Toward an effective field theory approach to ab-initio and energy density functional calculations

Chieh-Jen (Jerry) Yang (楊傑仁)

CYCU 5/3/2017

Collaborators: D. Phillips, Ch. Elster, Bingwei Long, B. Barrett, U. van Kolck, M. Grasso, D. Lacroix







UNIVERSITÀ DEGLI STUDI DI TRENTO



A simplified overview of nuclear physics

1 TeV 100 GeV Effective fundamental theories (QCD, QED, etc.) Nuclear physics Difficulty: Non-perturbative region By spontaneous symmetry breaking Lattice QCD 1 GeV Chiral perturbation theory 100 MeV NN data Effective field theory for low energy NN interaction.

Application: From QCD to nuclear structure

Part I: Nuclear Force

The Nuclear Force Problem: Is the Never-Ending Story Coming to an End?

R. Machleidt

Department of Physics, University of Idaho, Moscow, Idaho, U.S.A.

Table 1. Seven Decades of Struggle: The Theory of Nuclear Forces	
1935	Yukawa: Meson Theory
1950's	The "Pion Theories"
	One-Pion Exchange: o.k.
	Multi-Pion Exchange: disaster
1960's	Many pions ≡ multi-pion resonances:
	$\sigma, \rho, \omega,$
	The One-Boson-Exchange Model
1970's	Refine meson theory:
	Sophisticated 2π exchange models
	(Stony Brook, Paris, Bonn)
1980's	Nuclear physicists discover
	QCD
	Quark Cluster Models
	Nuclear physicists discover EFT
1990's	Weinberg, van Kolck
and beyond	Back to Meson Theory!
-	But, with Chiral Symmetry

Answer: Yes, almost!

EFT on NN: Weinberg's proposal

- Concept of EFT: symmetries, separation of scales, renormalization.
- Spontaneous symmetry breaking:

$$SU_L(2) \times SU_R(2) \rightarrow SU_V(2)$$
 (chiral sym)

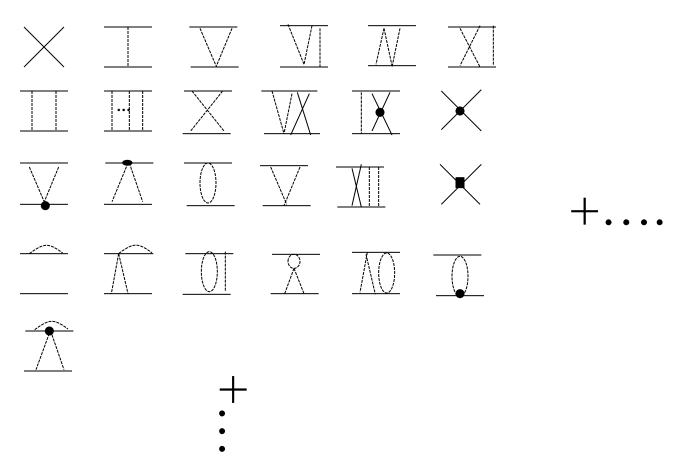
• Write down all possible terms in Lagrangian allowed by symmetry.



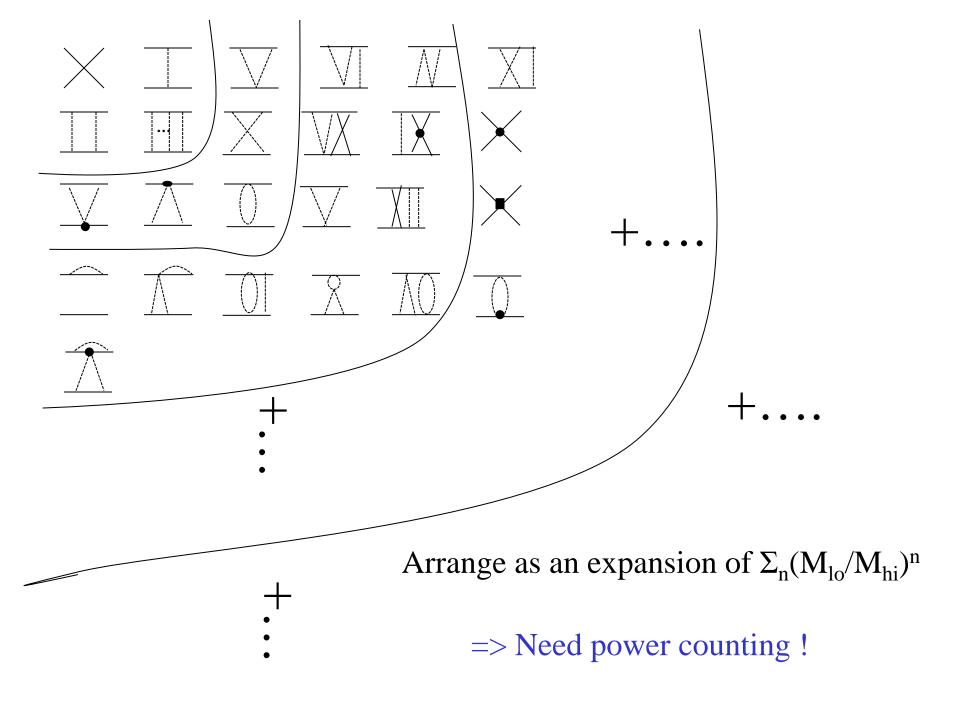
Chiral perturbation theory: works in $\pi\pi$, πN , but NN is too strong (infrared enhancement), still have open issues.

Nature of the problem: Chiral EFT at NN sector

- Infinitely many diagrams contribute, most of them require renormalization.
- Need to arrange a way to include them based on their importance (there maybe more than one consistent way).
- Weinberg counting is correct up to the potential level.
- Pure perturbation doesn't work.



Infinity many diagrams.



Conventional power counting

Epelbaum, Entem, Machleidt, Kaiser, Meissner, ... etc., ~90% of the people

- Arrange diagrams base on Weinberg's power counting (WPC): each derivative on the Lagrangian terms is always suppressed by the underlying scale of chiral EFT, $M_{hi}\sim m_{\sigma}$.
- Iterate potential to all order (in L.S. or Schrodinger eq.), with an ultraviolet Λ .

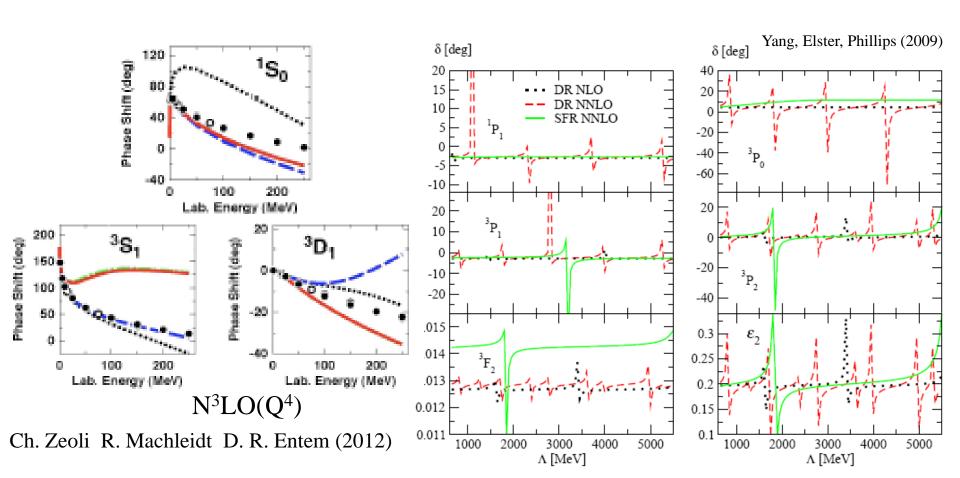
Carried out to $N^4LO(Q^5/M_{hi}^5)$ just last month!

D. R. Entem, R. Machleidt and Y. Nosyk, arXiv:1703.05454 [nucl-th].

 $V(N^3LO)$ performs as good as high accuracy $V_{CDBonn,\;AV18,\;etc.,...}$, if keep 500< $\Lambda < 875\;MeV$.

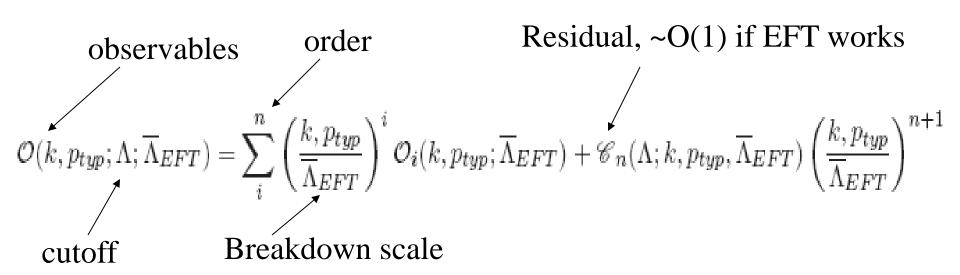
Problems in RG

- Singular attractive potentials demand contact terms. (Nogga, Timmermans, van Kolck (2005))
- Beyond LO: Has RG problem at $\Lambda > 1$ GeV (due to iterate to all order)



Why is that a problem?

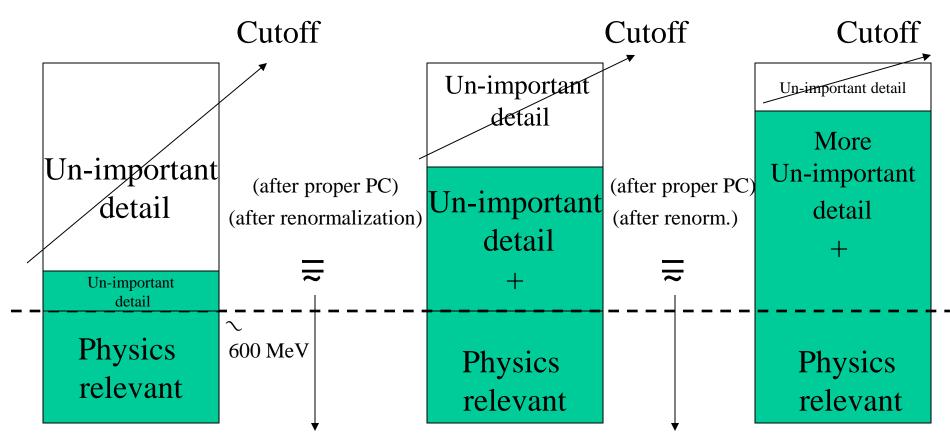
Essence of any EFT



H. W. Griesshammer, arXiv:1511.00490v3 [nucl-th].

Renormalization group (RG)

: included



*Only source of error: given by the high order terms.

If not so, the power counting isn't completely correct!

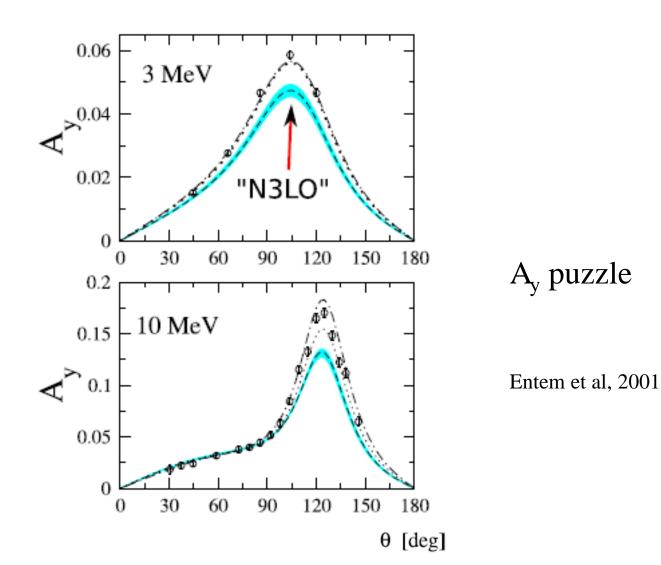
(unimportant are not really unimportant)

In the window of $500 < \Lambda < 875$ MeV

- Whether the conventional way happens to represent the reality, or, the problem just got hidden in the apparently o.k. fit of phase shifts?
- It is safest/more reasonable, to develop a new power counting, which is more EFT.
- The ultimate way to check is through few-body and ab-initio nuclear structure calculations.

Some indications

In the window: $500 < \Lambda < 875 \text{ MeV}$

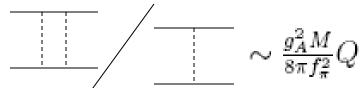


New power counting Long & Yang, (2010-2012)

LO: Still iterate to all order (at least for l < 2).

Reason: van Kolck, Bedaque,... etc.

Thus, $O(Q^0)$:



$$\sim \frac{g_A^2 M}{8\pi f_\pi^2} Q \qquad \boxed{ } + \boxed{ } + \ldots \boxed{ } \equiv \boxed{ \boxed{ } \qquad }$$

Start at NLO, do perturbation. $(T = T^{(0)} + T^{(1)} + T^{(2)} + T^{(3)} + ...)$

$$(T = T^{(0)} + T^{(1)} + T^{(2)} + T^{(3)} + \dots)$$

If V⁽¹⁾ is absent:

$$T^{(2)} = V^{(2)} + 2V^{(2)}GT^{(0)} + T^{(0)}GV^{(2)}GT^{(0)}.$$

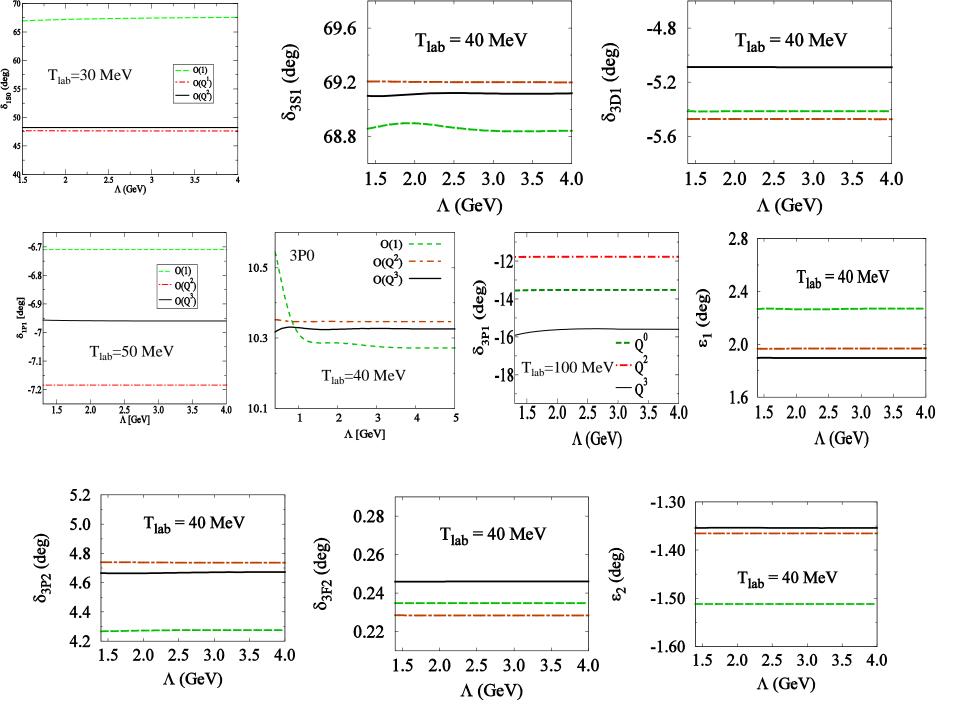
$$V^{(2)} = V^{(2)} + 2V^{(2)}GT^{(0)} + T^{(0)}GV^{(2)}GT^{(0)}.$$

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$$\overline{\left(\mathbf{T}^{(0)}\right)\left(\mathbf{V}^{(2)}\right)\left(\mathbf{T}^{(0)}\right)} \qquad G \equiv \frac{2M_N}{\pi} \int_0^{\Lambda} \frac{p^2 dp}{p_0^2 - p^2 + i\varepsilon}$$

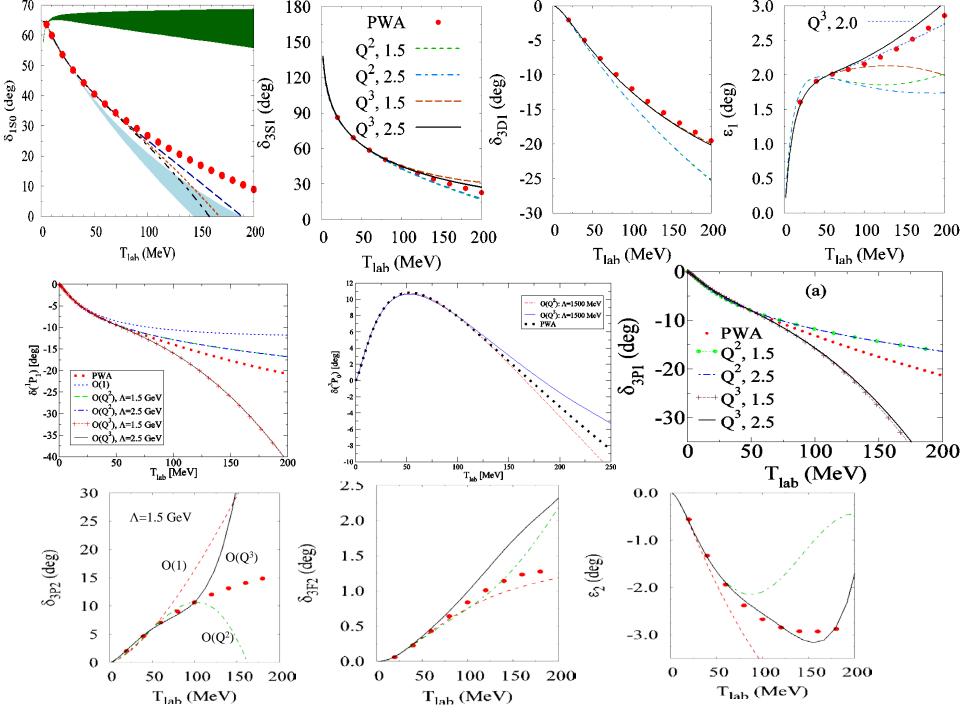
$$T^{(3)} = V^{(3)} + 2V^{(3)}GT^{(0)} + T^{(0)}GV^{(3)}GT^{(0)}.$$

Results (All RG-invariant)

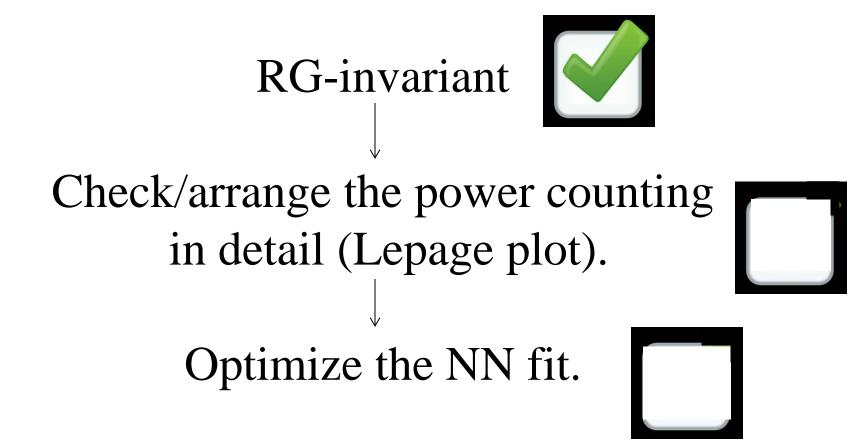


Quality of the fits

(comparable to WPC at the same order)



Road Map for the future



Practical calculations

From QCD to nuclear structure (Suppose we have the correct NN force)

Nuclear structure

4+ nucleons

Difficulty: Model space grow combinatorial.

Many-body

Reasonable truncation of prodel space

Unitary transformation of NN, NNN forces

Establish the (short-range) EFT in truncated model space

No-core shell model (NCSM)

EFT approach to NCSM ©

• Since, in practical, only a finite subset (n_{max}<20) of the basis can be used, need to obtain H_{eff} in very small model space.



Results needs to converge within the very limited model space

Results are only trustable if they converge w.r.t. number of basis!

For V not "soft" enough (e.g. N³LO, or almost every high precision potentials), it won't converge!



Unitary transformation to get effective interaction and operator. (e.g. Lee-suzuki)



``Soften" the potential, e.g., Similarity renormalization group (SRG) transformation: V_{lowk} .



Remarkable success for some light nuclei (A<12).

But...

Whenever a model space is truncated, (artificial) higher body forces arise

$$V_{ij} \xrightarrow{unitary \text{ trans.}} V_{ij} + V_{ijk} + V_{ijkl} + \dots$$
 $keep \xrightarrow{truncated?}$

$$O(1) \left| O(Q^1) \left| O(Q^2) \right| O(Q^3) \dots \xrightarrow[Unitary \ trans.]{Well-organized power counting in EFT could be destroyed! Especially when $V^{\text{subleading}}$ need to be treated perturbatively.}$$

EFT: separation of scale

Idea: Directly perform renormalization of EFT in the truncated model space

$$V = \underbrace{C_0 \delta(\vec{r})}_{LO} - \underbrace{C_2 \left[\nabla^2 \delta(\vec{r}) + 2(\overline{\nabla} \delta(\vec{r})) \cdot \overline{\nabla} + 2\delta(\vec{r}) \nabla^2 \right]}_{NLO} + \dots$$

Adjust $C_{0,2,...}$ so that $\langle \psi^{\text{truncated}} | V | \psi^{\text{truncated}} \rangle$ fit some physical observables.

Then can use $\psi^{\text{truncated}}$ and V to make predictions.

$$\Lambda = \sqrt{(2N_{\text{max}} + l + 3/2)M_N \omega}$$

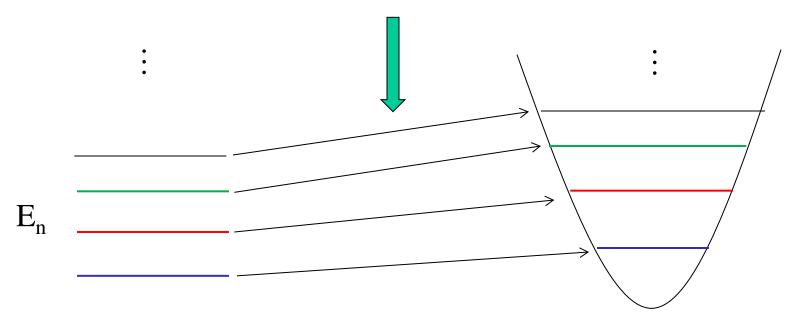
Good idea. But, not enough bound-state to decide $C_{0,2}$

Solution I: Use trapped space

HO basis in free space

HO basis in trapped space

Energy shift due to different b.c.



Busch's formula: through the E-shift, relates E_n to **phase shift**.

Analogy: Lattice QCD (Luscher formula)

Generalization of Busch formula

Uncoupled channels:
$$\frac{\Gamma(\frac{2l+3}{4} - \frac{E(\infty)}{2\omega})}{\Gamma(\frac{1-2l}{4} - \frac{E(\infty)}{2\omega})} = (-1)^{l+1} \left(\frac{bk}{2}\right)^{2l+1} \cot \delta_l(k)$$

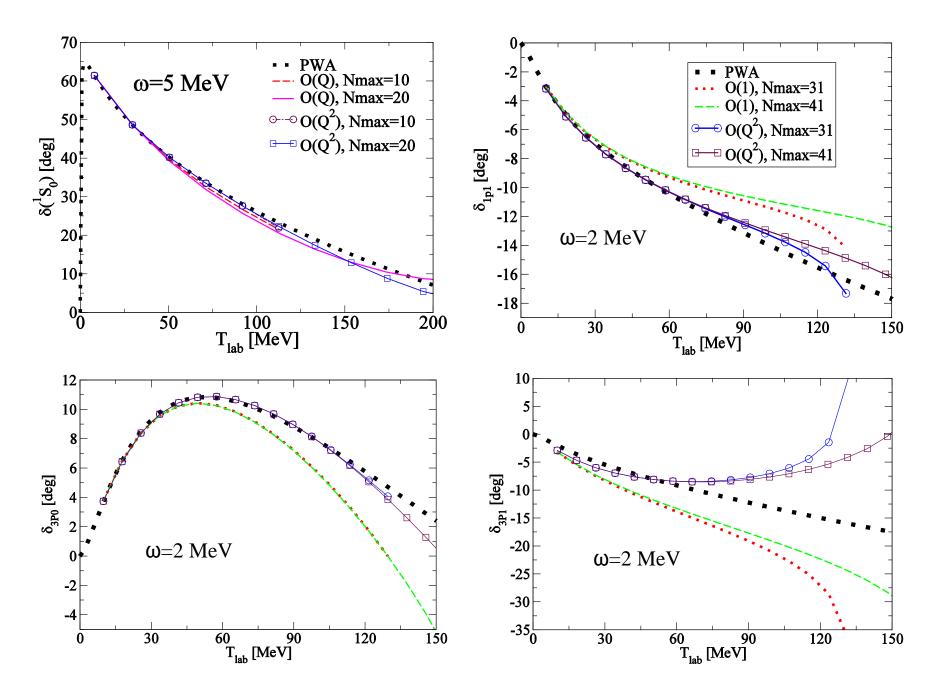
Exact only for $N_{max} \rightarrow \infty$, l=0 and zero-range interaction case.

Otherwise has error $\sim O(\mu \omega R^2)$. R: range of potential

$$\cot \delta_1 = R_1 - \tan^2 \delta_3 \left[\frac{\cot \delta_1 - R_2}{\cot \delta_2 - R_2} \right] (R_1 + \cot \delta_2),$$

$$R_{1} = -2\frac{\Gamma(\frac{3}{4} - \frac{\varepsilon}{2})}{\Gamma(\frac{1}{4} - \frac{\varepsilon}{2})} \frac{1}{bk}, R_{2} = -32\frac{\Gamma(\frac{7}{4} - \frac{\varepsilon}{2})}{\Gamma(-\frac{3}{4} - \frac{\varepsilon}{2})} (bk)^{-5}$$

Results up to $O(Q^2)$



Solution II

J-matrix formalism:

scattering in the oscillator basis

$$T + V$$

$$\sum_{n'=0}^{N} H^{l}_{nn'}\langle n'|\lambda\rangle = E_{\lambda}\langle n|\lambda\rangle, \quad n \leq N.$$

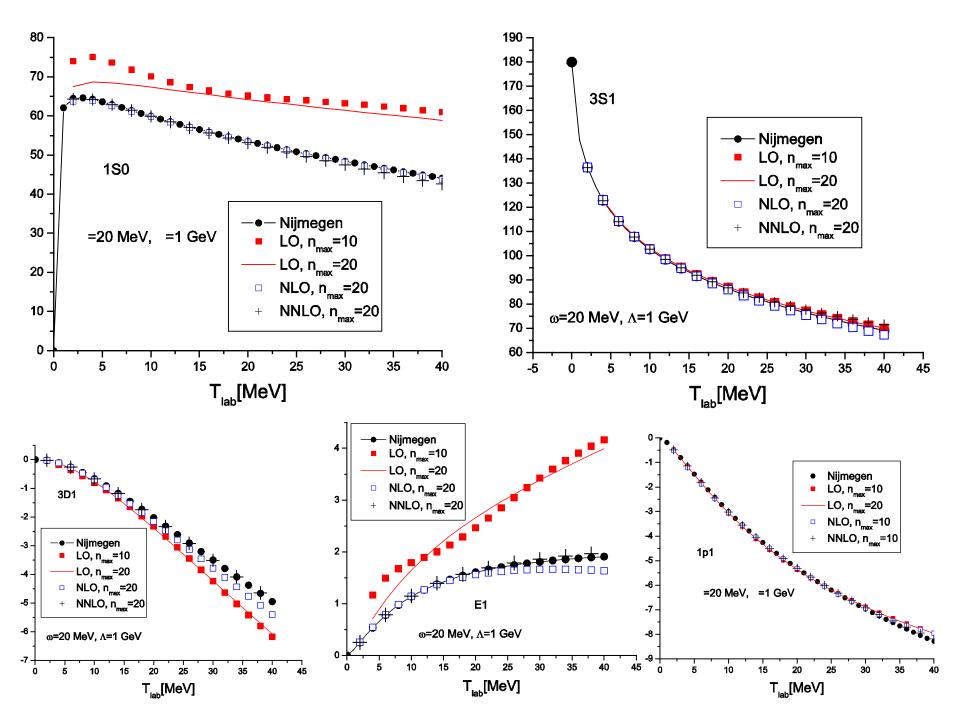
$$G_{NN}(E) = -\sum_{\lambda=0}^{N} \frac{\langle N|\lambda\rangle^2}{E_{\lambda} - E},$$

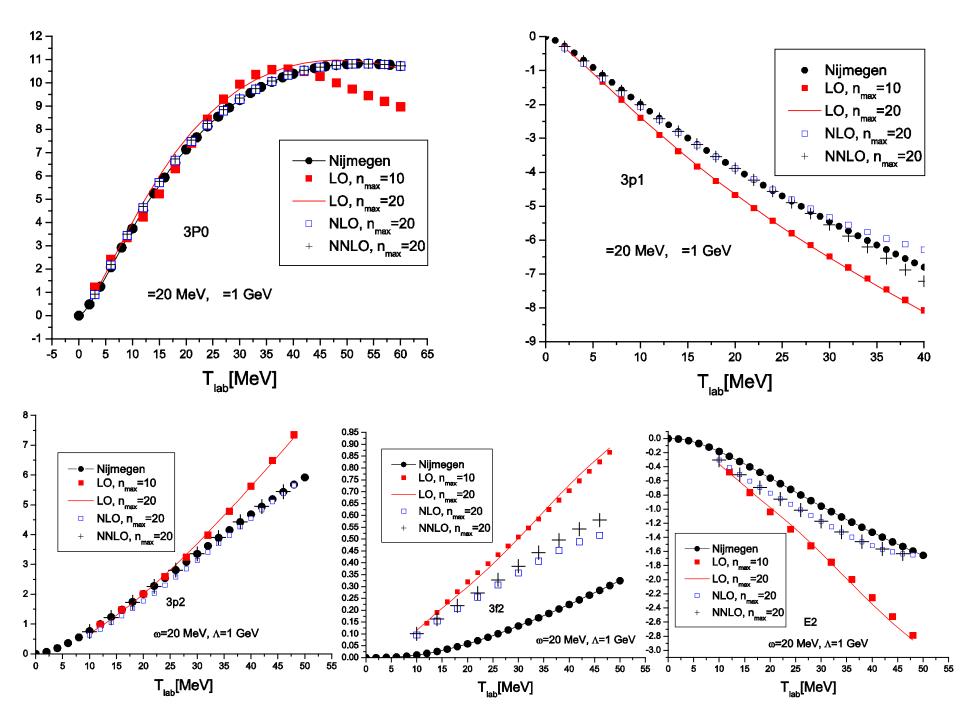
$$S = \frac{C_{NI}^{(-)}(q) - \mathcal{G}_{NN}(E) T_{N,N+1}^t C_{N+1,l}^{(-)}(q)}{C_{NI}^{(+)}(q) - \mathcal{G}_{NN}(E) T_{N,N+1}^t C_{N+1,l}^{(+)}(q)},$$

T

Results of J-matrix method

C.J. Yang, Phys.Rev. C94 (2016) no.6, 064004

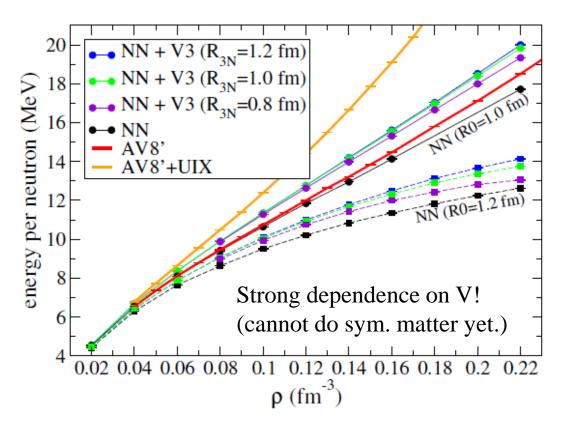




Part II: EFT approach to energy density functional (EDF)

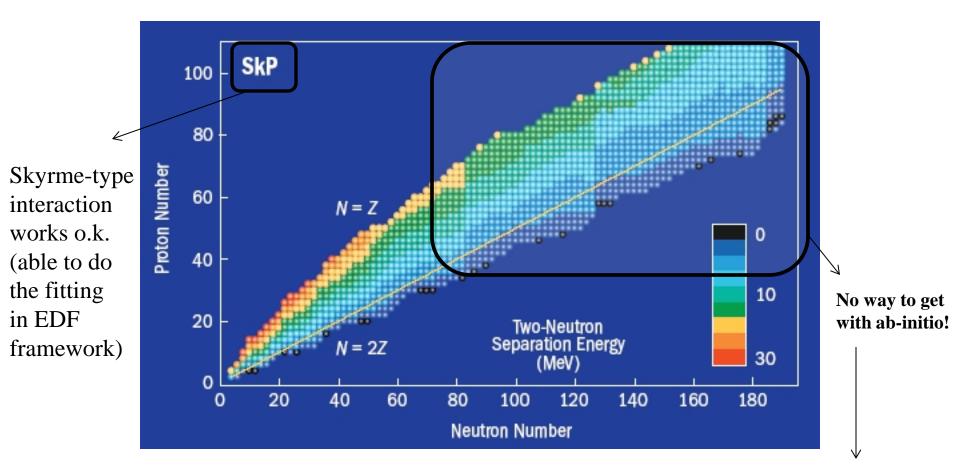
Nuclear matter: ab-inito

Equation of state of neutron matter at N^2LO .



S. Gandolfi, talk in ESNT workshop, 2017

Finite nuclei



Need to think about other expansion (than on NN d.o.f.).

EDF

• Energy density functional (EDF) framework gives reasonable results at mean field, when sufficient amount of parameters (~10) are included.

$$v(\mathbf{k}, \mathbf{k}') = t_0(1 + x_0 P_{\sigma}) + \frac{1}{2}t_1(1 + x_1 P_{\sigma})(\mathbf{k}'^2 + \mathbf{k}^2) + t_2(1 + x_2 P_{\sigma})\mathbf{k}' \cdot \mathbf{k} + \frac{1}{6}t_3(1 + x_3 P_{\sigma})\rho^{\alpha},$$

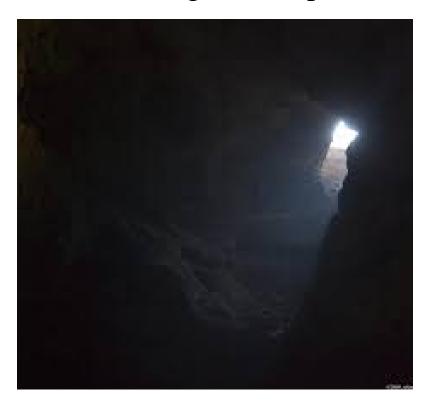
But,...

- Include more parameters won't necessarily help.
- → Limited predictive power.



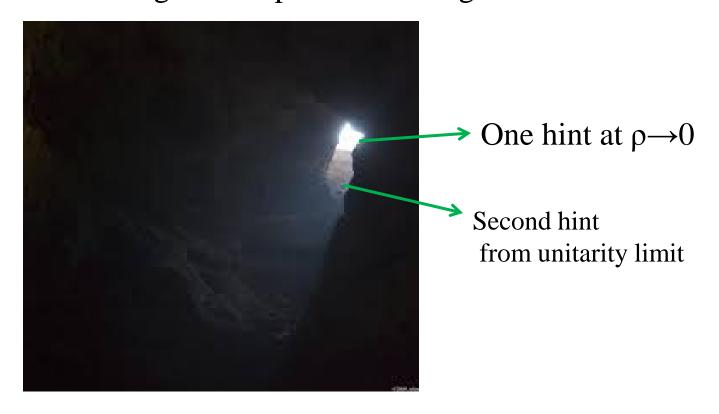
Is there a way to do EFT? (need to go beyond mean field to perform the test).

Turn off nucleon-nucleon d.o.f., Also, no EFT/ERE to guild the power counting



In term of power counting: Just like turn of the light in a cave.

Turn off nucleon-nucleon d.o.f., no EFT/ERE to guild the power counting



In term of power counting: Just like turn of the light in a cave.

First hint: a special case where an EFT expansion is known to works

Pure neutron matter at very low density ($k_Na<1$, $\rho<10^{-6}$ fm⁻³).

Lee & Yang formula (1957) describes the dilute system.

=> Can be re-derived by EFT with matching to ERE

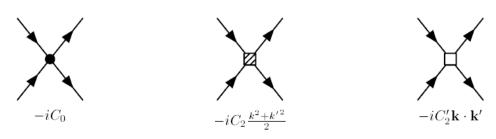
L. Platter, H. Hammer, Ulf. Meissner, Nucl. Phys. A714 (2003), 250-264, H. Hammer and R.J. Furnstahl, Nucl. Phys. A678 (2000) 277-294.

$$\frac{E_{NM}}{A} = \frac{\hbar^2 k_N^2}{2m} \left[\frac{3}{5} + \frac{2}{3\pi} (k_N a) + \frac{4}{35} (11 - 2\ln 2)(k_N a)^2 + \underbrace{O(k_N^3)}_{higher \text{ order}} \right]$$

Expansion in $\mathbf{k_N}\mathbf{a}$

But the valid ρ is way too low!

Diagrams gives V up to $O(k_F^8)$



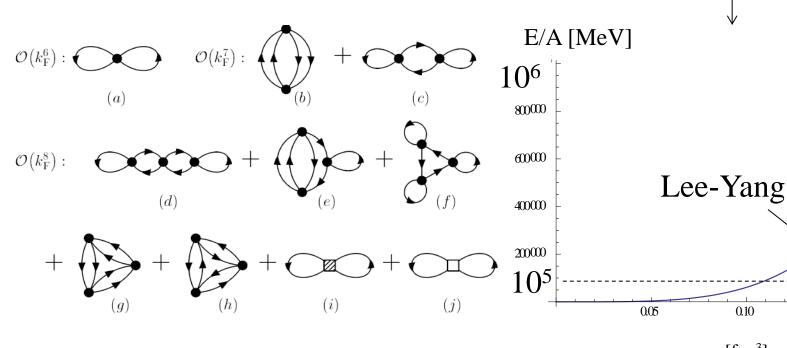
If take physical value of a=-18.9 fm, then impossible to fit pure neutron matter EoS outside region $k_Fa << 1$ (adding t1, t2, t3 terms doesn't help).

0.10

 ρ [fm⁻³]

0.15

0.20



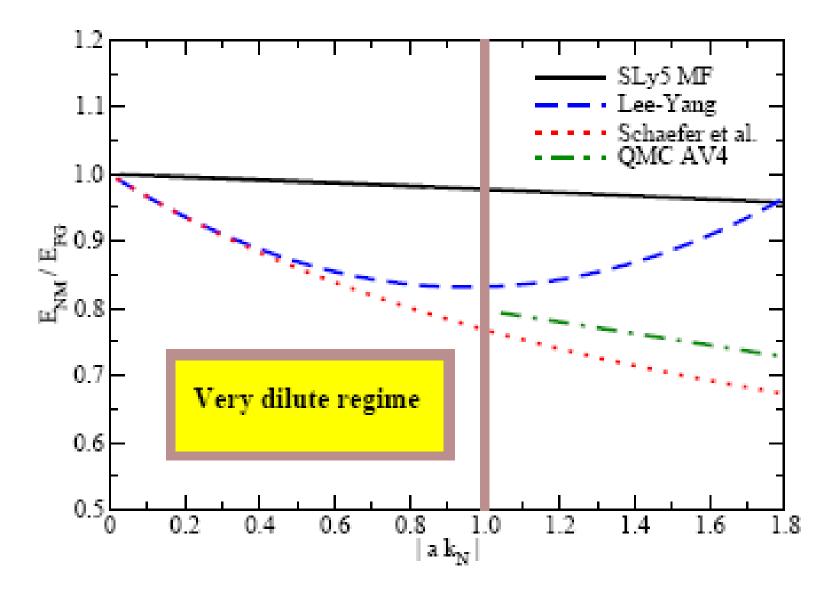
H. Hammer and R.J. Furnstahl, Nucl. Phys. A678 (2000) 277-294

Treatment: Re-sum

To be valid at higher ρ , $(k_N a)$ needs to be re-summed. (Steele (2000), Schafer, C.W. Kao, et al (2005), Kaiser (2011))

$$\frac{E_{NM}}{N} = \frac{\hbar^2 k_N^2}{2m} \left[\frac{3}{5} + \frac{2}{3\pi} \frac{k_N a}{1 - 6k_N a (11 - 2\ln 2)/(35\pi)} \right]$$

Neutron matter only



YGLO: Resumed-inspired functional

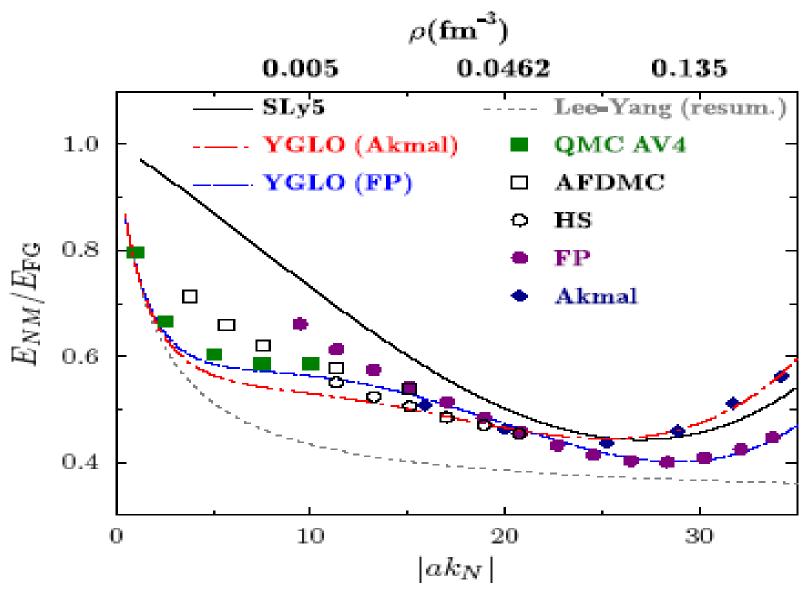
C.J. Yang, D. Lacroix, M. Grasso, Phys. Rev. C 94 034311(2016)

$$V = \frac{B_{\beta}}{1 - R_{\beta}\rho^{1/3} + \underbrace{C_{\beta}\rho^{2/3}}_{\text{higher order in L&Y to be resumed*}} + \underbrace{D_{\beta}\rho^{2/3}}_{\text{velocity-dep term*}} + \underbrace{F_{\beta}\rho^{\alpha}}_{3^{+}-body}$$

 B_{β} , R_{β} are fixed to reproduce first two term in Lee & Yang.

$$=> B_{\beta} = 2\pi \frac{\hbar^2}{m} \frac{v-1}{v} a_{\beta}, R_{\beta} = \frac{6}{35\pi} \left(\frac{6\pi^2}{v}\right)^{1/3} (11-2\ln 2) a_{\beta}.$$
(degeneracy: $v = 2(4)$ for $\beta = 0$ (1) pure n sym
$$a_0 = -18.9 \text{fm}, \quad a_{1} = -20 \text{ fm} \quad a_{2} = -20 \text{ fm}$$

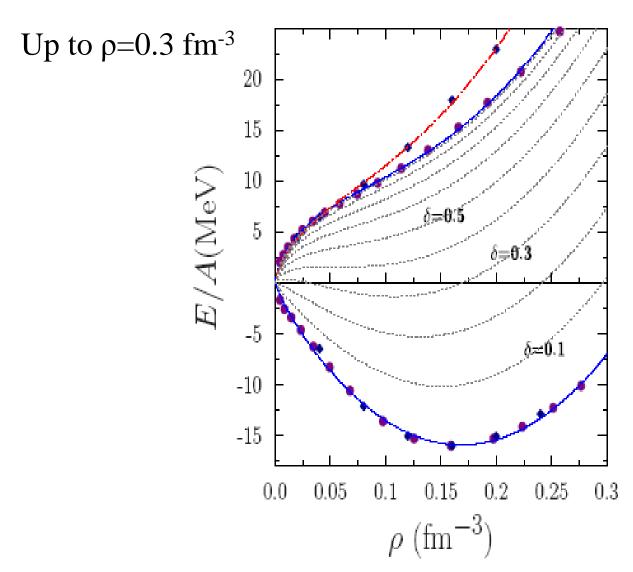
$$\frac{E}{A} = KE_{\beta} + \frac{B_{\beta}\rho}{1 - R_{\beta}\rho^{1/3} + C_{\beta}\rho^{2/3}} + D_{\beta}\rho^{5/3} + F_{\beta}\rho^{\alpha+1}$$



FP: B. Friedman and V. Pandharipande, Nucl. Phys. A361,502 (1981).

Akmal: A. Akmal, V. R. Pandharipande, and D. G. Ravenhall, Phys. Rev. C 58, 1804 (1998).

HS: K. Hebeler and A. Schwenk Phys. Rev. C 82, 014314(2010).



Able to describe both sym and pure neutron matter EoS up to $2\rho_0$ very well with only 4 free parameters each.

Asymmetric case

Parabolic approximation

$$\frac{E_{\delta}}{A}(\rho) = \frac{E_{sym}}{A}(\rho) + S(\rho)\delta^{2},$$

$$(\delta = (\rho_{N} - \rho_{p})/(\rho_{N} + \rho_{p}))$$

$$L = 3\rho_{0}(dS/d\rho)_{\rho=\rho_{0}}$$

Before: Lots of models fail

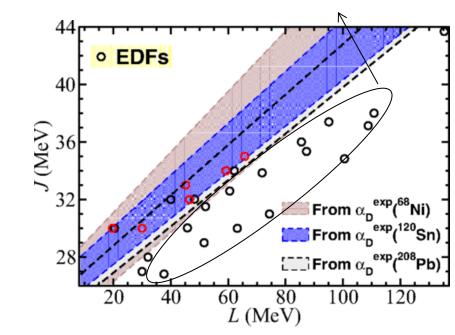


FIG. 4: Symmetry energy at saturation density as a function of its slope L. The black lines delimit the phenomenological area constrained by the experimental determination of the electric dipole polarizability in ²⁰⁸Pb. The blue dotted lines delimit the area constrained by the same measurement in ⁶⁸Ni, and the red dashed lines refer to the measurement done in ¹²⁰Sn. The yellow area is the overlap. Inset: density dependence of the Symmetry energy for the two YGLO parametrizations of this work.

X. Roca-Maza, et al., (2015).

Asymmetric case

Our result (prediction)

Satisfies the experimental constraint.

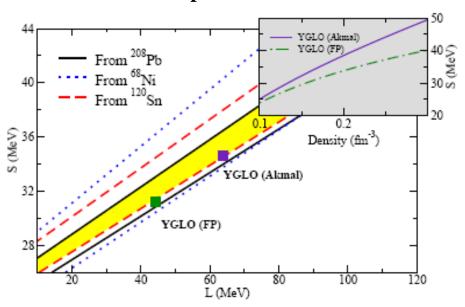


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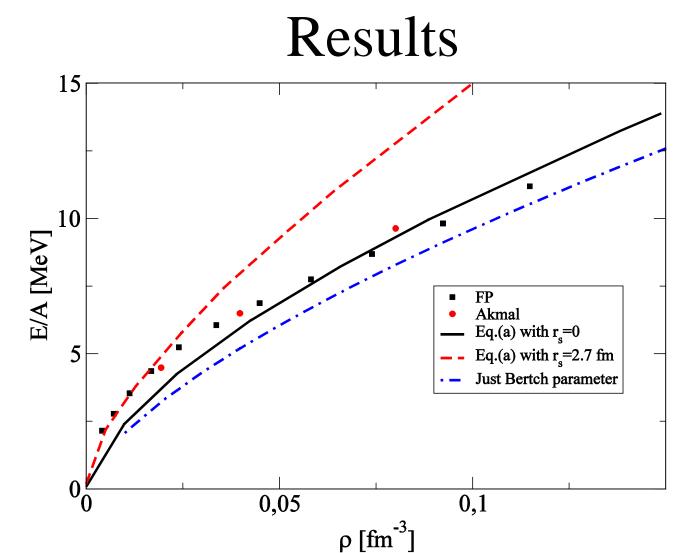
Second hint: Unitarity limit

D Lacroix, A. Boulet, M. Grasso, C. J. Yang, arXiv:1704.08454 (in press prc)

- Scale invariance tells $\frac{E}{E_{FG}} = \xi$ (Bertch parameter)
- Neutron system ($|a=-18.9 \, fm/>>R(range of interaction)$) can be approached by an expansion around UT.
- Validity: $\frac{1}{|a_s|} < k_F < \frac{1}{R} \Rightarrow 4*10^{-6} < \rho < 0.002 [fm^{-3}]$, or higher if there's an extra suppression in the coefficient of the range.

$$\begin{split} \frac{E}{E_{\text{FG}}} &= 1 - \frac{U_0}{1 - (a_s k_F)^{-1} U_1} \\ &+ \frac{R_0(r_e k_F)}{\left[1 - R_1(a k_F)^{-1}\right] \left[1 - R_1(a_s k_F)^{-1} + R_2(r_e k_F)\right]} \end{split}$$

No free parameters: U_i, R_i come from QMC data (with V_{unitarity})



Lesson:

- Nuclear (many-body) systems are not too far from the unitarity limit.
- Just a few more parameters might be sufficient to describe data up to ρ =0.3 fm⁻³, this explains why Skyrme works!

How to establish an EFT with a Skyrme-like interaction?

What will an EFT-based force look like?

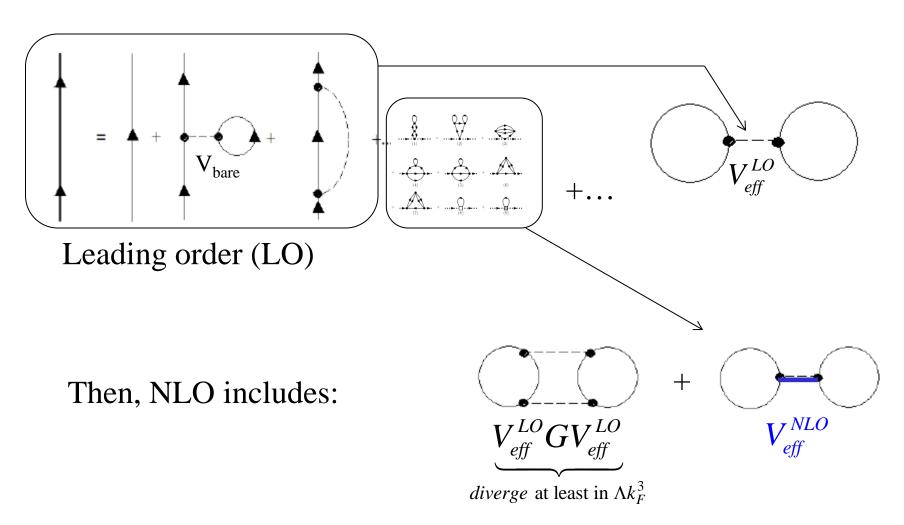
- Leading order (LO): Need to make a guess.
- Based on renormalizability analysis

C.J. Yang, M. Grasso, U. van Kolck, and K. Moghrabi, under review PRC

 \Rightarrow A good guess would be the t_0 - t_3 model (or t_0 model, but it gives a very bad EOS).

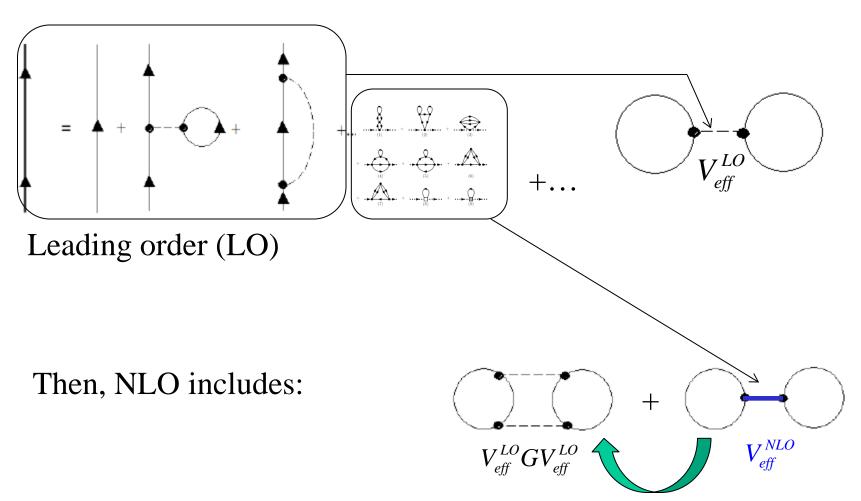
Diagrammatic explanation of How Skyrme works

Dressing of propagator→V_{eff}



 $V_{eff}^{Sly5}GV_{eff}^{Sly5}$ evaluated in: C.J. Yang, M. Grasso, X. Roca-Maza, G. Colo, and K. Moghrabi, PhysRevC.94.034311

Dressing of propagator→V_{eff}



^{*} V_{eff}^{NLO} contains (at least) contact terms to renormalize $V_{eff}^{LO}GV_{eff}^{LO}$.

Counter term part of the NLO potential

 V_{eff}^{NLO} : For t_0 - t_3 model, the divergence from $V_{eff}^{LO}GV_{eff}^{LO}$ is:

$$\underbrace{O(k_F^3), O(k_F^{3+3\alpha})}_{k_F^n-dep. \text{ appears in } MF}, \underbrace{O(k_F^{3+6\alpha})}_{new \ k_F^n-dep.}.$$

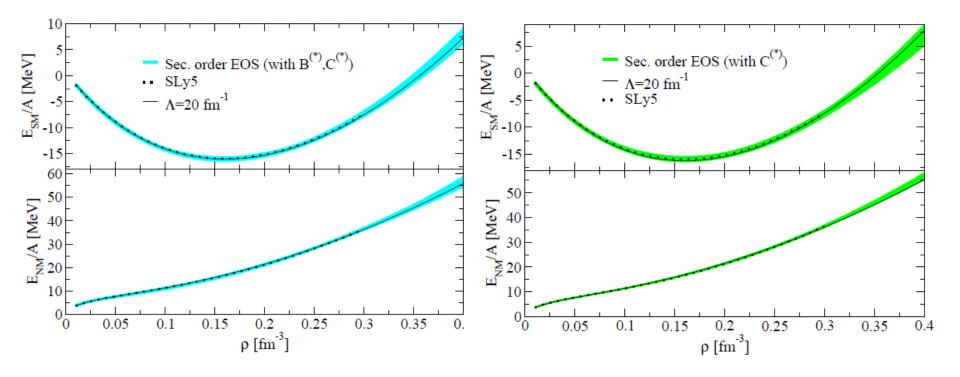
If want to keep α free, =>Minimun contact term required: $Ck_F^{3+6\alpha}$.

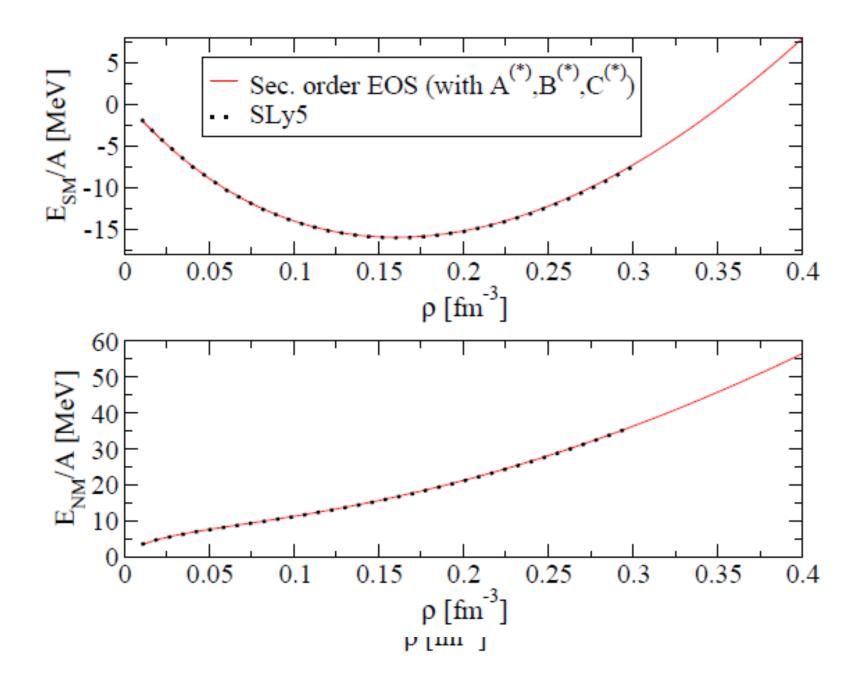
Most general case: Ak_F^3 , $Bk_F^{3+3\alpha}$, $Ck_F^{3+6\alpha}$.

In infinite matter, k_F^{3n} in-distinguishable with $3\pi^2\rho$

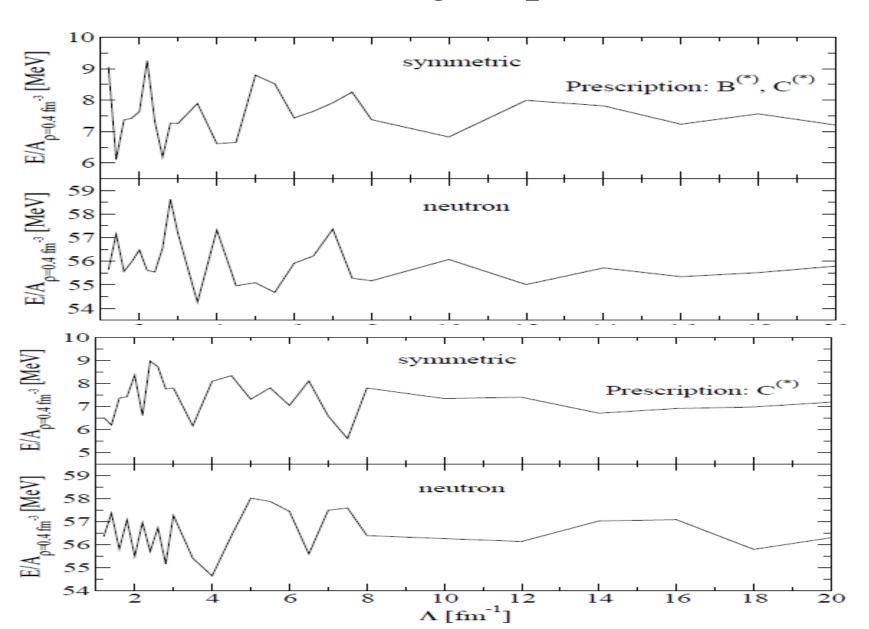
=> k_F^n -term in EOS *could* originated (at interaction level) from $(k - k')^{3n} \rho^{\nu}$, where ν is an extra parameter to be decided in the fitting to finite nuclei.

NLO results (based on t_0 - t_3 as LO) α <1/6 case*



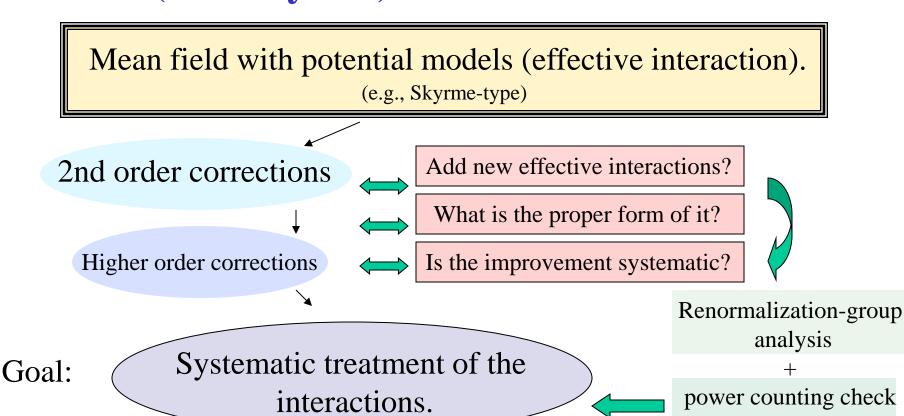


Renormalization group (RG) check

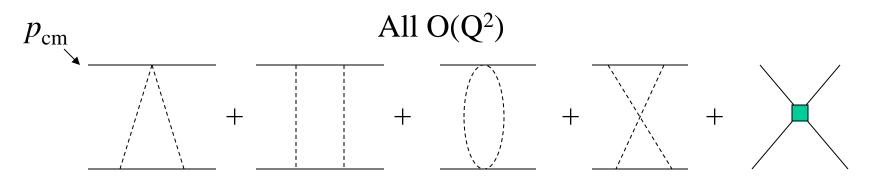


Future prospects

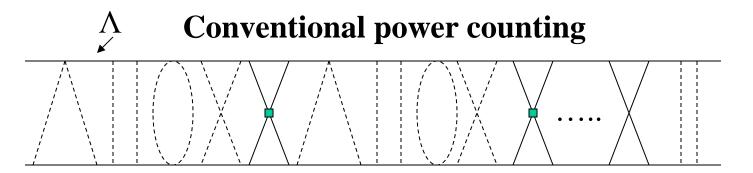
Try to bridge EFT ideas/techniques to mean field (and beyond) within EDF framework.



Thank you!



O.k., as long as p_{cm} is small enough, so that $\frac{p_{cm}}{M_{bi}} < 1$



Has problem, as Λ -dependence enter here; contact term aren't enough.

The expansion parameter is no longer $\frac{p_{cm}}{M_{bi}}$!

Problems at $\Lambda>1$ GeV also imply that WPC might not give you (to make use of) all the counter terms which are legitimate (according to a truly RG-invariant theory) to be used.

$$V^{(n)} = V_{Long}^{(n)} + V_{Short}^{(n)};$$

$$V_{Long}^{(n)}: \text{ pion-exchange at } O\left(\left(\frac{Q}{M_{hi}}\right)^n\right)$$

$$V_{Short}^{(n)}: \text{ counter terms,}$$

$$C_0 + C_2 q^2 + C_4 q^4 + \dots$$

value of C's decided from renormalization

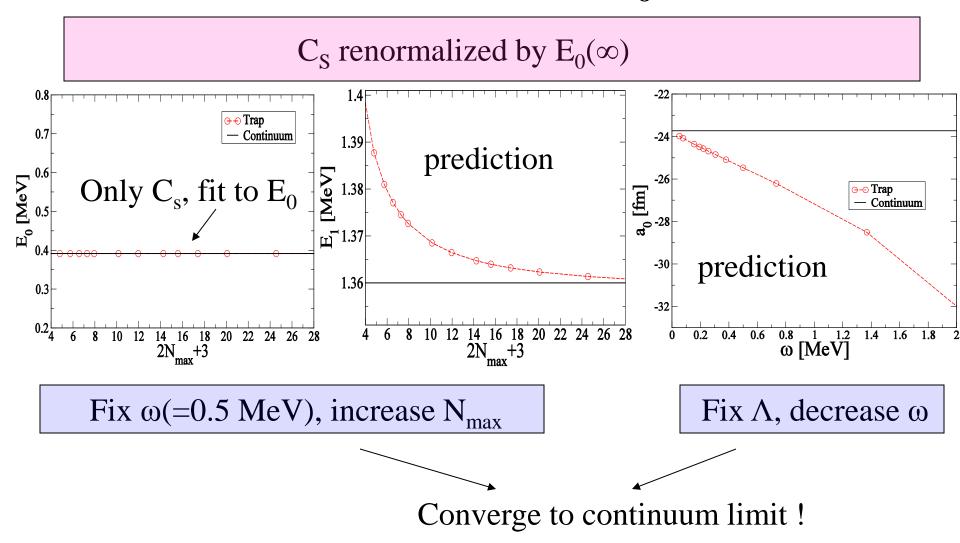
3 types of counter terms (determined by RG)

- 1. Primordial: Those renormalize the pion-exchange diagrams. (always there if survived from partial-wave decomposition)
- 2. Distorted –wave counter terms

3. Residual counter terms: Decided by the requirement from RG.

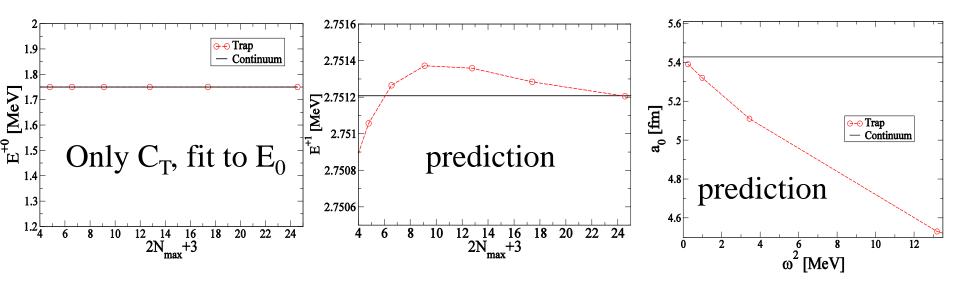
e.g., if
$$|T^{(n)}(k;\Lambda) - T^{(n)}(k;\infty)| \ge O(\frac{Q^{n+2}}{M_{bi}^{n+2}})$$
, then need V_{Short}^{n+1} at order n+1.

LO results: ¹S₀



LO results: ${}^3S_1 - {}^3D_1$

C_T renormalized by $E_0(\infty)$



Fix $\omega(0.5 \text{ MeV})$, increase N_{max}

Fix Λ , decrease ω

How to apply to finite nuclei

• One simple version of beyond mean field interaction has been applied via PVC (with the phonon replaced by p-h pair).

(M. Brenna, G. Colo, X. Roca-Maza, Phys. Rev. C 90, 044316 (2014))

• In principle, a general refitting is needed.

One either perform the fit directly in the chosen beyond mean field scheme, or use subtraction.

• To be fully consistent, **n parameters in the** interaction means **n subtractions** are needed.

Advantages

Enable direct fitting of contact terms to phase shifts; thus, no effect of $\frac{1}{2}\mu r^2\omega^2$ on A>2 system.

Leave us to deal with pure UV and IR dependence

Problem

The formula is based on eigenvalues of <H>, thus cannot be directly applied to treatments involve perturbation.

"Folk theorem"

The quantum field theory generated by the most general Lagrangian with some assumed symmetries will produce the most general Smatrix incorporating quantum mechanics, Lorentz invariance, unitarity, cluster decomposition and those symmetries, with no further physical content.

S. Weinberg '79

(could be disproven in the future ...
... but not yet)