

Nuclear ab-initio Theories and Neutrino Physics

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From dilute matter to the equilibrium point in the energy-density-functional theory







Present collaborators along this research line

- ENSAR2, JRA TheoS (Theoretical Support for Nuclear Facilities in Europe) Task: Development of suitable effective interactions in mean-field and BMF theories



- International Laboratory LIA COLL-AGAIN (France-Italy collaborations)



- <u>J. Bonnard</u>, A. Boulet, U. van Kolck, D. Lacroix, O. Vasseur (IPN Orsay)
- J. Yang (George Washington University), 3 years spent at IPN
- G. Colò, X. Roca-Maza (Univ. of Milano)

Density Functional Theory in chemistry and solid state physics





Nuclear many-body problem with effective interactions

Energy Density Functional (EDF) theory (functionals derived in most cases from effective phenomenological interactions) ... since several decades



Mean-field models and beyond

Double counting, divergences, ...

Work on EDF designed for beyond-mean-field models <u>Nuclear</u> <u>matter</u> <u>Bridging with EFT/</u> <u>ab initio (borrowing</u> <u>concepts and</u> <u>techniques</u> <u>->less</u> phenomenological)



OUTLINE

<u>Starting point. Work on EDF designed for beyond-mean-field models.</u>
 <u>Beyond mean field: second order in the Dyson perturbative many-body expansion for nuclear matter with Skyrme-type interactions.</u>

<u>Divergences, double counting -></u> regularization procedures and parameters adjustment (for 'usual' nuclear density scales)



Properties of matter: relevant for constraining energy density functionals for finite nuclei and neutron stars



Properties of matter: relevant for constraining energy density functionals for finite nuclei and neutron stars

Around the saturation point and beyond.

The structure of neutron stars may be calculated by solving the Tolmann-Oppenheimer-Volkoff equations.

Pressure (first derivative of the EOS) enters in such equations. The total radius is provided by the point where the pressure vanishes:

neutron star mass/radius



- Moghrabi, Grasso, Colo', Van Giai, PRL 105, 262501 (2010)
- Yang, Grasso, Roca-Maza, et al., PRC 94, 034311 (2016)
- Grasso, Lacroix, van Kolck, Invited Comment, Phys. Scr. 91, 063005 (2016)
- Yang, Grasso, and Lacroix, PRC 96, 034318 (2017)
- Yang, Grasso, et al., PRC 95, 054325 (2017)

Equation of state of nuclear matter with a Skyrme-type interaction.

The perturbative many-body problem:



Skyrme interaction for matter (no spin orbit at the mean-field level)

$$v = t_0(1 + x_0P_{\sigma}) + \frac{1}{2}t_1(1 + x_1P_{\sigma})(\mathbf{k}'^2 + \mathbf{k}^2) + t_2(1 + x_2P_{\sigma})\mathbf{k}' \cdot \mathbf{k} + \frac{1}{6}t_3(1 + x_3P_{\sigma})\rho^{\alpha}$$

Spin-exchange operator $P_{\sigma} = \frac{1}{2}(1 + \sigma_1 \cdot \sigma_2)$

Second-order contribution to the EOS (symmetric matter)

$$\int d^3k_1 \int d^3k_2 \int d^3q(vGv)$$

v -> interaction

- G -> propagator
- q -> transferred momentum

$$\begin{split} G &= \frac{-1}{\epsilon'_1 + \epsilon'_2 - \epsilon_1 - \epsilon_2}, \ \epsilon_i^{(')} = \frac{\hbar^2 k_i^{(')2}}{2m_i^*} \longleftarrow \begin{array}{l} & \text{Effective mass} \\ \mathbf{k'_1} &= \mathbf{q} + \mathbf{k_1}, \ \mathbf{k'_2} = \mathbf{k_2} - \mathbf{q}, \end{split}$$

$$|\mathbf{k_1}| < k_{F1}, |\mathbf{k_2}| < k_{F2},$$

 $\mathbf{q} + \mathbf{k_1}| > k_{F1}, |\mathbf{k_2} - \mathbf{q}| > k_{F2}$

k_{F1} and k_{F2} -> Fermi momenta of the two nucleons

In symmetric matter, neutron and proton Fermi momenta are the same:

$$k_F = \left(\frac{3\pi^2}{2}\rho\right)^{1/3}$$

EOS of symmetric matter and cutoff regularization

First order

$$\frac{E_S}{A}^{(1)} = \frac{3}{10} \frac{\hbar^2}{m} \left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \rho^{\frac{2}{3}} + \frac{3}{8} t_0 \rho + \frac{3}{80} \left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \Theta_S \rho^{\frac{5}{3}} + \frac{1}{16} t_3 \rho^{\alpha+1}$$

 $\Theta_S = 3t_1 + t_2(5 + 4x_2)$

Second order

Convenient change of variables: using the incoming and outgoing relative momenta k and k'

$$\mathbf{k} = \frac{\mathbf{k_1} - \mathbf{k_2}}{2}, \ \mathbf{k}' = \frac{\mathbf{k_1}' - \mathbf{k_2}'}{2} = \frac{\mathbf{k_1} - \mathbf{k_2}}{2} + \mathbf{q}$$

Then the propagator can be simplified and written as

$$G = \frac{-m^*}{\hbar^2(k'^2 - k^2)}$$

Second-order contribution for symmetric matter (without the spinorbit and the tensor terms). Sum of the two following terms (cutoff on k')

$$\frac{E_{l=0}^{S(2)}}{A} = -\frac{mk_F^4}{110880\hbar^2\pi^4} \left\{ \begin{array}{c} -6534 + 1188ln[2] + 3564\lambda - 19602\lambda^3 - 5940\lambda^5 \\ +(1782 - 20790\lambda^4)ln[\frac{\lambda-1}{\lambda+1}] \\ +(24948\lambda^5 - 5940\lambda^7)ln[\frac{\lambda^2-1}{\lambda^2}] \\ -14696 + 2112ln[2] + 5280\lambda - 2860\lambda^3 \\ -48840\lambda^5 - 18480\lambda^4 + (2640 - 55440\lambda^6)ln[\frac{\lambda-1}{\lambda+1}] \\ +(71280\lambda^7 - 18480\lambda^9)ln[\frac{\lambda^2-1}{\lambda^2}] \\ +(71280\lambda^7 - 18480\lambda^9)ln[\frac{\lambda^2-1}{\lambda^2}] \\ -9886 + 1128ln[2] + 2520\lambda + 147\lambda^3 - 3654\lambda^5 \\ + 35280\lambda^4 - 15120\lambda^9 + (1260 - 41580\lambda^8)ln[\frac{\lambda-1}{\lambda+1}] \\ +(55440\lambda^9 - 15120\lambda^{11})ln[\frac{\lambda^2-1}{\lambda^2}] \end{array} \right] \begin{pmatrix} 4_F \widetilde{T}_1^2 \\ 4_F \widetilde{T}_1^2 \end{pmatrix}$$

$$\frac{E_{l=1}^{S(2)}}{A} = -\frac{mk_F^8}{73920\hbar^2\pi^4} \left\{ \begin{bmatrix} -1033 + 156ln[2] - 420\lambda + 140\lambda^3 - 840\lambda^5 \\ -5880\lambda' - 2520\lambda'' + (-210 + 6930\lambda^8)ln[\frac{\lambda-1}{\lambda+1}] \\ +(9240\lambda^9 - 2520\lambda^{11})ln[\frac{\lambda^2-1}{\lambda^2}] \end{bmatrix} \left| \widetilde{T}_2^2 \right|,$$

Asymptotic behavior:

$$E_{l=0,poly}^{sym(2)} = -\frac{18mk_s^4}{4\hbar^2\pi^4} \left[\begin{array}{c} +\frac{k_s^4\tilde{T}_1^2}{300}\lambda^5 + (\frac{k_s^2\tilde{T}_{03}\tilde{T}_1}{108} + \frac{k_s^4\tilde{T}_1^2}{240})\lambda^3 + (\frac{\tilde{T}_{03}}{12} + \frac{k_s^2\tilde{T}_{03}\tilde{T}_1}{60} + \frac{k_s^4\tilde{T}_1^2}{140})\lambda}{44k_s^2\tilde{T}_{03}\tilde{T}_1(-167+24ln[2]) + k_s^4\tilde{T}_1^2(-4943+564ln[2]) + 297\tilde{T}_{03}^2(-11+2ln[2])}{-(\frac{\tilde{T}_{03}^2}{240} + \frac{k_s^2\tilde{T}_{03}\tilde{T}_1}{140} + \frac{k_s^4\tilde{T}_1^2}{270})/\lambda + O(\lambda^{-2})} \right]$$

$$E_{l=1,poly}^{sym(2)} = -\frac{18mk_s^8}{4\hbar^2\pi^4} \left[\begin{array}{c} \frac{1}{720}\lambda^3 + \frac{1}{560}\lambda + \left(\frac{-1033 + 156ln[2]}{332640}\right) \\ -\left(\frac{1}{1080}\right)/\lambda + O(\lambda^{-2}) \end{array} \right] \widetilde{T}_2^2 \; .$$

Combinations of Skyrme parameters

$$\begin{split} \widetilde{T}_{03}^2 &= \left[t_0(1-x_0) + \frac{1}{6} t_3(1-x_3)\rho^{\alpha} \right]^2 + \left[t_0(1+x_0) + \frac{1}{6} t_3(1+x_3)\rho^{\alpha} \right]^2 \\ \widetilde{T}_1^2 &= \left[\frac{1}{4} t_1^2 \left[(1-x_1)^2 + (1+x_1)^2 \right] = \frac{1}{2} t_1^2 (1+x_1^2) \\ \widetilde{T}_{03} \widetilde{T}_1 &= \left[\frac{t_1}{2} \left[\left[t_0(1-x_0) + \frac{1}{6} t_3(1-x_3)\rho^{\alpha} \right] (1-x_1) + \left[t_0(1+x_0) + \frac{1}{6} t_3(1+x_3)\rho^{\alpha} \right] (1+x_1) \right] \\ \widetilde{T}_2^2 &= \left[t_2^2 (1-x_2)^2 + 9 t_2^2 (1+x_2)^2 \right] / 9 \\ &= \left[\frac{2}{9} t_2^2 (5+8x_2+5x_2^2) \right]. \end{split}$$

Double counting and ultraviolet divergence (equation of state of symmetric matter)



Second-order equation of state compared with SLy5 mean-field

Second-order correction

(a) Second-order EOS of symmetric matter computed for several values of the cutoff Λ and compared with the mean-field EOS; (b) second-order correction to the energy per particle for symmetric matter. The used parameters are those of SLy5.

Double counting and ultraviolet divergence (pressure and incompressibility)



(a) Second-order pressure; (b) second-order incompressibility modulus. The used parameters are those of SLy5.

Cutoff-regularized and readjusted EOSs. <u>Simultaneous fit for symmetric,</u> asymmetric and neutron matter (benchmark: SLy5 mean field)



Pressure and incompressibility (not entering in the fit)



Pressure (a) and incompressibility modulus (b) computed with the parameters of the simultaneous fit and compared with the mean-field curves.

Remaining at leading order in the perturbative expansion ... new functionals for nuclear matter

YGLO functional (resummation at leading order)

Low-density for neutron matter (EFT satisfies this regime -> Hammer, Furnstahl, NPA 678, 277 (2000))

Lee-Yang expansion in (ak_N). Low-density EOS Lee and Yang, Phys. Rev. 105, 1119 (1957)



We have to constrain the parameters in the following way:

$$t_0(1-x_0) = 4\pi\hbar^2 a/m.$$

$$t_3(1-x_3) = \frac{\hbar^2}{m} \frac{144}{35} (3\pi^2)^{1/3} (11-2\ln 2)a^2.$$

$$t_{0} = \frac{-9849.45}{1 - x_{0}} MeV fm^{3},$$

$$t_{3} = \frac{1812705.02}{1 - x_{3}} MeV fm^{4}.$$

It is possible to constrain the <u>low-density behavior</u> of neutron matter, with α =1/3, and to adjust x0 and x3 for reproducing a <u>reasonable EOS for symmetric</u> <u>matter (at ordinary densities)</u>



<u>Neutron matter at 'usual'</u> <u>density scales.</u> Example of Lyon-Saclay forces adjusted on the neutron EOS

Low-density regime

$$\frac{E}{N} = \frac{\hbar^2 k_N^2}{2m} \left[\frac{3}{5} + \frac{2}{3\pi} (k_N a) + \frac{4}{35\pi^2} (11 - 2ln^2) (k_N a)^2 \right]$$



(1997); 635, 231 (1998), 643, 441 (1998) Akmal et al. -> PRC 58, 1804 (1998)

Neutron matter energy divided by the free gas energy

Some indications from second-order calculations: the second-order contribution has the required k_F^4 term (second term of Lee-Yang exp.)

... but only second order is not enough (if one wants to keep the correct value of the scattering length)



Available online at www.sciencedirect.com



Nuclear Physics A 762 (2005) 82-101

Resummation techniques

- Steele, arXiv: nucl-th/0010066v2
- Kaiser, NPA 860, 41 (2011)
- Schaefer, NPA 762, 82 (2005)

Many body methods and effective field theory

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Available online 30 August 2005

Effective field theories capable of describing systems with anomalously large scattering lengths require summing an infinite number of Feynman diagrams at leading order ... **Guided by:**

- The fact that the second-order t₀ contribution leads to the correct dependence on the Fermi momentum in neutron matter;
- 2) The resumed formulae;
- 3) Good properties of Skyrme functionals

A hybrid functional, YGLO (Yang, Grasso, Lacroix, Orsay): Matching the low-density limit with the Lee-Yang expansion of the energy

$$\mathcal{V} = \frac{B_{\beta}\rho^2}{1 - R_{\beta}\rho^{1/3} + C_{\beta}\rho^{2/3}} + D_{\beta}\rho^{8/3} + F_{\beta}\rho^{\alpha+2}$$

Beta = 1 - > symmetric matter Beta =0 -> neutron matter

YGLO functional: Inspired by resumed expressions (resumed functional) (EFT)



Other parameters adjusted on QMC results at extremely low densities and on Friedman et al. or Akmal et al. EOSs at higher densities

Yang, Grasso, Lacroix, PRC 94 , 031301(R) (2016)

B and R are fixed by imposing to recover the Lee-Yang formula (the analog for symmetric matter may be found in Fetter-Walecka book)

$$B_{\beta} = 2\pi \frac{\hbar^2}{m} \frac{(\nu - 1)}{\nu} a, \quad R_{\beta} = \frac{6}{35\pi} \left(\frac{6\pi^2}{\nu}\right)^{\frac{1}{3}} (11 - 2\ln 2) a,$$

 $\nu = 2$ (4) is the degeneracy for $\beta = 0$ (1)

	C_{β} (fm ²)	D_{β} (MeV fm ⁵)	F_{β} (MeV fm ^{3+3α})
$\beta = 0 \text{ (FP)}$ $\beta = 0 \text{ (Akmal)}$	100.87	-9264.18 -8377.83	9571.90 8743.85
$\beta = 0$ (FRIIIII) $\beta = 1$ (FP)	8.188	-6624.87	6995.46

YGLO functional. In all cases, $\alpha = 0.7$.

Benchmark data are (i) for neutron

matter, the QMC AV4 results of Ref. [17] for values of $|ak_N| < 10 \ (\rho < 0.05 \ \text{fm}^{-3})$, and two different sets of results for $|ak_N| > 10$: the Friedman *et al.* results (FP) of Ref. [18] or the Akmal *et al.* results (stiffer EOS) of Ref. [19] [we call here the corresponding parameter sets YGLO (FP) and YGLO (Akmal), respectively]. (ii) For symmetric matter, the FP results and those of Akmal *et al.* are very close from each others and we made a fit using only the FP points.

YGLO. Very low-density behavior of neutron matter



Yang, Grasso, Lacroix, PRC 94, 031301(R) (2016)

Asymmetric matter

Parabolic approximation



Asymmetric matter



EOSs from Akmal *et al.* [19] (blue diamonds) and Friedman *et al.* (purple circles) in symmetric and neutron matter compared to the YGLO (Akmal) (red dot-dashed curve) and YGLO (FP) (blue dashed curve) results. The different gray dotted curves correspond to the YGLO(FP) EOSs obtained for different asymmetry δ from 0.1 to 0.9 by steps of 0.1 (see text).

Neutron stars Experiments

Neutron skin thickness (difference between rms radii of neutrons and protons)

Dipole polarizability versus neutron skin thickness

Dipole polarizability times symmetry energy versus neutron skin thickness



Roca-Maza et al, PRC 92, 064304 (2015)

Symmetry energy and its slope L= $3\rho_0 (dS/d\rho)_{\rho=\rho_0}$

Strong correlation observed between the neutron skin thickness and the slope L of the symmetry energy (see for instance: Warda et al. PRC 80, 024316 (2009), Centelles et al. PRL 102, 122502 (2009) ->

This correlation is thus expected to exist between the electric dipole polarizability times the symmetry energy and the slope of the symmetry energy

Recent experimental determinations of the electric dipole polarizability:

- ²⁰⁸Pb (polarized proton inelastic scattering at forward angles, RCNP) (Tamii et al. PRL107, 062502 (2011)). Combining all available data: $\alpha_D = 20.1 \pm 0.6 \text{ fm}^3$
- - ¹²⁰Sn (polarized proton inelastic scattering at forward angles, RCNP) (Hashimoto et al. PRC 92, 031305 (2015)). Combining all available data: α_D =8.93 \pm 0.36 fm³
- ⁶⁸Ni (Coulomb excitation in inverse kinematics and invariant mass in one- and two-neutron decay channels, GSI) (Wieland et al, PRL 102, 092502 (2009); Rossi et al. PRL 111, 242503 (2013)). α_D =3.40 ± 0.23 fm³

Using the experimental values of the electric dipole polarizability in the three nuclei

Roca-Maza et al, PRC 92, 064304 (2015)

Lines delimit the phenomenological areas constrained by the exp. determination of the electric dipole polarizability



Yang, Grasso, Lacroix, PRC 94, 031301(R) (2016)

No resummation. Imposing a Lee-Yang regime at all densities at leading order ... Without resummation, how to handle the different density scales ?

... A Lee-Yang type expression for the EOS of neutron matter-> if the low-density regime is always satisfied



We choose to keep terms containing only the s-wave scattering length. The next term in the Lee-Yang expansion contains the p-wave scattering length

Grasso, Lacroix, Yang, Phys. Rev. C 95, 054327 (2017)

Neutron-neutron scattering length.

Low-density regime:

$$|ak_F| < 1$$

We impose a low-density constraint: - a k_F=1 ->

a =-18.9 fm up to a max momentum so that 18.9 k_F=1.

 Beyond this value, we tune the scattering length so that –a = 1/k_F

Neutron-neutron scattering length



Grasso, Lacroix, Yang, PRC 95, 054327 (2017).

Interdisciplinary bridges

Analogy with atomic gases close to Feshbach energy in the case of a density-dependent scattering length



We introduce a Skyrme-type functional containing only s-wave terms and leading, at the mean-field level, to a neutron matter EOS given by the LY expression, with the relations :

$$\begin{split} t_0(1-x_0) &= \frac{4\pi\hbar^2}{m}a, \\ t_3(1-x_3) &= \frac{144\hbar^2}{35m}(3\pi^2)^{1/3}(11-2\ln 2)a^2 \\ t_1(1-x_1) &= \frac{2\pi\hbar^2}{m}(a^2r_s+0.19\pi a^3), \end{split}$$

The power of the density-dependent term is chosen equal to 1/3

Grasso, Lacroix, Yang, PRC 95, 054327 (2017).

We require that: (i) The functional correctly describes neutron matter at all density scales (ii) The functional leads to a reasonable EOS for symmetric matter around the equilibrium point

This may be obtained by imposing a low-density regime everywhere (with a density-dependent neutron-neutron scattering length) The parameters x_i do not enter in the EOS of symmetric matter.

We may thus adjust the parameters t_i to have a reasonable EOS of symmetric matter and tune the neutron-neutron scattering length by imposing, at each density scale, a low-density constraint



Density dependence of the parameters x_0 and x_3



Grasso, Lacroix, Yang, Phys. Rev. C 95, 054327 (2017)

First two terms of the Lee-Yang expansion. EOS of neutron matter



Including the s-wave k_F⁵ terms and adjusting the effective range



Low-density behavior



Grasso, Lacroix, Yang, Phys. Rev. C 95, 054327 (2017)

Towards finite-size systems. Applications to neutron drops trapped in isotropic harmonic potentials of frequency ω

Energy of neutron drops in a trap with $h\omega$ =10 MeV, scaled by $h\omega$ N ^{4/3}



Zhao, Gandolfi, Phys. Rev. C 94, 041302 (2016).

Adding spin-orbit and pairing to our functionals Adjusting to preudodata: using the average of the results shown in the figure below (except Brueckner HF Bonn A)



Bonnard, Grasso, Lacroix, in progress

Adding spin-orbit and pairing to our functionals Adjusting to preudodata: using the average of the results shown in the figure below (except Brueckner HF Bonn A)



Bonnard, Grasso, Lacroix, in progress

Additional parameters in finitesize systems:

- Harmonic shell closures N=8, 20 (no spin orbit, no pairing) (disentangle density-dep. and velocitydep. Terms for k_F⁵)
- Spin orbit coupling constant: adjusting to N ± 1
- Pairing strength (densitydependent mixed surfacevolume interaction): midshell systems 12, 14, 16
- Rest will be predictions

Lee-Yang inspired functional. HF calculations (no spin orbit, no pairing). Lee-Yang regime with - a $k_F = \Lambda$



After adjustment of spin-orbit and pairing

$$\mathcal{E}_{\mathrm{pp}}(\vec{r}) = V_{\mathrm{pp}} \Big(1 - \frac{1}{2} \frac{
ho(\vec{r})}{
ho_c} \Big) \tilde{
ho}(\vec{r})$$



Root-mean-square radius

Bonnard, Grasso, Lacroix, in progress



Pairing potential

Bonnard, Grasso, Lacroix, in progress



Conclusions

 New functionals valid at all density scales for neutron matter and at densities around saturation for symmetric matter

-> YGLO (resummation from EFT and good properties of Skyrme forces : a hybrid functional)

-> without resummation -> density-dependent neutron-neutron scattering length

-> not only nuclear matter. Towards finite-size systems: preliminary results for neutron drops