_{PNM} > 0 \\ \langle V_E^{\tau_{12}} \rangle_{PNM} < 0 \end{cases}$$

Fixing only one of the contact terms of NNLOL on low energy observables leads to ambiguity in PNM.

NNLOL contact term issue in nuclear matter

Assume that reproducing the binding energies of light nuclei and $2a_{\text{nd}}$ and requires a repulsive V_E

$$\Rightarrow \begin{cases} c_E^T < 0 \\ c_E^I > 0 \end{cases}$$

Symmetric Nuclear Matter (SNM)

Infinite cutoff

$$\frac{\langle V_E^{\tau_{12}} \rangle_{SNM}^{FG}}{A} = -\frac{3}{16} \rho^2 V_0^E$$

$$\frac{\langle V_E^I \rangle_{SNM}^{FG}}{A} = \frac{3}{16} \rho^2 V_0^E$$

Finite cutoff

Λ (MeV)	$\langle V_E^{\tau_{12}} \rangle_{SNM}^{FG}/A$ (MeV)	$\langle V_E^I \rangle_{SNM}^{FG}/A$ (MeV)
300	-2.61	10.21
400	-3.61	8.15
500	-4.37	6.93
600	-4.87	6.30
700	-5.15	5.98
800	-5.30	5.81
∞	-5.55	5.55

The two contact term are equivalent in the limit of infinite cutoff only

3-body potential analysis

Kievsky et al. in 2010 have found the best-fit values for the TM' and NNOL 3-body potentials plus Argonne v_{18} NN potential to simultaneously reproduce

$$\left\{ \begin{array}{l} B(^3H) = -8.482 \text{ MeV} \\ B(^4He) = -28.30 \text{ MeV} \\ {}^2a_{nd} = 0.645 \pm 0.003 \pm 0.007 \text{ fm} \end{array} \right.$$

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Chiral NNLOL potential

Potential	c_3 (MeV $^{-1}$)	c_4 (MeV $^{-1}$)	c_D	c_E
NNLOL $_1$	-0.00448	-0.001963	-0.5	0.100
NNLOL $_2$	-0.00448	-0.002044	-1.0	0.000
NNLOL $_3$	-0.00480	-0.002017	-1.0	-0.030
NNLOL $_4$	-0.00544	-0.004860	-2.0	-0.500

MIXED APPROACH

Fit of all c_i required

$$\left\{ \begin{array}{l} c_1 = 0.00081 \text{ MeV}^{-1} \\ \Lambda_\chi = 700 \text{ MeV} \\ \Lambda = 500 \text{ MeV} \end{array} \right.$$

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TM' potential

Potential	$b(m_\pi^{-3})$	$d(m_\pi^{-3})$	c_E	$\Lambda(m_\pi)$
TM' ₁	-8.256	-4.690	1.0	4.0
TM' ₂	-3.870	-3.375	1.6	4.8
TM' ₃	-2.064	-2.279	2.0	5.6

$$a = -0.87 m_\pi^{-1}$$

Correlated basis function

The correlated basis ground state is defined by $|\Psi_0\rangle = \frac{\hat{F}|\Phi_0\rangle}{\langle\Phi_0|\hat{F}^\dagger\hat{F}|\Phi_0\rangle^{1/2}}$

The Fermi gas wave function is a Slater determinant of plane waves

$$\Phi_0 = \mathcal{A}[\phi_1(x_1) \dots \phi_A(x_A)]$$

The correlation operator reflects the structure of the NN potential

$$F = \mathcal{S}\left(\prod_{j>i=1}^A F_{ij}\right) = \mathcal{S}\left(\prod_{j>i=1}^A \sum_{p=1}^6 f^p(r_{ij}) O_{ij}^p\right)$$

Variational approach!

Variational principle holds

$$E_V = \langle\Psi_0|H|\Psi_0\rangle = \frac{\langle\Phi_0|F^\dagger H F|\Phi_0\rangle}{\langle\Phi_0|F^\dagger F|\Phi_0\rangle} \geq E_0$$

Exact ground state energy

The correlation functions are determined variationally by minimizing E_V

Correlated basis function

Hamiltonian expectation value

$$E_V = \frac{\int dx_1 \dots dx_A \Phi_0^*(x_1 \dots x_A) F^\dagger H F \Phi_0(x_1 \dots x_A)}{\int dx_1 \dots dx_A \Phi_0^*(x_1 \dots x_A) F^\dagger F \Phi_0(x_1 \dots x_A)}$$

Integration over the coordinates of a huge number of particles.



Cluster expansion

Key point of the cluster decomposition: expansion of $F^\dagger F$ in powers of

$$h_{ij} \equiv f_{ij}^c - 1 \quad , \quad 2f_{ij}^c f_{ij}^p \quad , \quad f_{ij}^{p>1} f_{ij}^{q>1}$$

The expansion can be **represented by generalized Mayer diagrams**

Massive summation of relevant diagrams

- Scalar diagrams: FHNC

No elementary diagrams

- Operatorial diagrams: SOC

At most two operators arrive at a given point of the diagram.

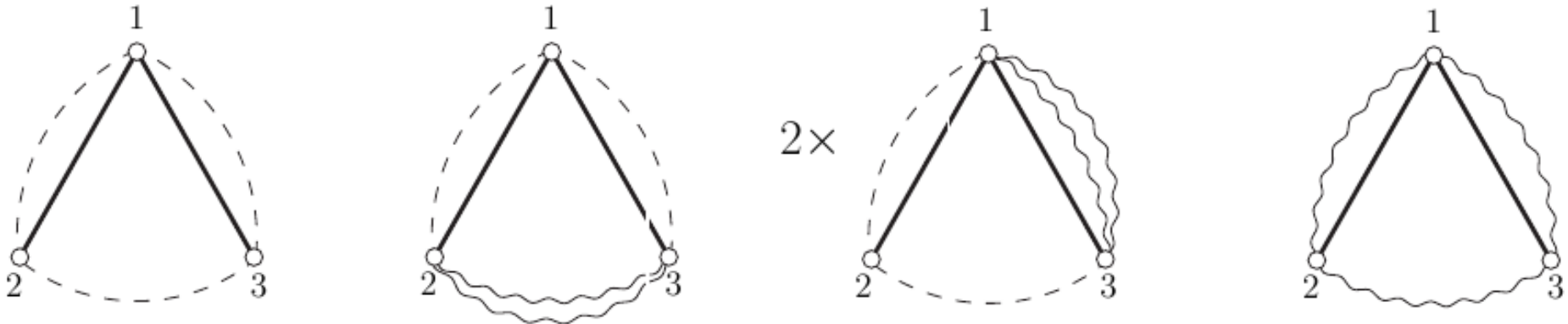
Violation of variational principle?

3-body potentials in CBF

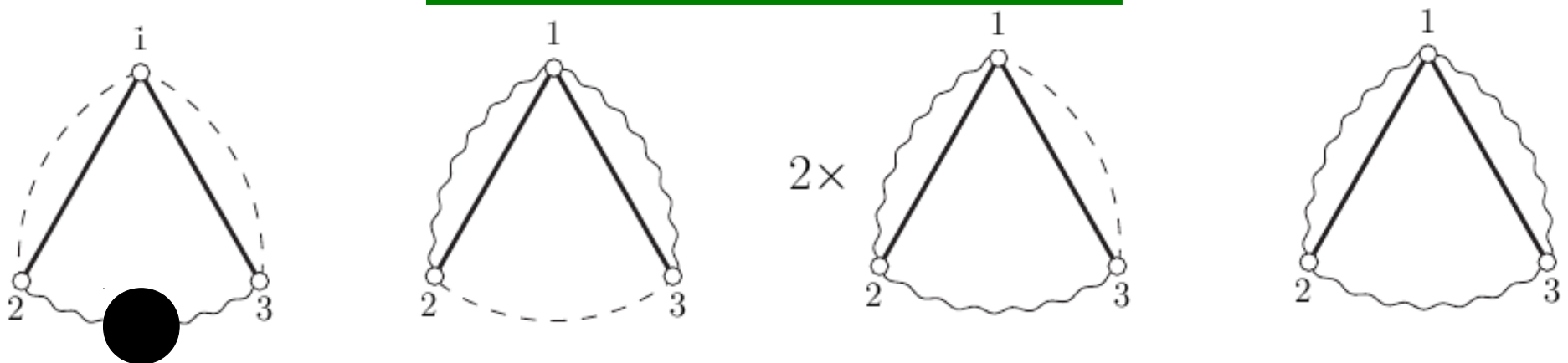
Expectation value of the three body potential

$$\langle V \rangle = \frac{\int dx_1 \dots dx_A \Phi_0^*(x_1 \dots x_A) F^\dagger V_{123} F \Phi_0(x_1 \dots x_A)}{\int dx_1 \dots dx_A \Phi_0^*(x_1 \dots x_A) F^\dagger F \Phi_0(x_1 \dots x_A)}$$

Diagrams involved for the contact term V_E



Diagrams for TPE and OPE



3-body potentials in CBF: simulated annealing

Variational energy depends on a set of parameters

$$E_V = E_V(d_c, d_t, \beta_p, \alpha_p)$$

For the minimization of E_V



Simulated annealing procedure

3-body potentials in CBF: simulated annealing

Variational energy depends on a set of parameters

$$E_V = E_V(d_c, d_t, \beta_p, \alpha_p)$$

For the minimization of E_V



Simulated annealing procedure




3-body potentials in CBF: simulated annealing

Variational energy depends on a set of parameters

$$E_V = E_V(d_c, d_t, \beta_p, \alpha_p)$$

For the minimization of E_V  **Simulated annealing procedure**

Metropolis algorithm



$$s = \{d_c, d_t, \beta_p, \alpha_p\} \quad s' = \{d'_c, d'_t, \beta'_p, \alpha'_p\} \quad \text{with} \quad P_{s,s'} = \exp \left[- \frac{E(s') - E(s)}{T} \right]$$

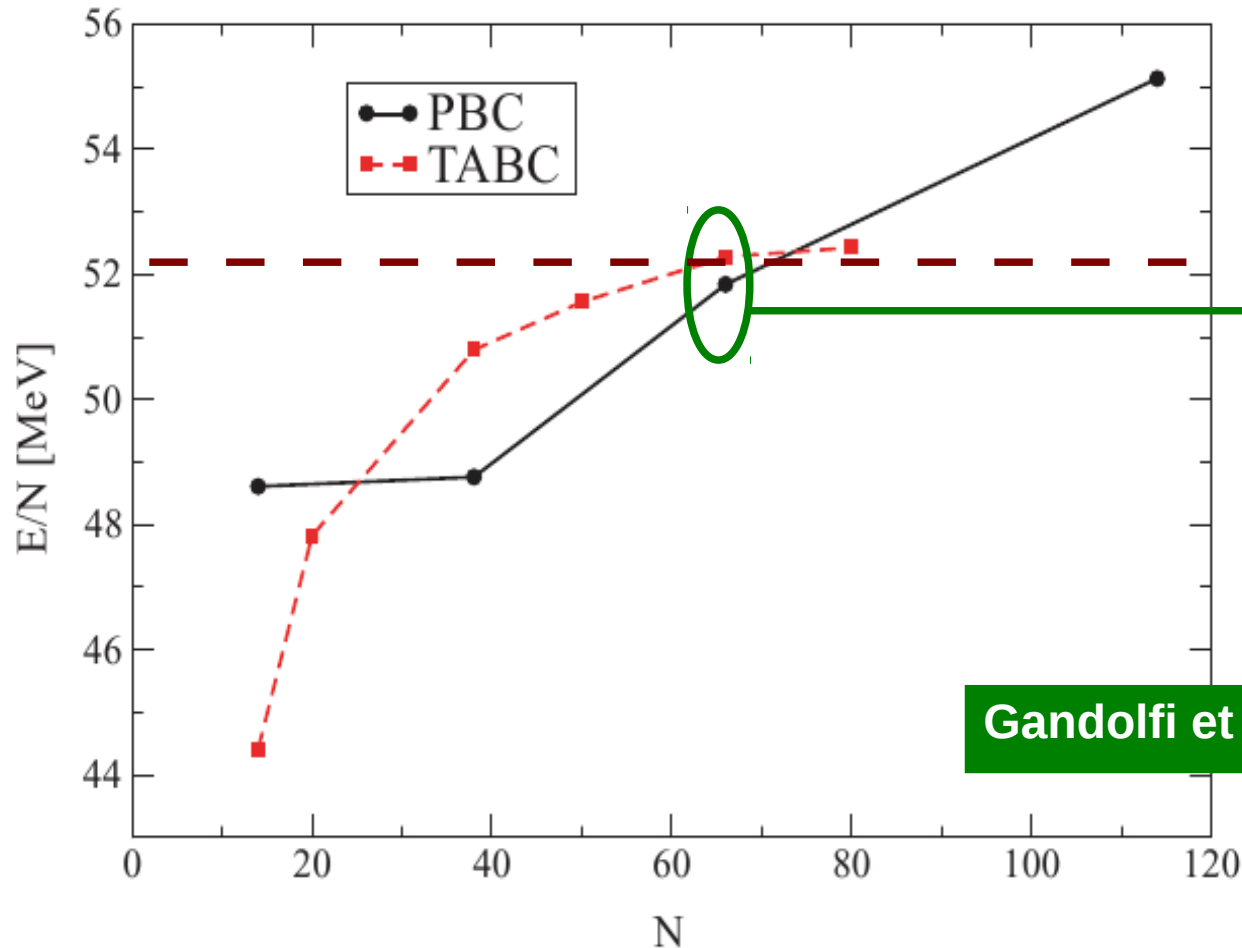
As T is lowered, the parameters stay closer to the minimum of E_V

To keep the violations under control  Constrained optimization

$$\left\{ \begin{array}{l} |E_{PB} - E_{JF}| < 10\% T_F \\ \left| \rho \int d\vec{r}_{12} (g^c(r_{12}) - 1) + 1 \right| < 0.03 \\ \left| \frac{\rho}{3} \int d\vec{r}_{12} g^T(r_{12}) + 1 \right| < 0.03 \end{array} \right.$$

3-body potentials AFDMC

AFDMC simulations for PNM with **66 neutrons in periodic box system**.

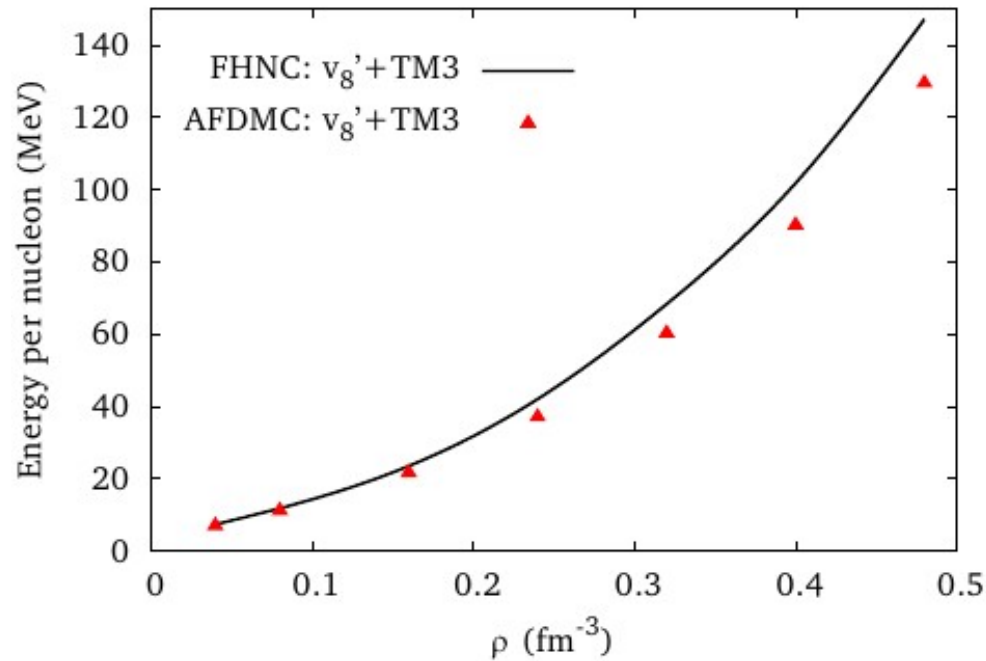
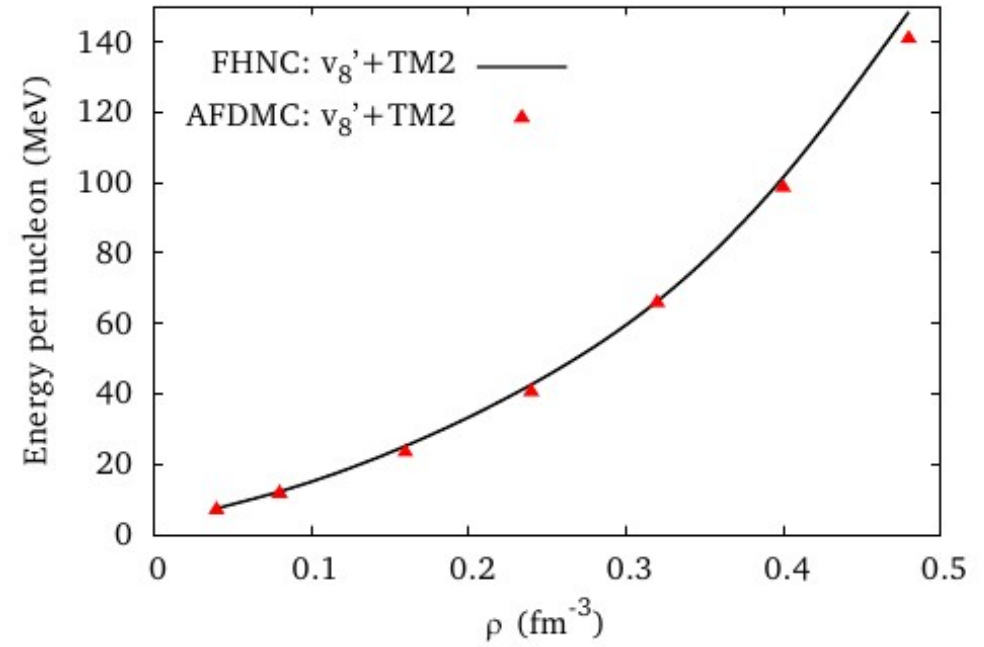
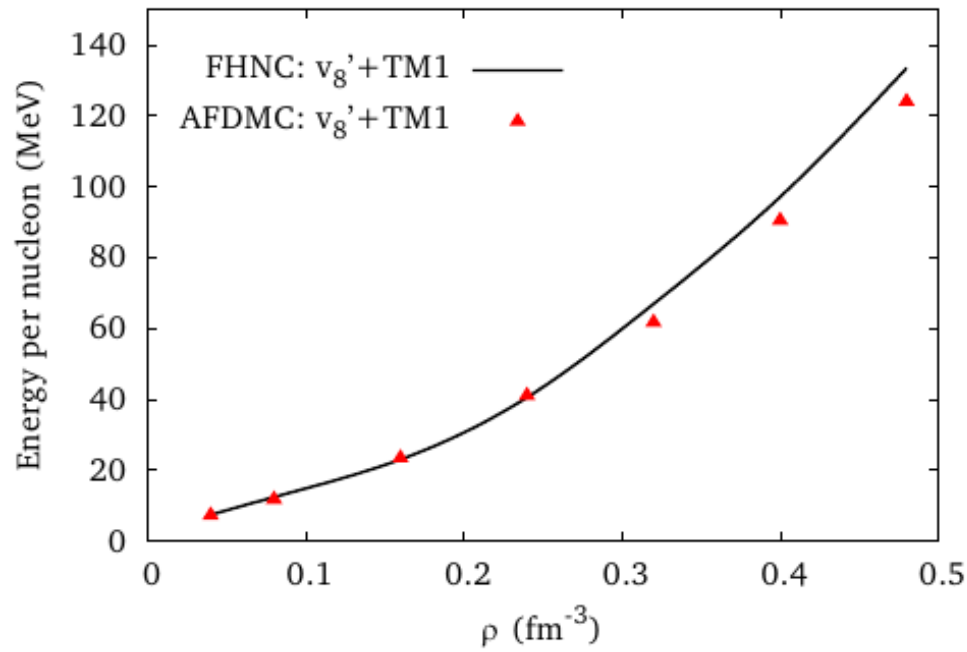


For 66 fermions
difference around 2%
of the asymptotic
value of TABC

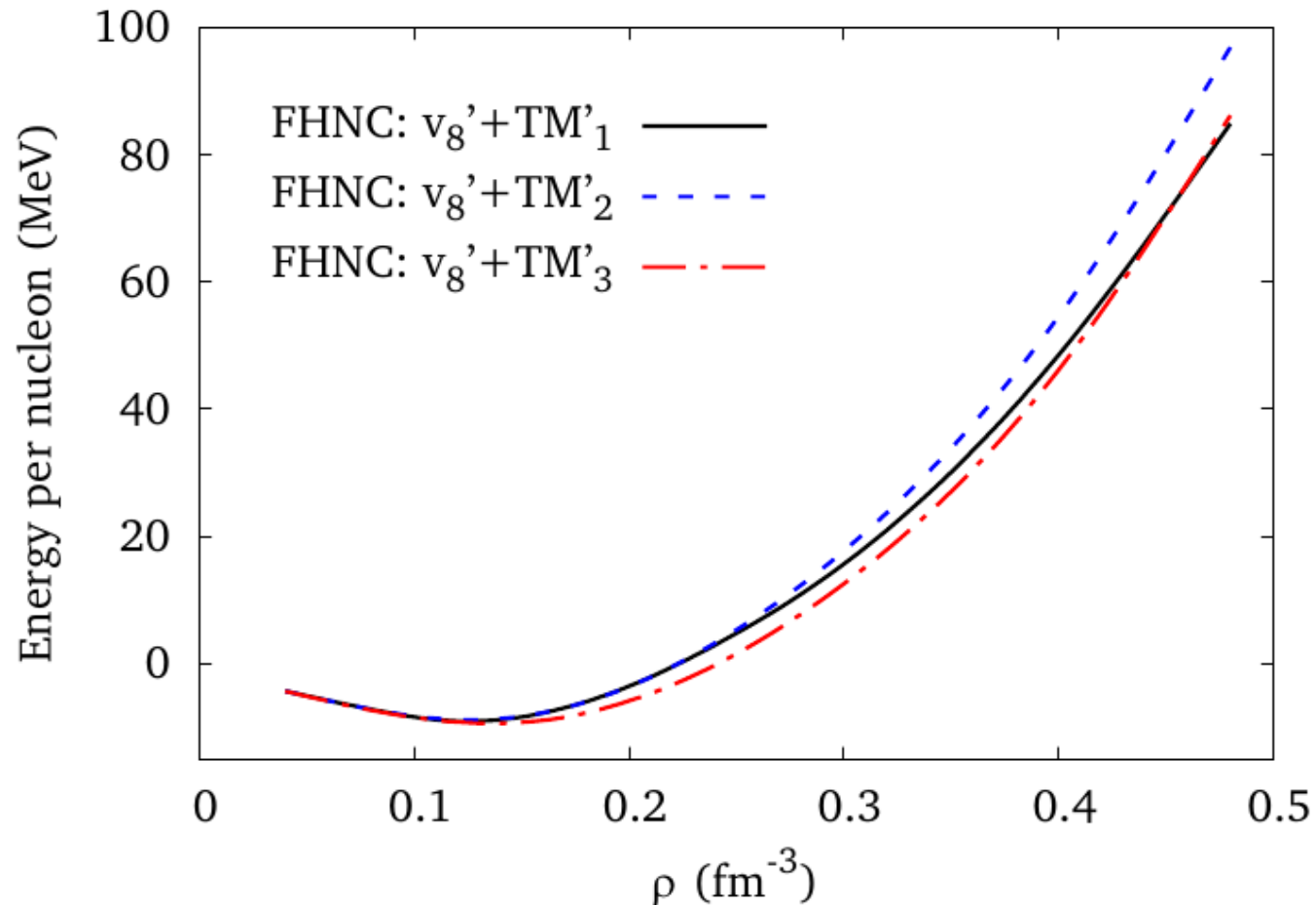
Gandolfi et al. 2009

	$A = 14$	$A = 38$	$A = 66$	$A = 114$	∞
$E/A(\text{MeV})$	56.51	53.50	55.43	56.58	55.71

TM' results for PNM



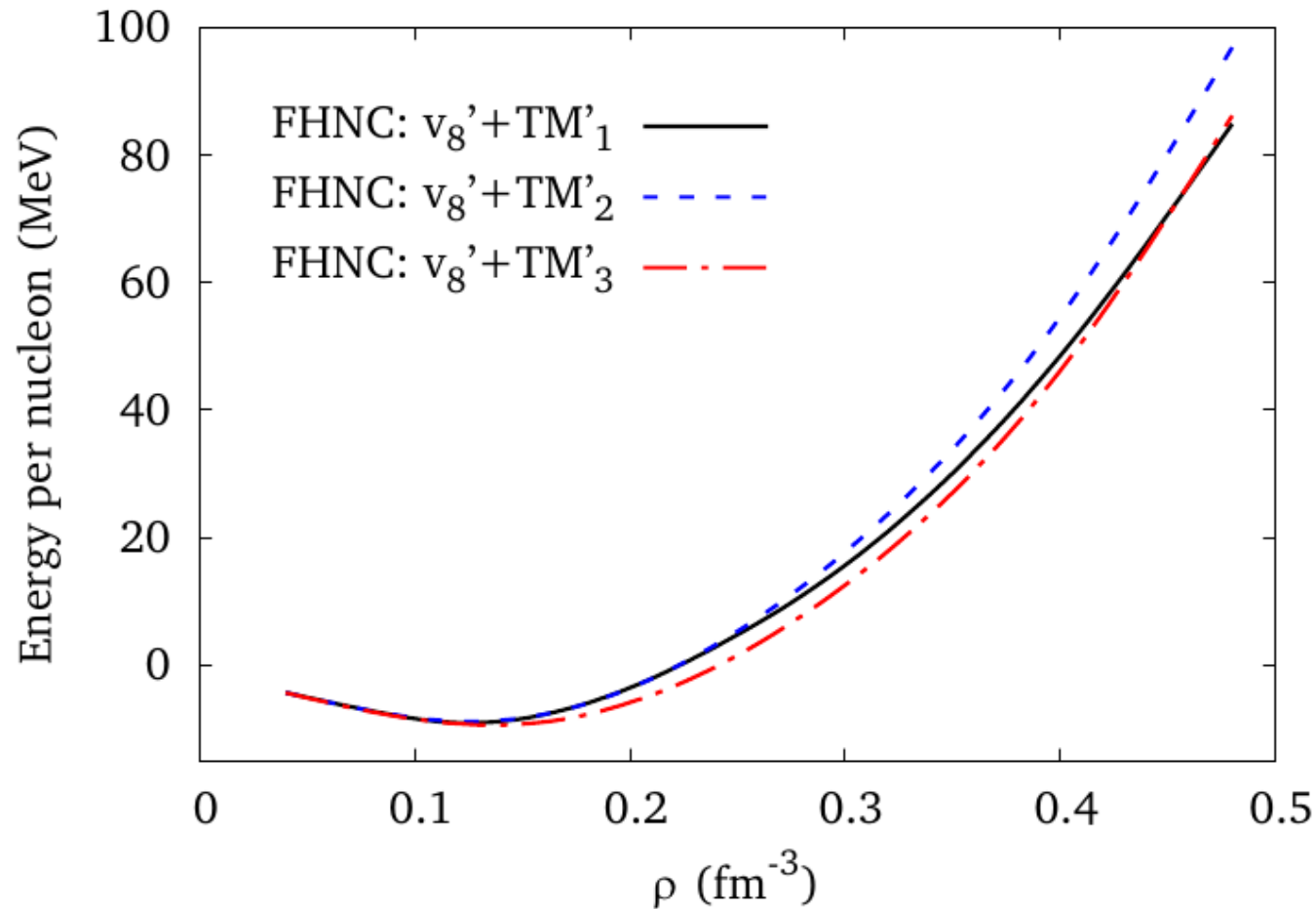
TM' results for SNM



Equations of State very close to each other

Is this happening because three body force are designed to reproduce $^2a_{nd}$ also?

TM' results for SNM



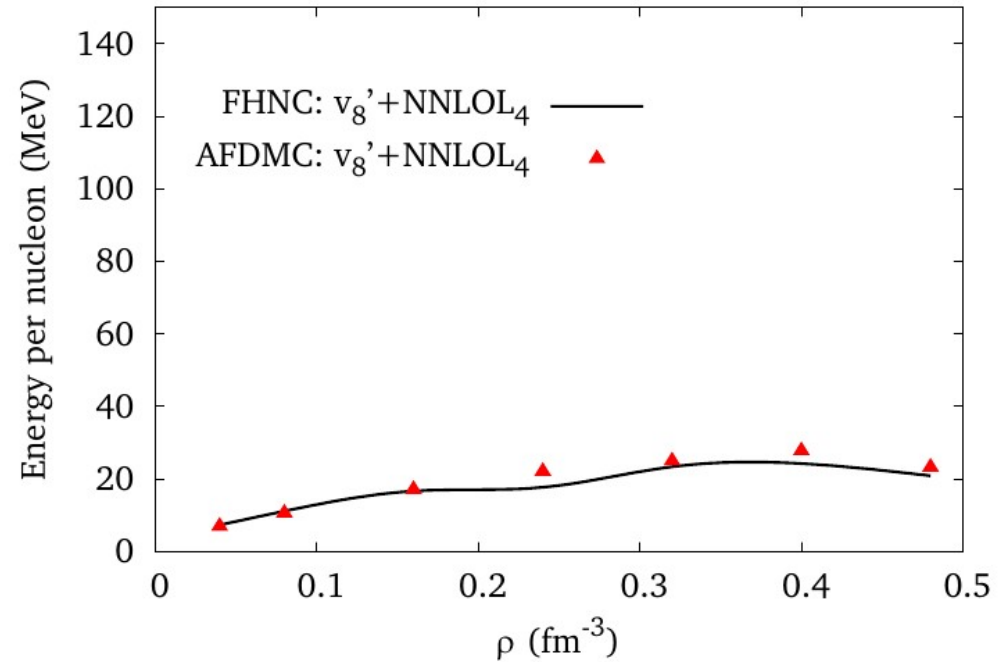
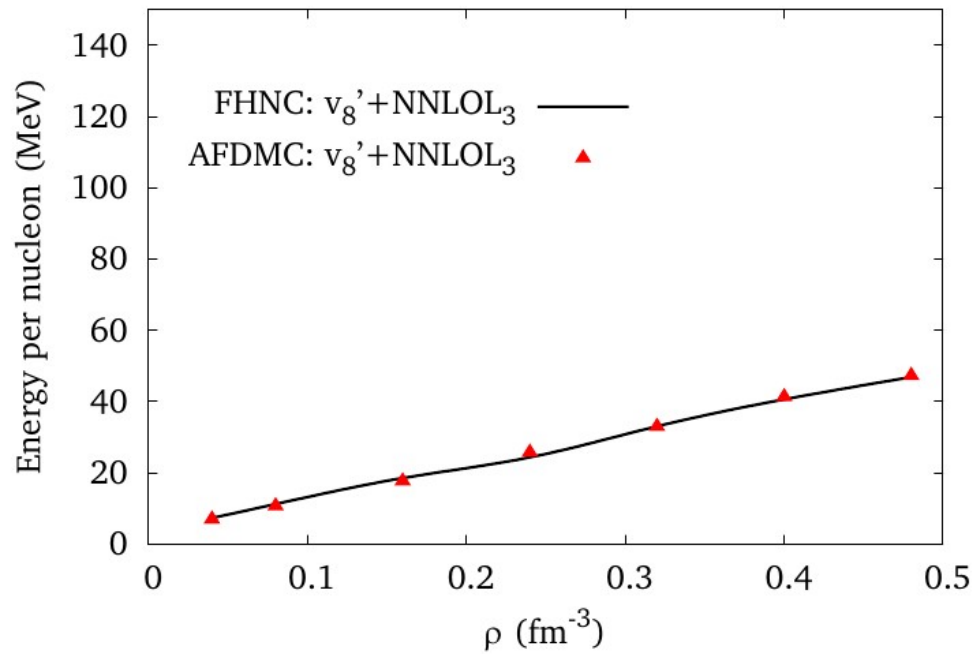
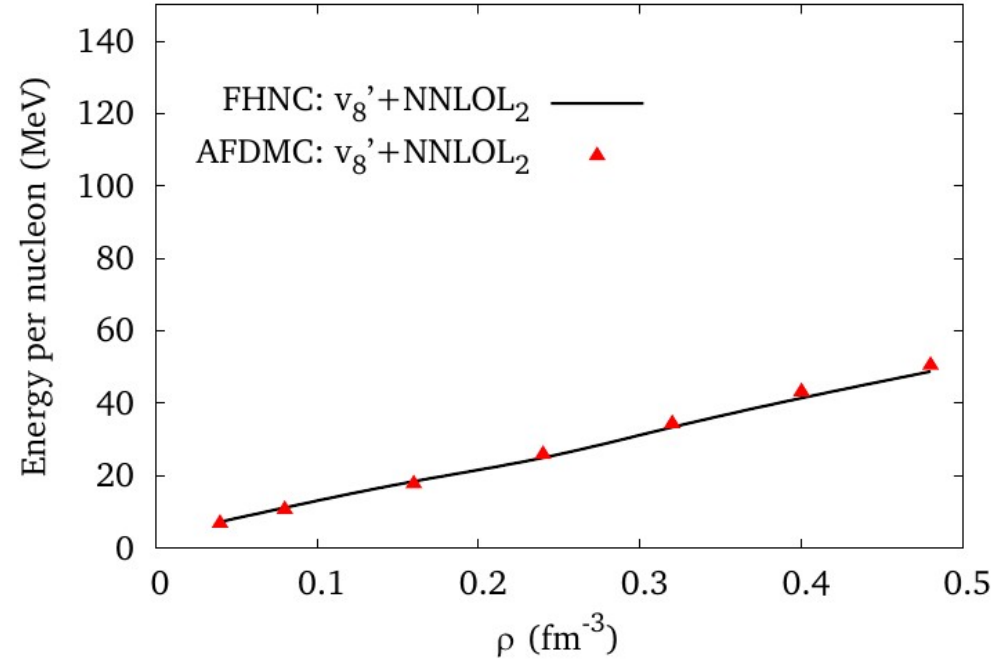
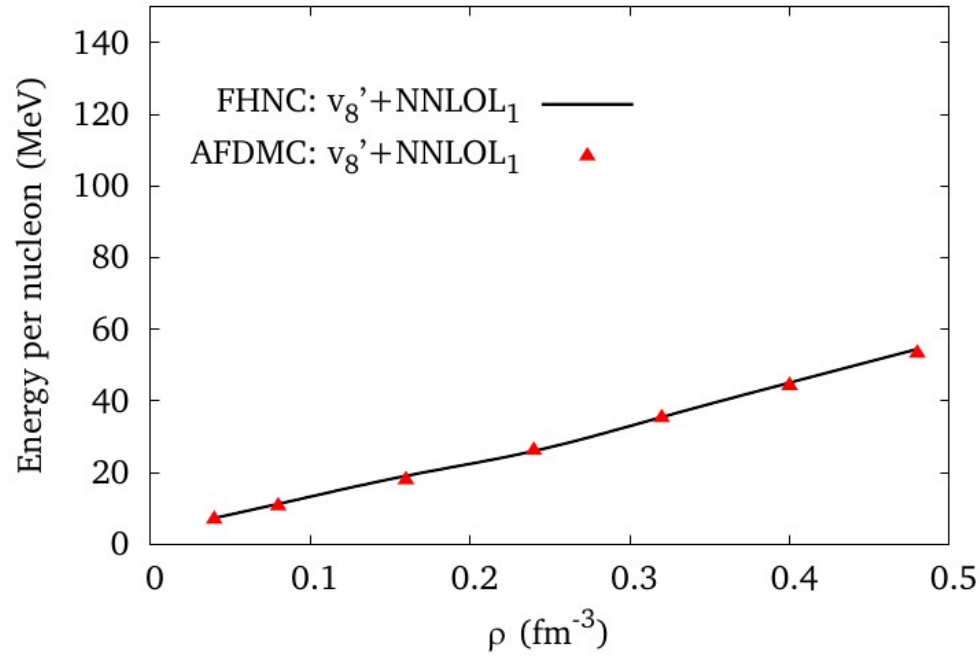
	TM'₁	TM'₂	TM'₃
ρ_0 (fm ⁻³)	0.12	0.13	0.14
E_0 (MeV)	-9.0	-8.8	-9.4
K (MeV)	266	243	249



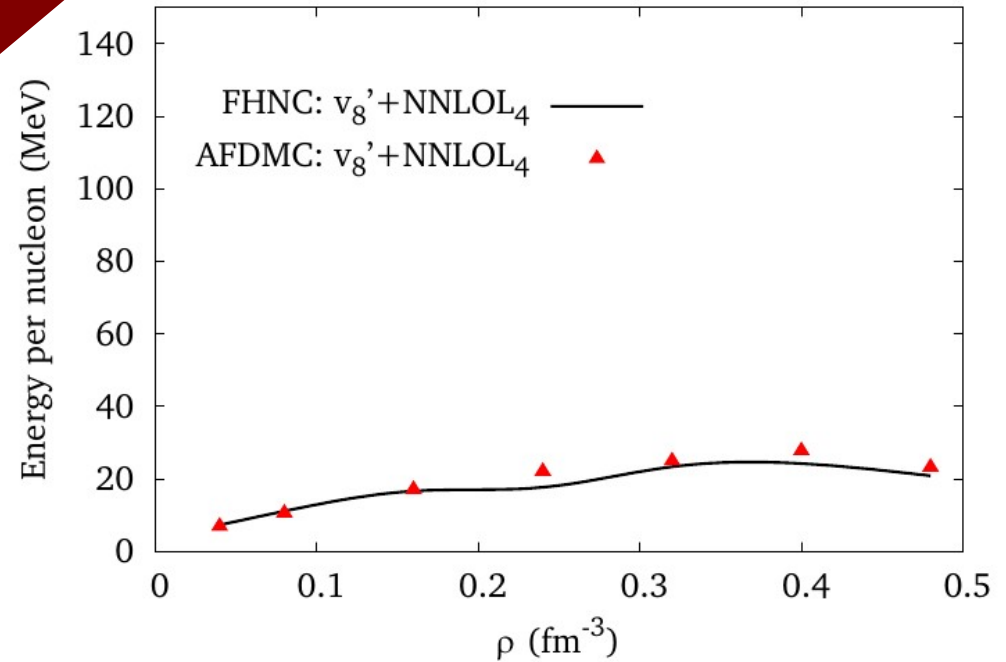
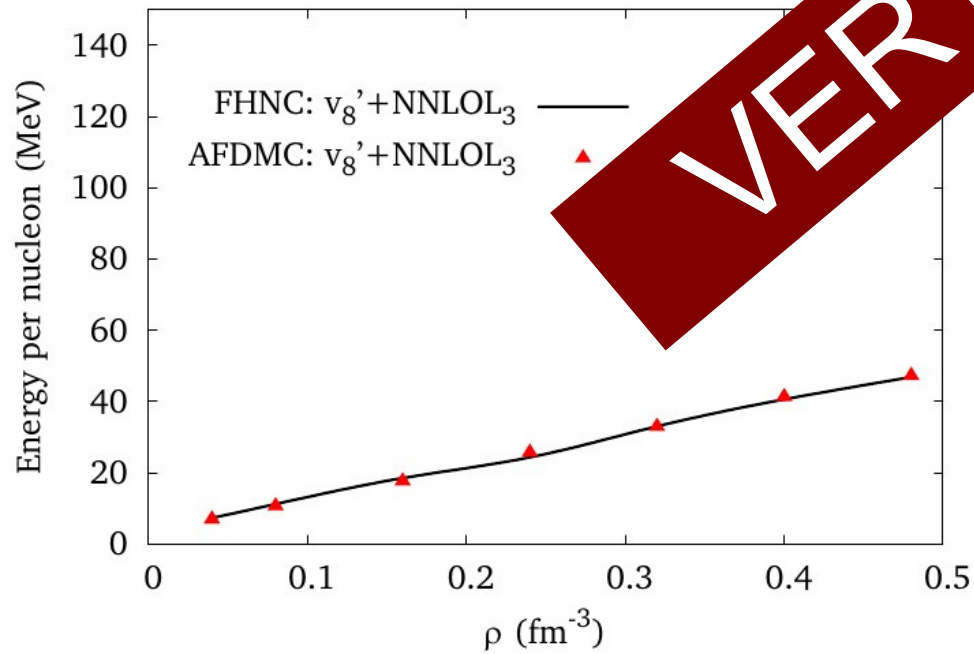
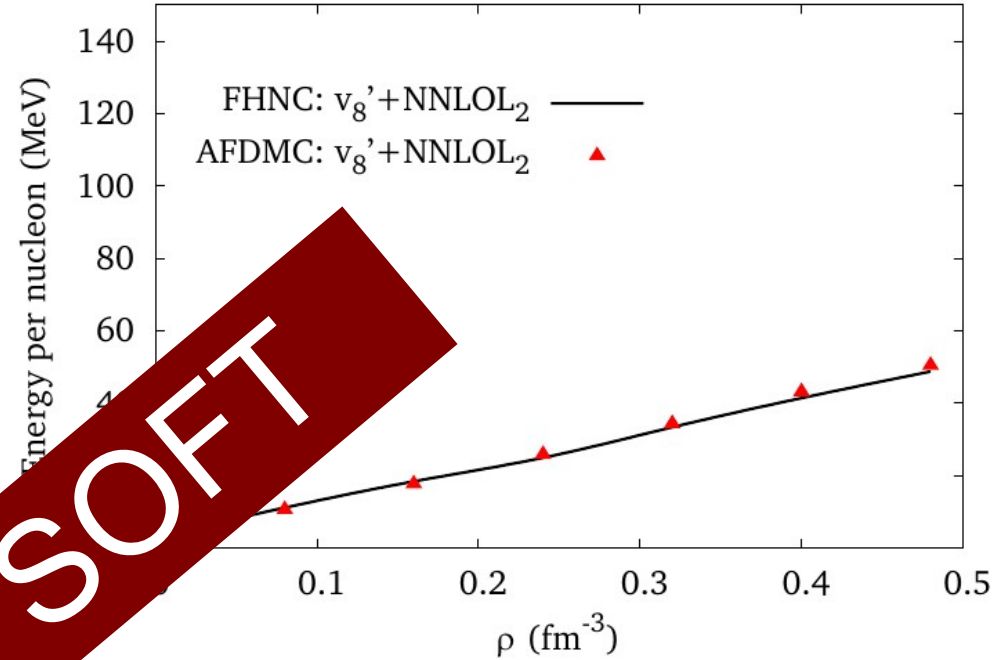
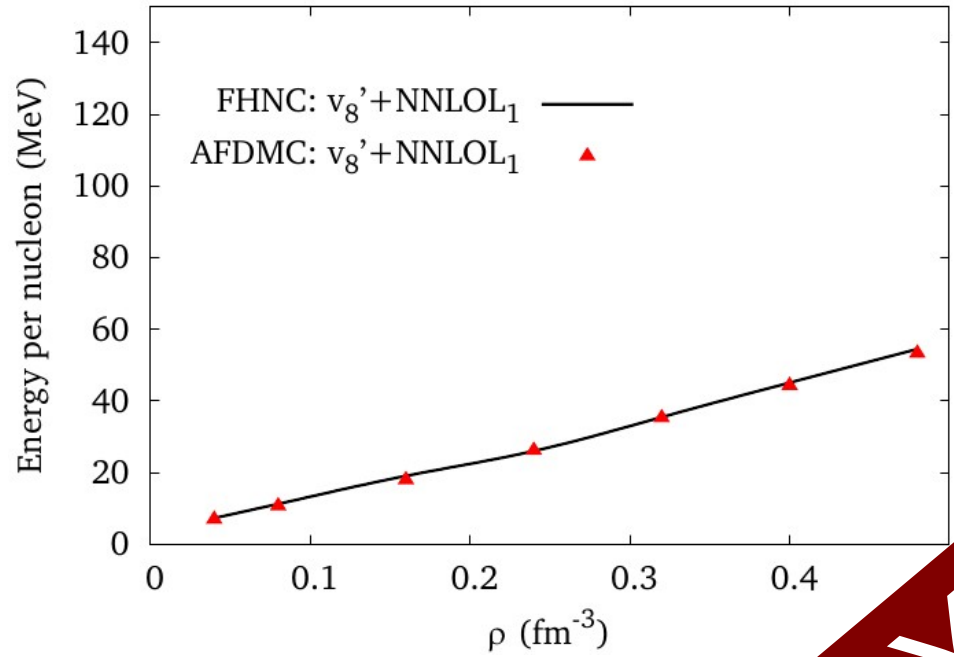
Experimental values

ρ_0 (fm ⁻³)	0.16
E_0 (MeV)	-16.0
K (MeV)	240

Chiral NNLOL results for PNM

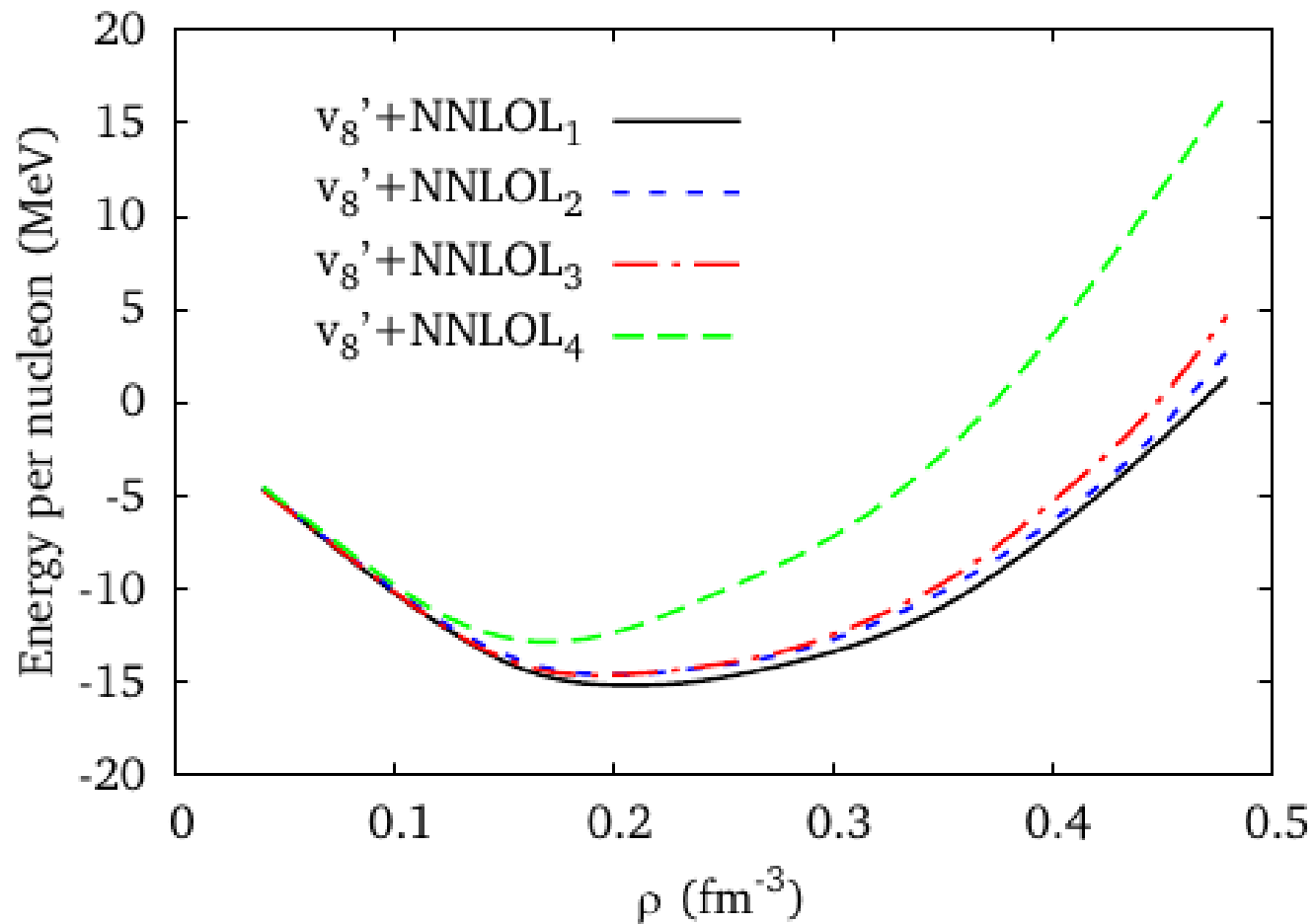


Chiral NNLOL results for PNM



VERY SOFT

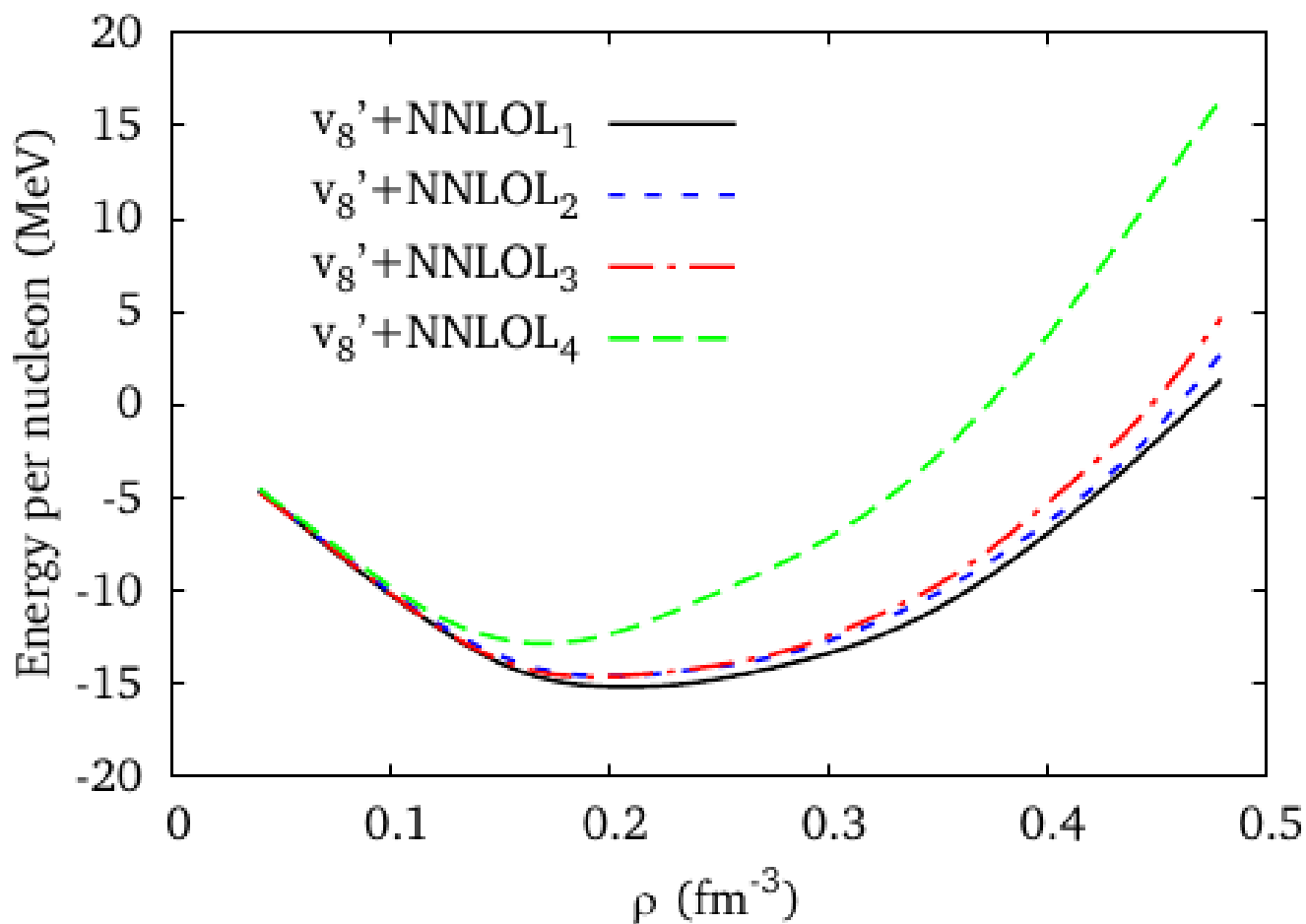
Chiral NNLOL results for SNM



NNLOL₄ has a large negative c_E

- stiffest SNM EoS
- softest PNM EoS

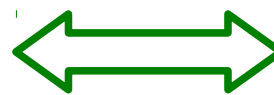
Chiral NNLOL results for SNM



	NNLOL ₁	NNLOL ₂	NNLOL ₃	NNLOL ₄
ρ_0 (fm^{-3})	0.21	0.20	0.19	0.17
E_0 (MeV)	-15.2	-14.6	-14.6	-12.9
K (MeV)	198	252	220	310

Experimental values

ρ_0 (fm^{-3})	0.16
E_0 (MeV)	-16.0
K (MeV)	240



Conclusions

- Contact term of NNLOL potential suffers of cutoff dependence.
Its contribution in nuclear matter cannot be evaluated fitting low energy observables.
- No one of the potential considered simultaneously explains the binding energy and the saturation density of SNM.
- NNLOL₄ and TM'₃ potentials provide reasonable value for the saturation density of SNM although **not involving any parameters adjusted to reproduce it.**
- Deriving potential from chiral perturbation theory is still a promising approach.

NNLO potential is now available as well as NNNLO contact terms!

More low energy observables are needed