Equation of state of nuclear matter: ab initio versus nuclear DFT approaches

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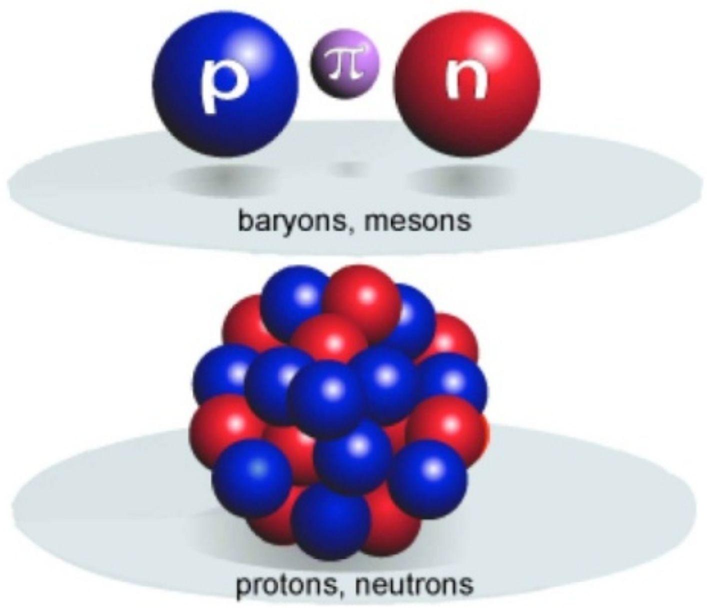
Outline:

- Brief discussion on DFT and ab-initio methods in nuclear systems
- Open problems and eventual solutions
- EFT guiding the construction of DFT: Regularisation, resummation…
- Novel generation of DFT/EDF
- Neutron systems as quasi Unitary systems (from unitary gas to neutron matter)
- Discussion

Coll: J. Bonnard, A. Boulet, M. Grasso and C.J. Yang

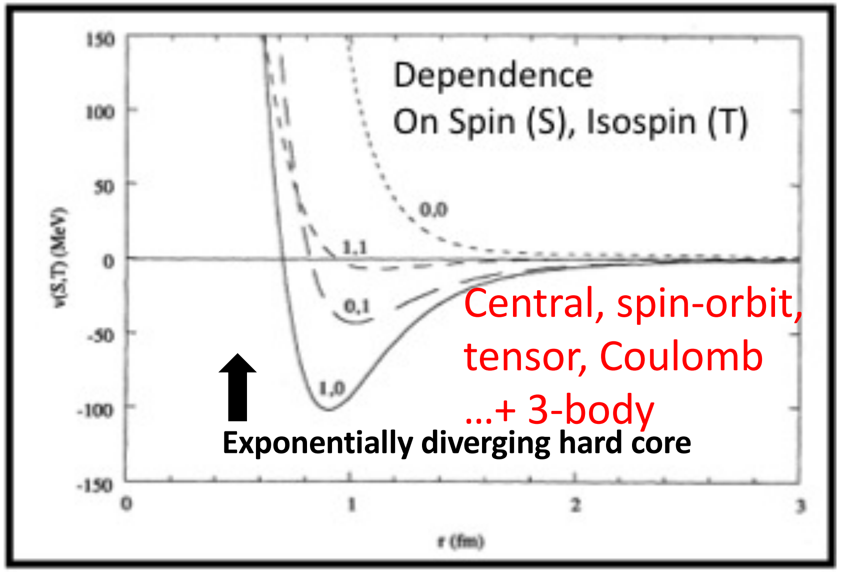
Equation[s] of state of infinite nuclear matter: generalities



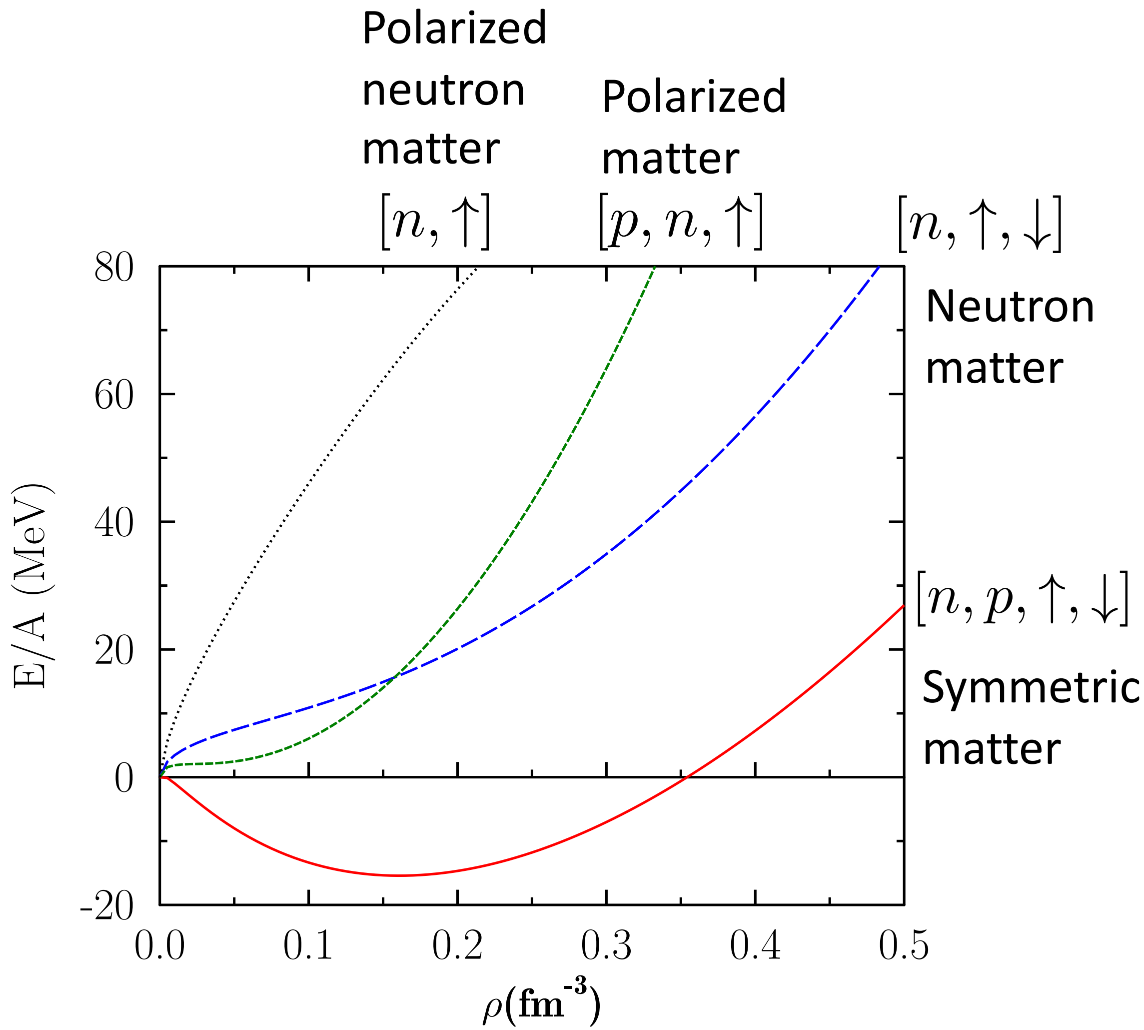
The nucleon-nucleon interaction is complex

$$\phi_{\text{nucleon}} \equiv \phi(\mathbf{r}, \sigma, \tau)$$

$$\boxed{\begin{array}{ll} \sigma = \uparrow, \downarrow & \text{spin} \\ \tau = n, p & \text{isospin} \end{array}}$$

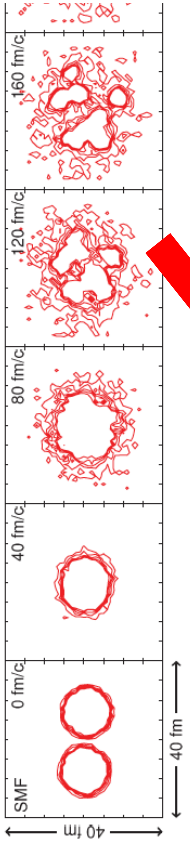


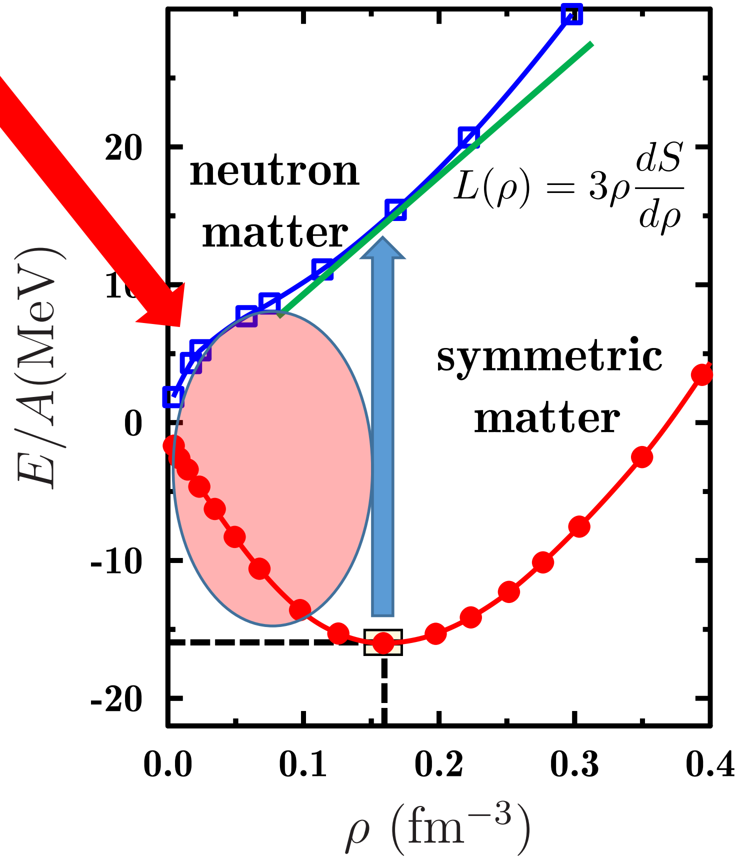
Wiringa, Rev. Mod. Phys. 1993



Equation[s] of state of infinite nuclear matter: and observations (what is known)

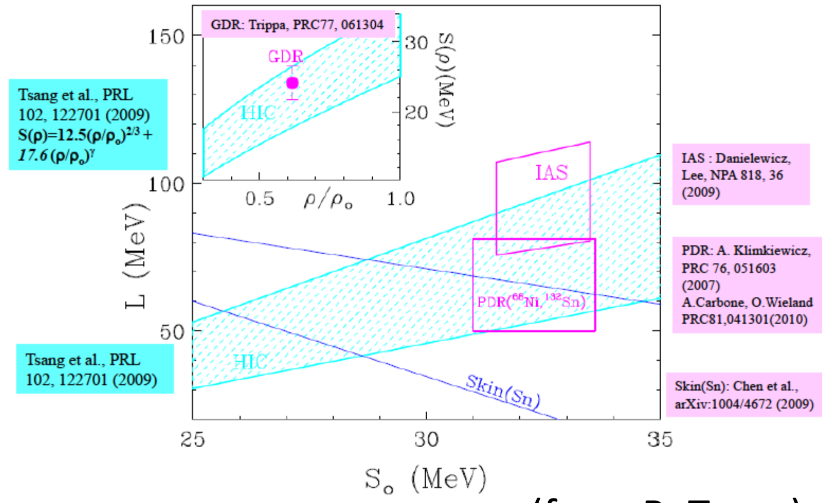
Colonna, Ono, and Rizzo, PRC82 (2010).





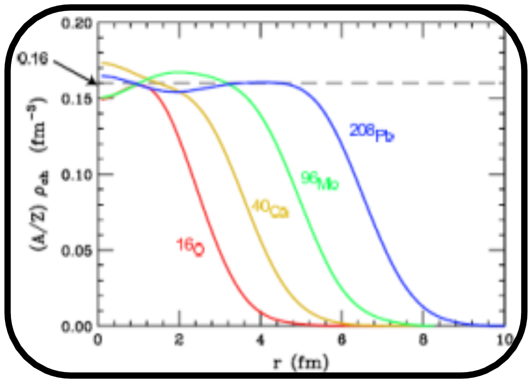
N/Z physics (symmetry energy)

$$S(\rho) \simeq \frac{E_{SM}(\rho)}{A} - \frac{E_{NM}(\rho)}{A}$$



(from B. Tsang)

Nuclei are mainly N~Z



Equilibrium and near-equilibrium point

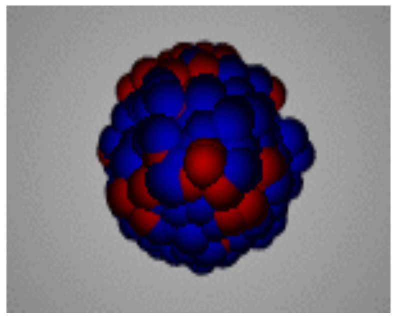
$$\rho_0 \simeq 0.16\ \mathrm{fm}^{-3}$$

$$E/A \simeq 16.0\ \mathrm{MeV}$$

Incompressibility/compressibility

$$K_\infty \simeq 230/270\ \mathrm{MeV}$$

Response to external perturbations

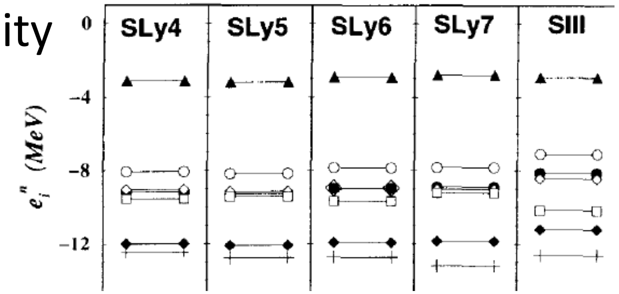


Equation[s] of state of infinite nuclear matter: and observations (quasi-particle properties)

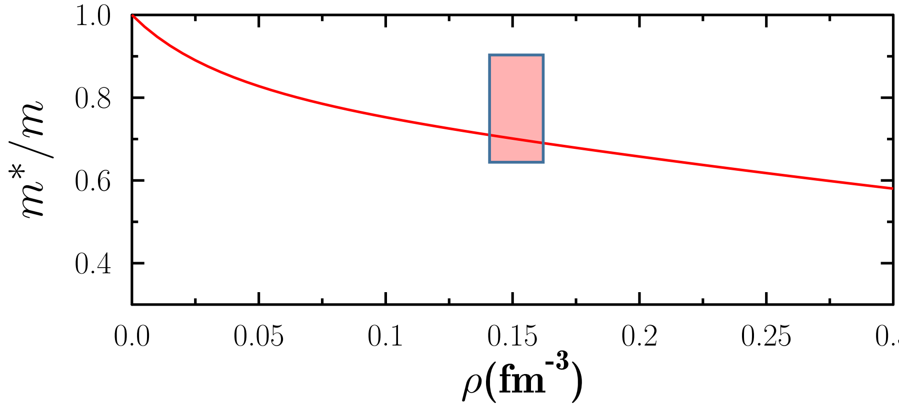
Effective Masses

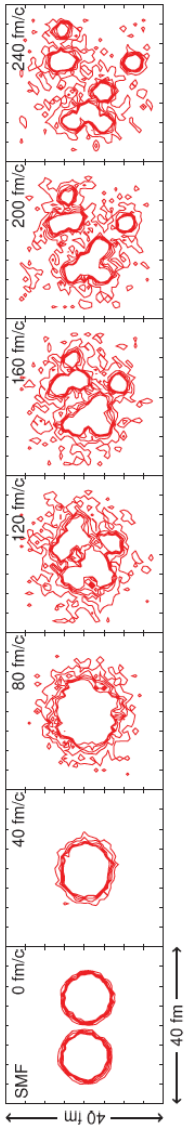
(see discussion J. Meyer, Ann Phys. (Fr), 2003)

Level density

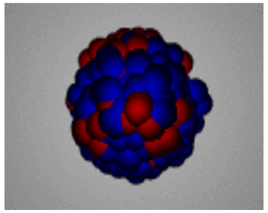


Chabanat et al, NPA (1998)

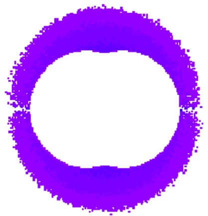




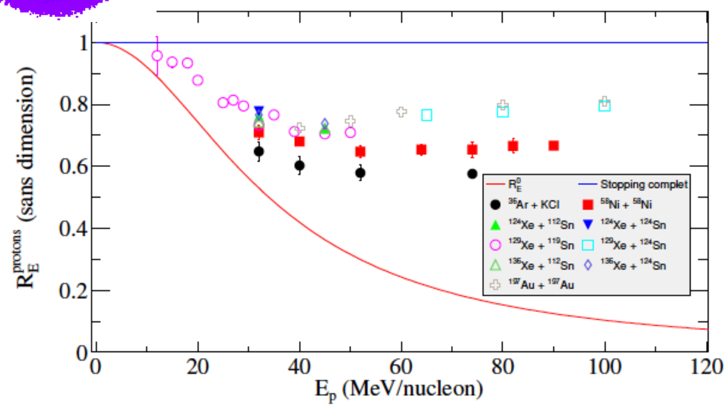
GQR

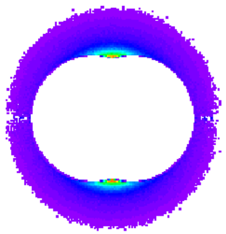


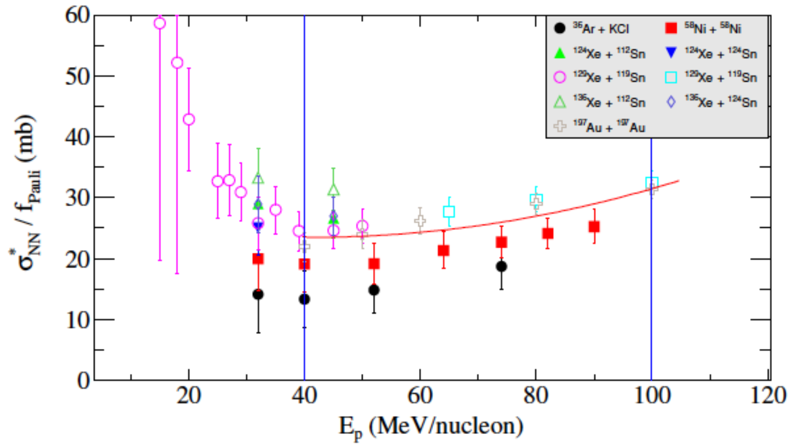
Transport properties (in medium nucleon-nucleon collisions)



Isotropic ratio



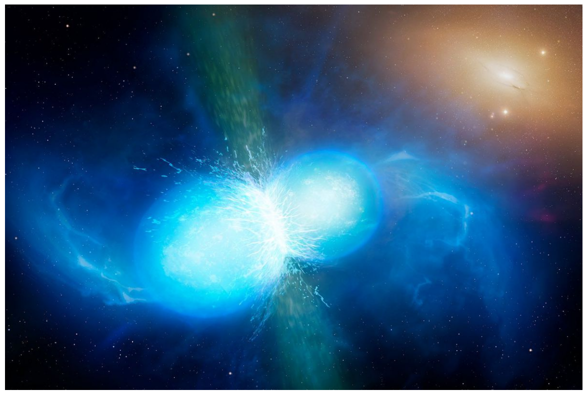




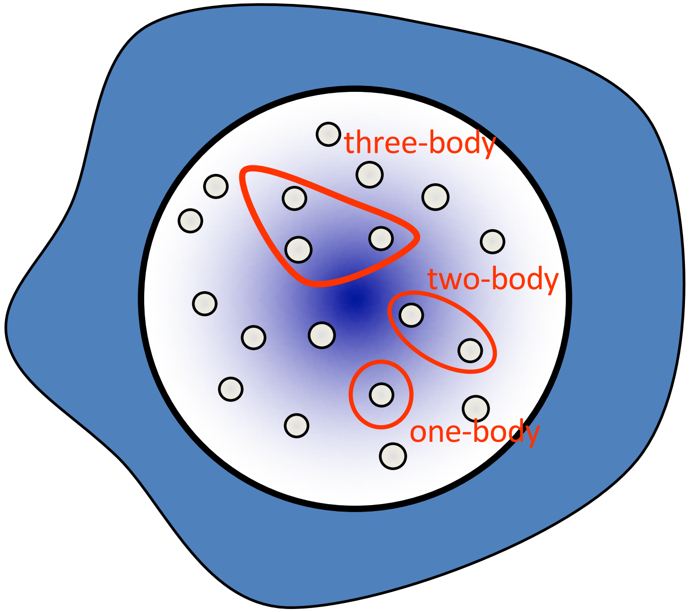
(M. Henri, Thesis 2018)

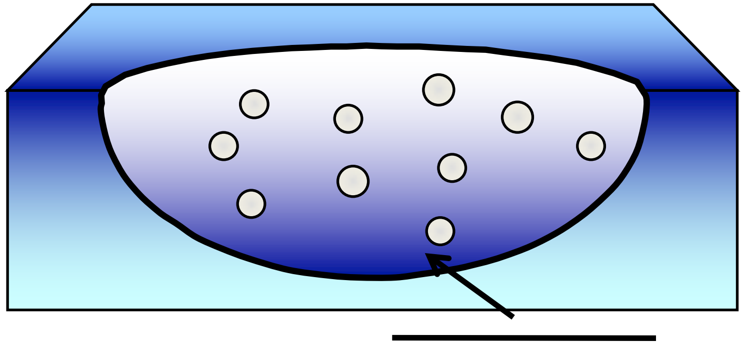
Equation[s] of state of infinite nuclear matter:
Some evident challenges for theory

- Identify as much as possible “well-controlled” observation that could be confronted to theory.
- Theory (whatever) should at least reproduce the observed quantities.
- Ultimately, theory should be able to provide reliable/predictive EOS especially where no observation can be made.
- Can ab-initio theory be considered as proper pseudo-data (see later)?
- One cannot a priori disconnect the EOS from global nuclei properties.
  In nuclei, there are large finite size effects (Mass<500 nucleons).
- New impulse given by the astrophysics observation?



Schematic view of ab-initio versus DFT strategy





Ab-initio strategy

Start from the best controlled many-body interaction (2-body, 3-body)

Major breakthrough (2005)
New generation of soft int.

Perform the best "exact" N-body calculation:
FY, CC, SCGF, MBPT, VMC, …

Applicability:
EOSs, static (spectroscopy) finite systems
(few-body reaction)

Density-functional theory strategy

Start from a set of properties (exp.)
(infinite matter, nuclei)

Major breakthrough (1972)
Predictive LDA DFTs

Guess a functional form and impose the "exact" constraint.
N-body correlation are included.

Applicability: >90% of nuclear physics today

Static, dynamics (small and large amplitude), thermo…

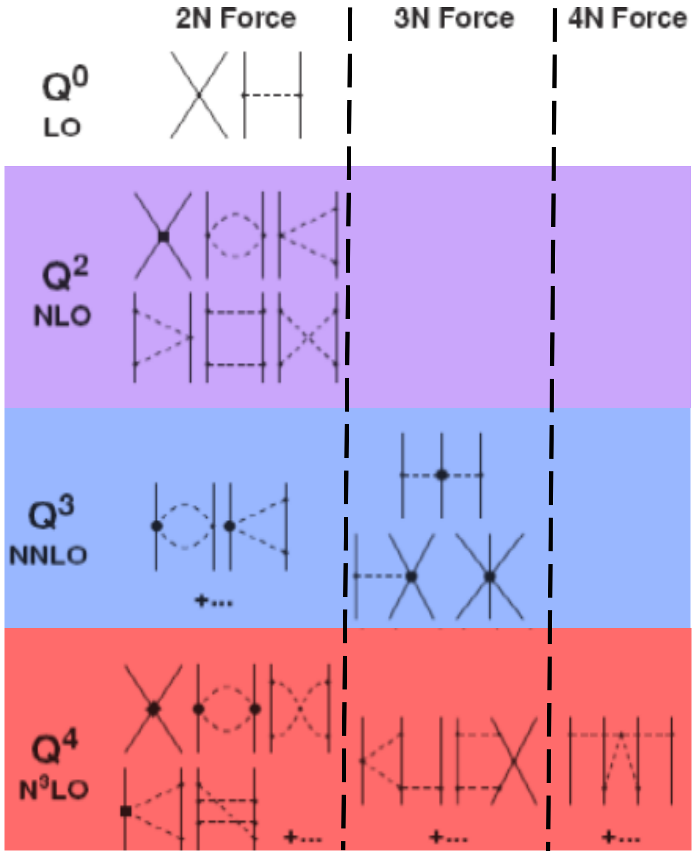
Nuclear physics today

Towards less-empirical approach to low energy nuclear physics

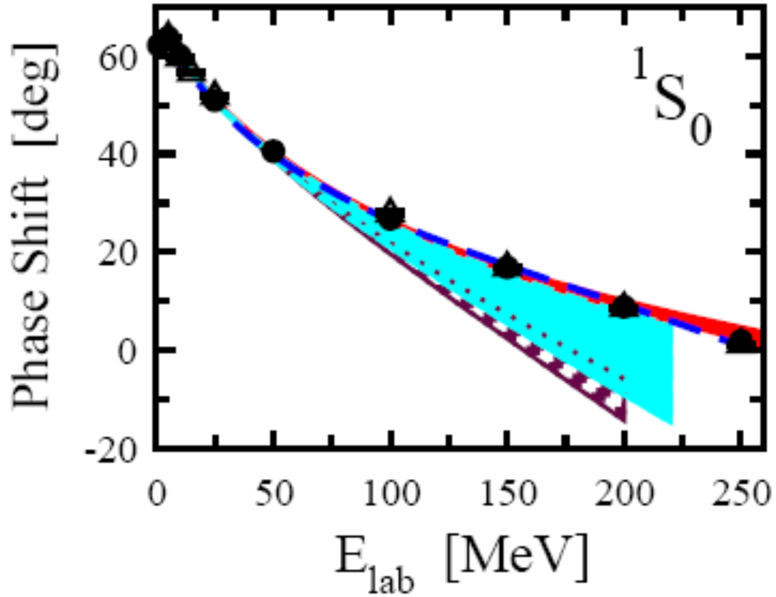
Starting point : Chiral Lagrangian

$$\mathcal{L}_{QCD} \longrightarrow \mathcal{L}_{EFT} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN} + \cdots$$

Feynman diagrams

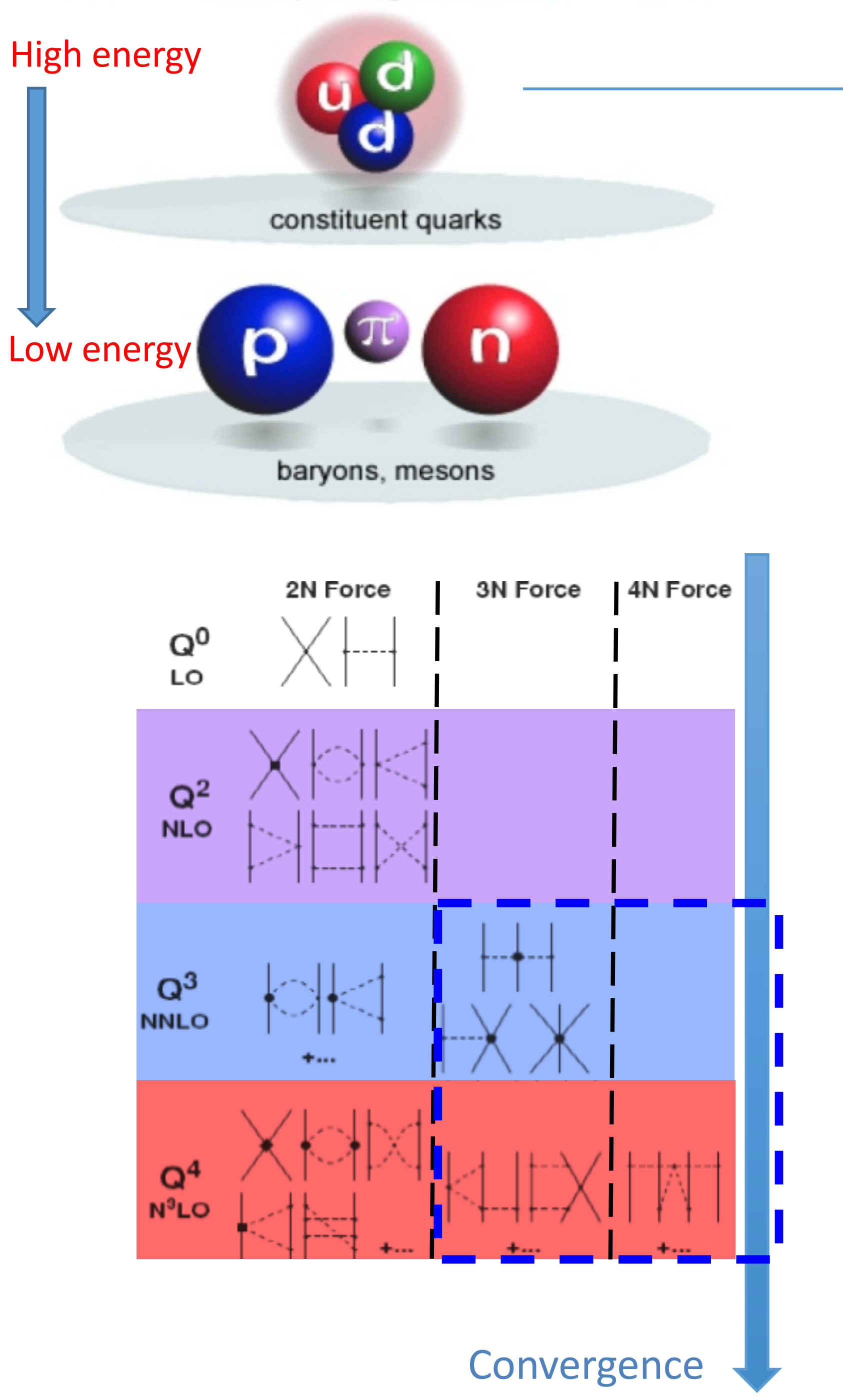


Epelbaum et al, arXiv:0811.1338



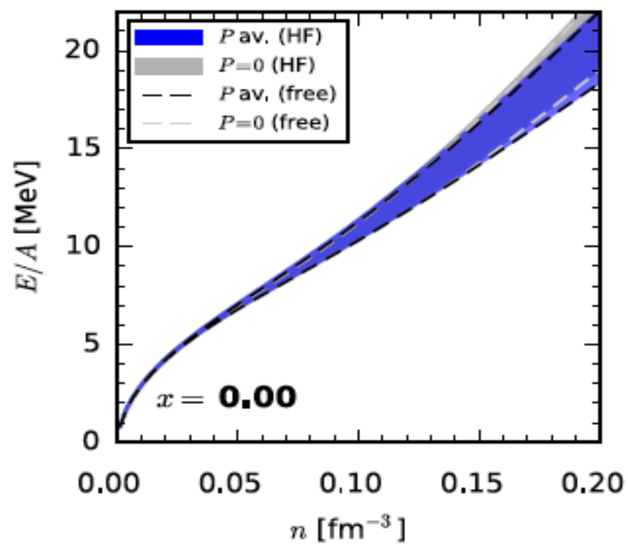
- Direct link to QCD (chiral)
- Systematic Constructive method
- Consistent NN, 3N, 4N ...

Ab-initio technique applied to infinite matter

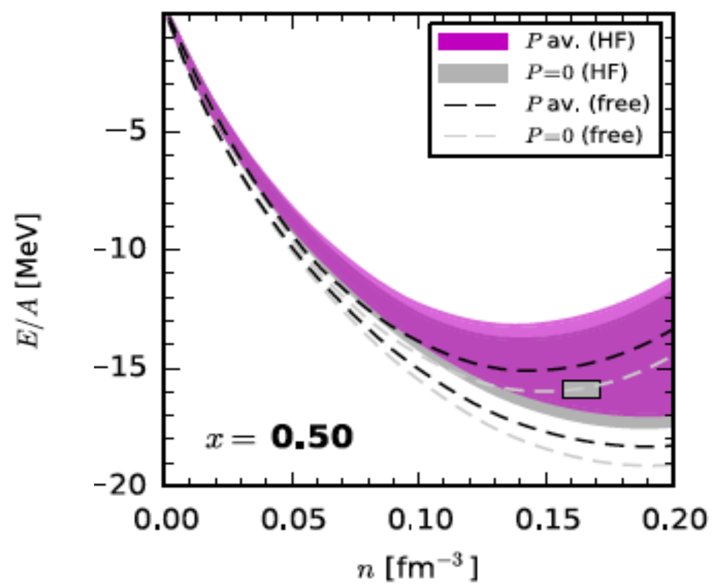


Convergence
and power counting

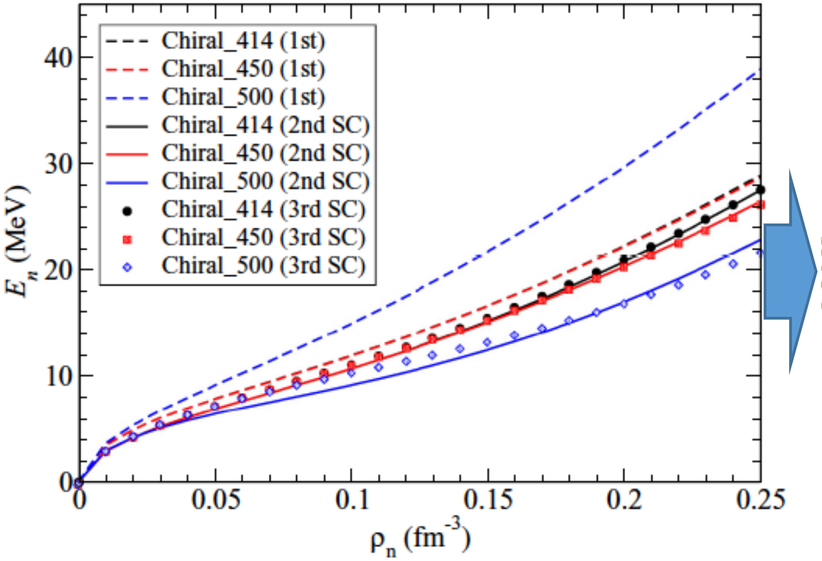
Neutron matter EOS

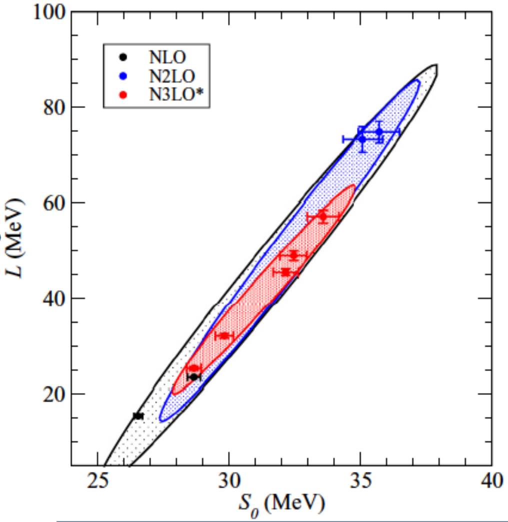


Symmetric matter EOS

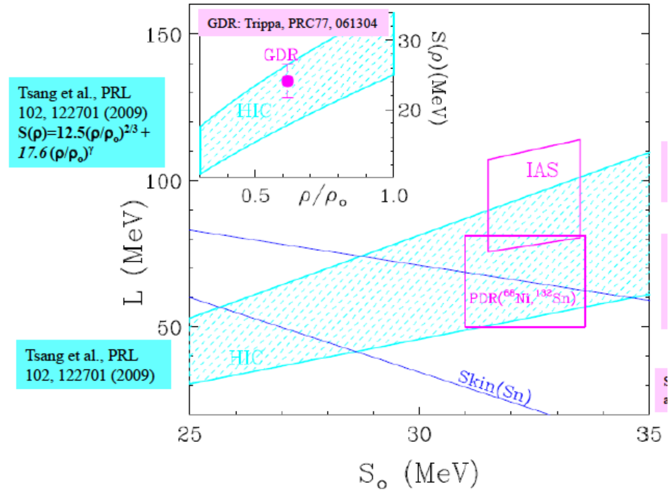


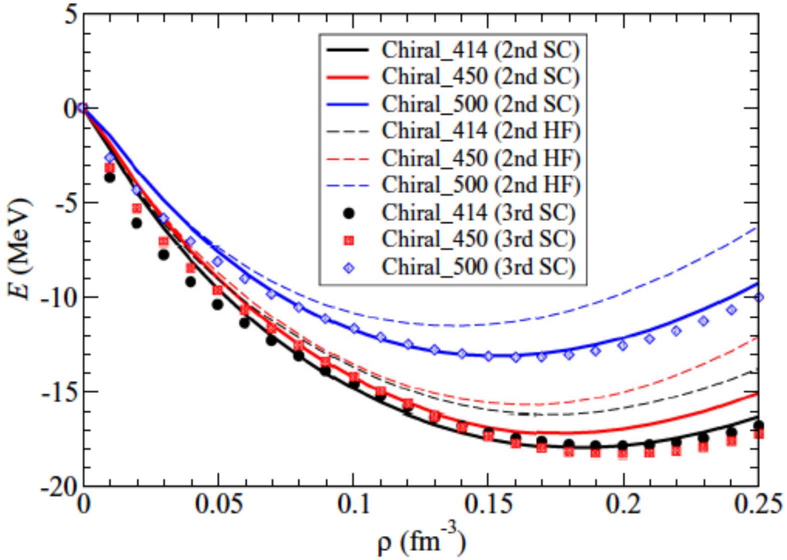
Drischler, Hebeler, and Schwenk Phys. Rev. C 93 (2016)
Drischler, Carbone, Hebeler and Schwenk Phys. Rev. C 94 (2016)





Remember





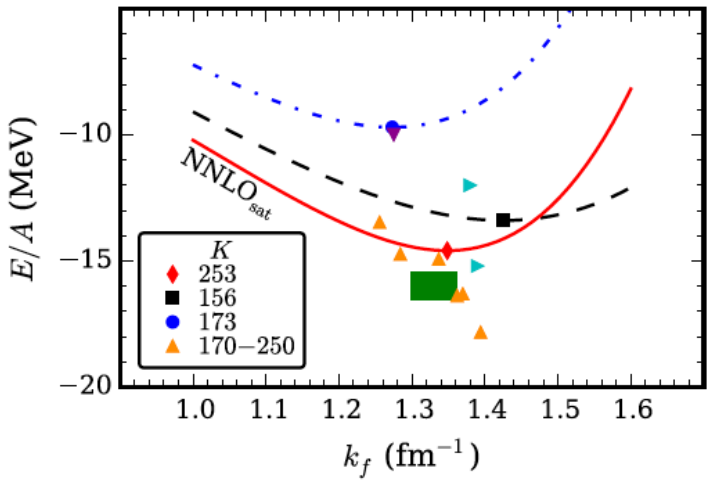
Holt and Kaiser, PRC 95 (2017)

Errorbars for saturation points are large (NLOsat)

Still for scarcely known quantities (below exp errorbars)

Tendency

Add constraint from nuclei



Ekstrom et al, PRC91 (2015).

The DFT concept: simplicity and efficiency

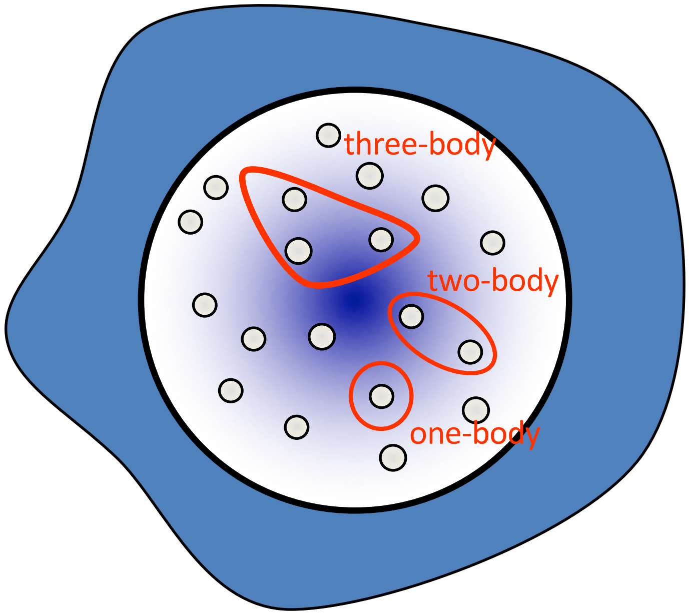
Simplicity

Many aspects of nuclei can be fairly well understood assuming that nucleons behaves like independent particles in an external one-body field

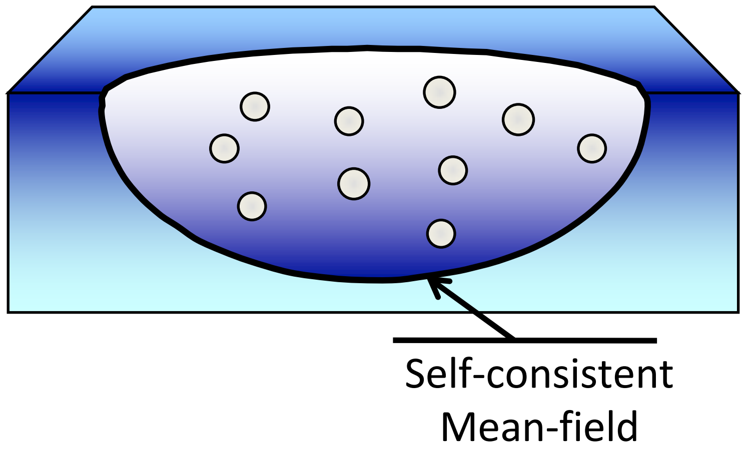
Complexity

The natural approach to map a many-boby problem into a one-body theory (HF) does not work in nuclear physics

The Energy Density Functional approach



Mean-field:
(DFT/EDF)



Complex many-body states:

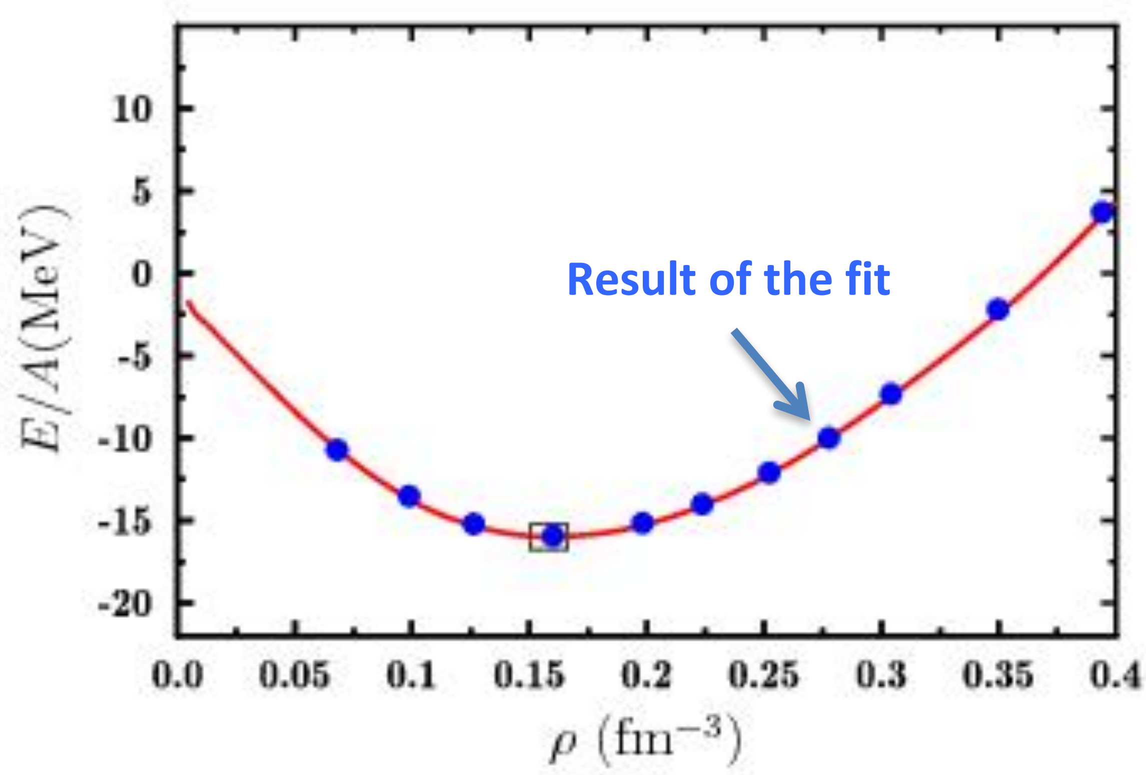
$$\Psi(r_1, \cdots, r_{12}, \cdots, r_{123}, \cdots)$$

Independent particles or quasi-particle states

Parameters of the functional are directly adjusted on data

Link to underlying bare Hamiltonian is lost

DFT from a simple perspective



Exercise : fit the curve with

$$E = \left\langle \frac{p^2}{2m} \right\rangle + U[\rho]$$

In nuclear matter:

$$\left\langle \frac{p^2}{2m} \right\rangle = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{2/3} \rho^{5/3}$$

Fit with 5th order polynomial of the density (Local density approximation)

- **An excellent fit is obtained**
- **Coefficients contains many-body physics**
- **Contains resummation of many-body effects to all orders**

Nuclear Energy Density Functional based on effective interaction

Illustration with the Skyrme Functional

Vautherin, Brink, PRC (1972)

$$
\begin{aligned}
v(\mathbf{r}_1 - \mathbf{r}_2) &= t_0\,(1 + x_0 \hat{P}_\sigma)\,\delta(\mathbf{r}) \\
&+ \tfrac{1}{2}\,t_1\,(1 + x_1 \hat{P}_\sigma)\left[\mathbf{P}'^2\,\delta(\mathbf{r}) + \delta(\mathbf{r})\,\mathbf{P}^2\right] \\
&+ t_2\,(1 + x_2 \hat{P}_\sigma)\,\mathbf{P}' \cdot \delta(\mathbf{r})\,\mathbf{P} \\
&+ iW_0 \sigma . \left[\mathbf{P}' \times \delta(\mathbf{r})\,\mathbf{P}\right] \\
&+ \tfrac{1}{6}\,t_3\,(1 + x_3 \hat{P}_\sigma)\,\rho^\alpha(\mathbf{R})\,\delta(\mathbf{r})
\end{aligned}
$$

$$
\mathcal{E} = \langle \Psi | H(\rho) | \Psi \rangle = \int \mathcal{H}(r) d^3\mathbf{r}
$$

$$
\begin{aligned}
\mathcal{H} = \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_3 + \mathcal{H}_{\text{eff}} \\
+ \mathcal{H}_{\text{fin}} + \mathcal{H}_{\text{so}} + \mathcal{H}_{\text{sg}} + \mathcal{H}_{\text{Coul}}
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{H}_0 &= \tfrac{1}{4} t_0 \left[(2 + x_0)\rho^2 - (2x_0 + 1)(\rho_p^2 + \rho_n^2)\right] \\
\mathcal{H}_3 &= \tfrac{1}{24} t_3 \rho^\alpha \left[(2 + x_3)\rho^2 - (2x_3 + 1)(\rho_p^2 + \rho_n^2)\right] \\
\mathcal{H}_{\text{eff}} &= \tfrac{1}{8}\left[t_1(2 + x_1) + t_2(2 + x_2)\right]\tau\rho \\
&+ \tfrac{1}{8}\left[t_2(2x_2 + 1) - t_1(2x_2 + 1)\right](\tau_p\rho_p + \tau_n\rho_n) \\
\mathcal{H}_{\text{fin}} &= \tfrac{1}{32}\left[3t_1(2 + x_1) - t_2(2 + x_2)\right](\nabla\rho)^2 \\
&- \tfrac{1}{32}\left[3t_1(2x_1 + 1) + t_2(2x_2 + 1)\right]\left[(\nabla\rho_p)^2 + (\nabla\rho_n)^2\right] \\
\mathcal{H}_{\text{so}} &= \tfrac{1}{2} W_0 \left[\mathbf{J}.\nabla\rho + \mathbf{J}_p.\nabla\rho_p + \mathbf{J}_n.\nabla\rho_n\right] \\
\mathcal{H}_{\text{sg}} &= -\tfrac{1}{16}(t_1 x_1 + t_2 x_2)\mathbf{J}^2 + \tfrac{1}{16}(t_1 - t_2)\left[\mathbf{J}_p^2 + \mathbf{J}_n^2\right]
\end{aligned}
$$

Functional of $\rho, \rho_n, \rho_p, \tau, \tau_n, \tau_p, \mathbf{J}, \ldots$

Around 10-14 parameters to be adjusted

Nuclear Energy Density Functional based on effective interaction

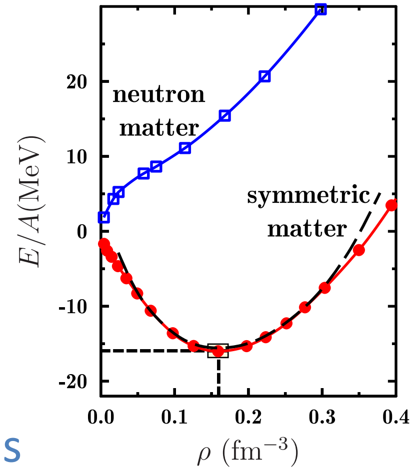
Constraining the functional

See for instance, Meyer EJC1997

Vautherin, Brink, PRC (1972)

$$
\begin{aligned}
v(\mathbf{r}_1-\mathbf{r}_2) &= t_0\,(1+x_0\hat{P}_\sigma)\,\delta(\mathbf{r}) \\
&+\tfrac{1}{2}\,t_1\,(1+x_1\hat{P}_\sigma)\left[\mathbf{P}'^2\,\delta(\mathbf{r})+\delta(\mathbf{r})\,\mathbf{P}^2\right] \\
&+t_2\,(1+x_2\hat{P}_\sigma)\,\mathbf{P}'\cdot\delta(\mathbf{r})\,\mathbf{P} \\
&+iW_0\sigma.\left[\mathbf{P}'\times\delta(\mathbf{r})\,\mathbf{P}\right] \\
&+\tfrac{1}{6}\,t_3\,(1+x_3\hat{P}_\sigma)\,\rho^\alpha(\mathbf{R})\,\delta(\mathbf{r})
\end{aligned}
$$

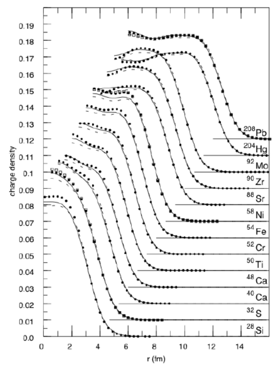
Infinite nuclear matter and Nuclear Masses



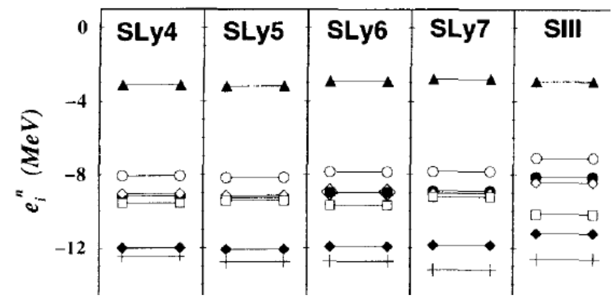
Constraints

$$E_0,\ \left.\frac{\partial E}{\partial \rho}\right|_{\rho_0},\ \left.\frac{\partial^2 E}{\partial \rho^2}\right|_{\rho_0}$$

Densities



Shell effect

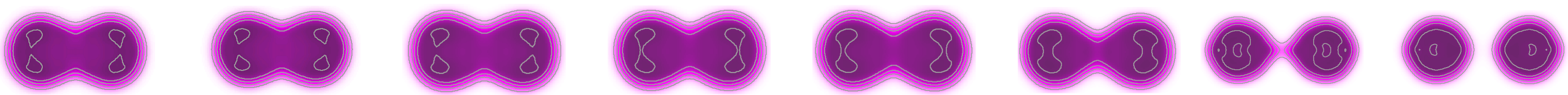


Chabanat et al, NPA (1998)

Dynamics

Time (fm/c)

1000 2000 3000 4000 5000 5300 5500 5600



Scamps, Simenel, Lacroix, PRC 92 (2015)
Tanimura, Lacroix, Scamps, PRC 92 (2015)

Nuclear Energy Density Functional based on effective interaction

Limitation and drawback

$$
\begin{aligned}
v(\mathbf{r}_1 - \mathbf{r}_2) &= t_0\,(1 + x_0 \hat{P}_\sigma)\,\delta(\mathbf{r}) \\
&+ \tfrac{1}{2} t_1\,(1 + x_1 \hat{P}_\sigma)\left[\mathbf{P}'^2\,\delta(\mathbf{r}) + \delta(\mathbf{r})\,\mathbf{P}^2\right] \\
&+ t_2\,(1 + x_2 \hat{P}_\sigma)\,\mathbf{P}' \cdot \delta(\mathbf{r})\,\mathbf{P} \\
&+ i W_0 \sigma . \left[\mathbf{P}' \times \delta(\mathbf{r})\,\mathbf{P}\right] \\
&+ \tfrac{1}{6} t_3\,(1 + x_3 \hat{P}_\sigma)\,\rho^\alpha(\mathbf{R})\,\delta(\mathbf{r})
\end{aligned}
$$

Since we directly fit on experiments
Complex correlation much beyond
Hartree-Fock are included

😀

Since we directly fit on experiments
there is no more link with the
interaction and associated low
energy constants…

😟

Selected shortcomings or hot topics

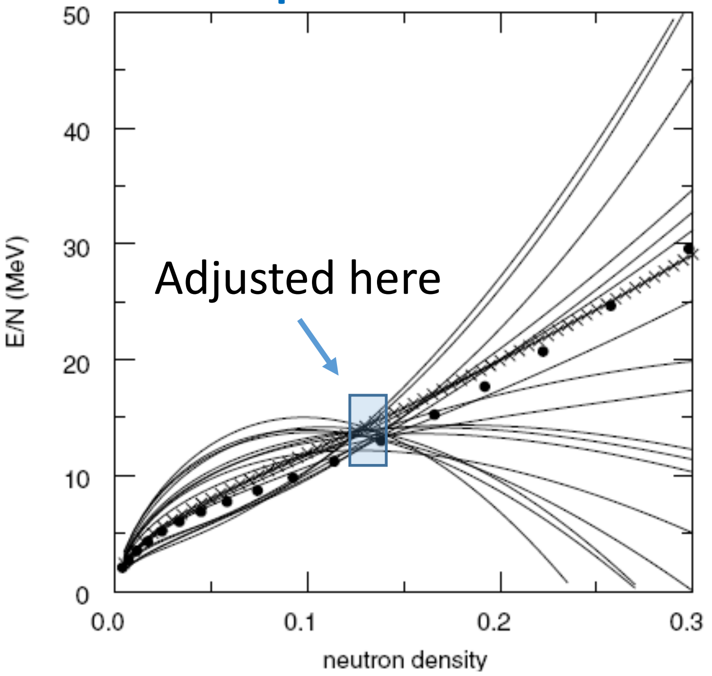
- ➡ Practical challenge: While DFT results are already amazingly good, there is a *relative* lack of predictive power away from known areas.
- ➡ DFT is in other areas considered as an (exact) *ab-initio* theory. Can what we call ab-initio help to render the ab-initio DFT more ab-initio?
- ➡ Formal challenge: DFT for self-bound systems (a bit exaggerated in my opinion)
- ➡ From Mean-field (HF like) to beyond mean-field (Beyond HF like)?
- ➡ Can we define a systematic framework for our Hamiltonian guided DFT theory?

Nuclear Energy Density Functional based on effective interaction

Relative lack of predictive power

Typical Illustration

EOS of pure neutron matter



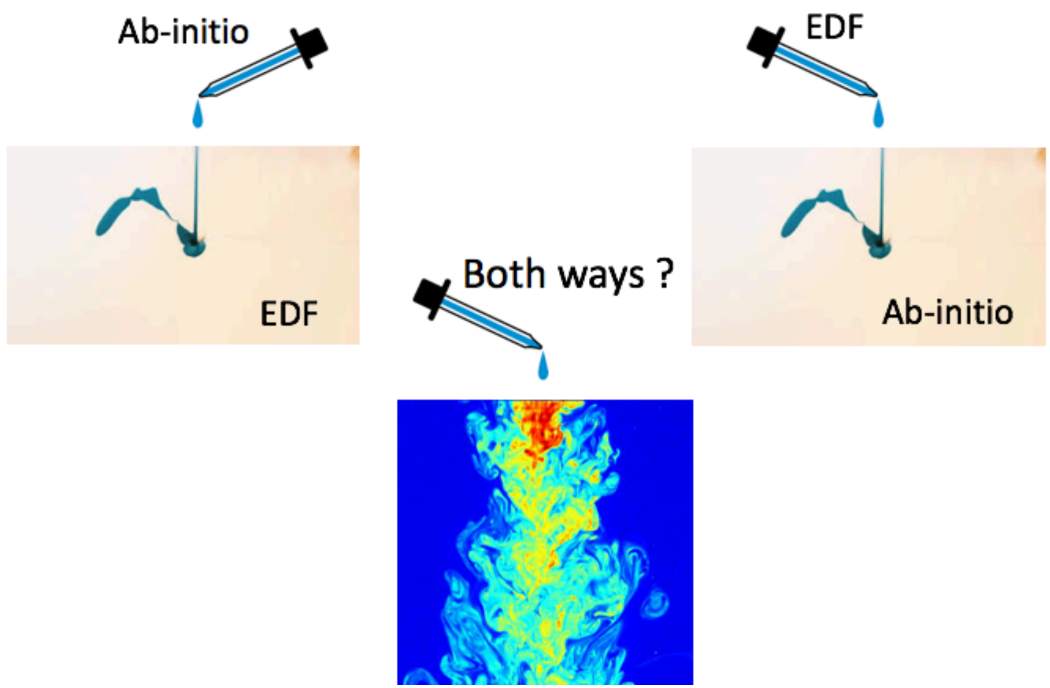
Brown, PRL85 (2000).

The Skyrme DFT is simple (maybe too simple) approach; many sets of parameters.

(see for instance Dutra et el, PRC 85 (2012) where 240 sets have been considered)

Ab-initio inputs can obviously render functionals less-empirical.

From ab-initio to Energy Density Functional (and vice-versa)



Ab-initio methods helping nuclear DFT approach

Some illustrations

Ab-initio calculations have been standardly used to adjust DFT (ex: Friedman-Pandharipande EOSs)

One challenge: To get systematic *well-controlled* reference exact calculations can provide important information for DFT where data are missing as well as well-defined techniques to match the two approaches.

Illustration of cross-fertilization

(From Roggero et al, PRC92 (2015)))

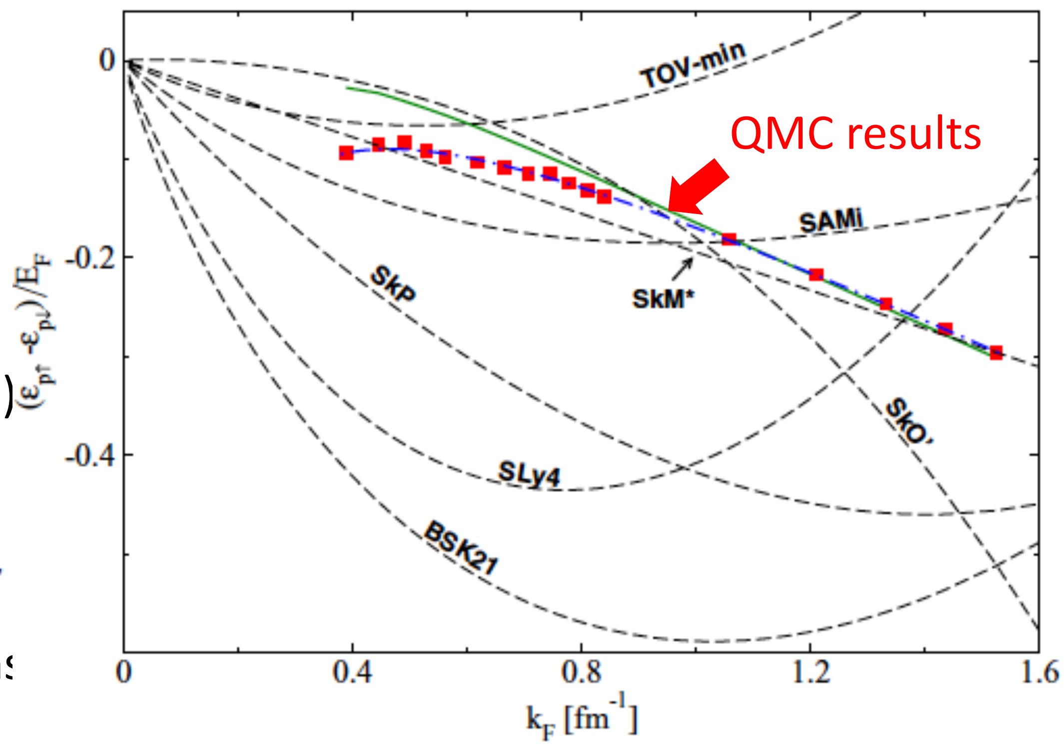
From Skyrme DFT

$$\mathcal{E} = \mathcal{E}_{\text{kin}} + \sum_{t=0,1} \left(C_t^\rho \rho_t^2 + C_t^\tau \rho_t \tau_t + C_t^s s_t^2 + C_t^T s_t T_t \right)$$

One spin-down in a polarized (spin up) matter

$$\frac{\varepsilon_{p\uparrow} - \varepsilon_{p\downarrow}}{E_F} = \frac{4m(C_0^s - C_1^s)}{3\pi^2\hbar^2} k_F - \frac{2m(C_0^T - C_1^T)}{5\pi^2\hbar^2} k_F^3$$

Constraint the time-odd terms



➡ Still not systematic

Ab-initio methods helping nuclear DFT

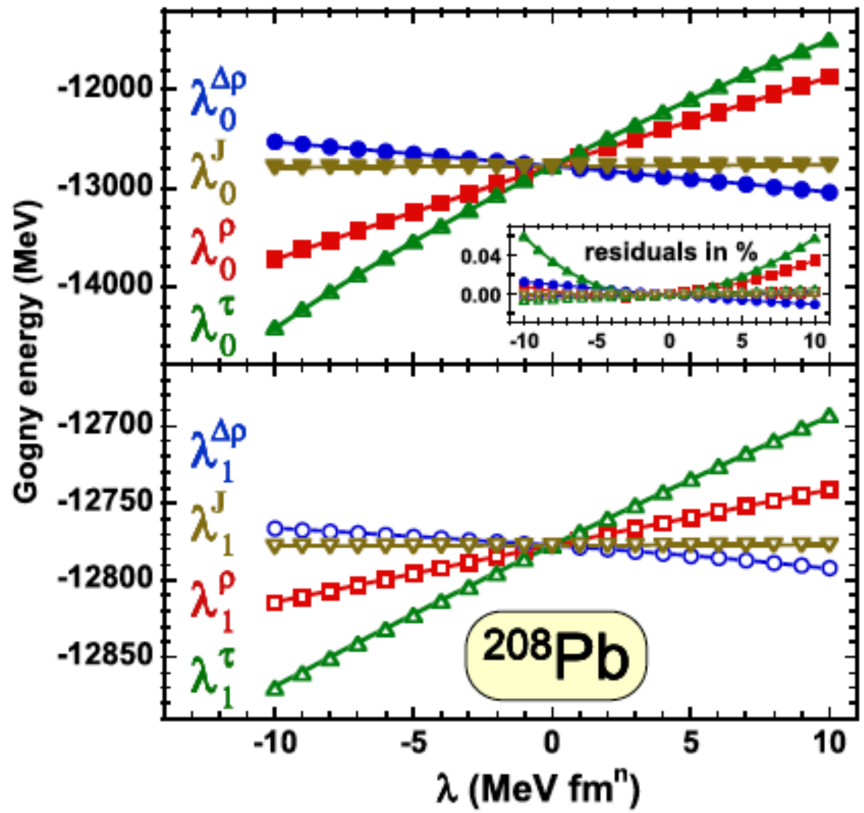
Some illustrations

Perform ab-initio calculations with
A set of independent constraints

$$\delta E' = \delta \langle \Psi | \hat{H} - \sum_{j=1}^{m} \lambda^j \hat{V}_j | \Psi \rangle = 0$$

Perform DFT calculations with
same constraints and adjust
coefficients of the DFT
to match the reference calculation

Illustration with constraint reference Gogny DFT



Dobaczewski, J. Phys. G43 (2016)

Still waiting for ab-initio/DFT some validation

Ab-initio methods helping nuclear DFT approach

Some illustrations

The Density-Matrix Expansion + MBPT approach

(Negele, Vautherin, PRC 5 (1972), PRC 11 (1975))

Take your favorite N-body Hamiltonian

↓

Use for instance the HF+MBPT framework

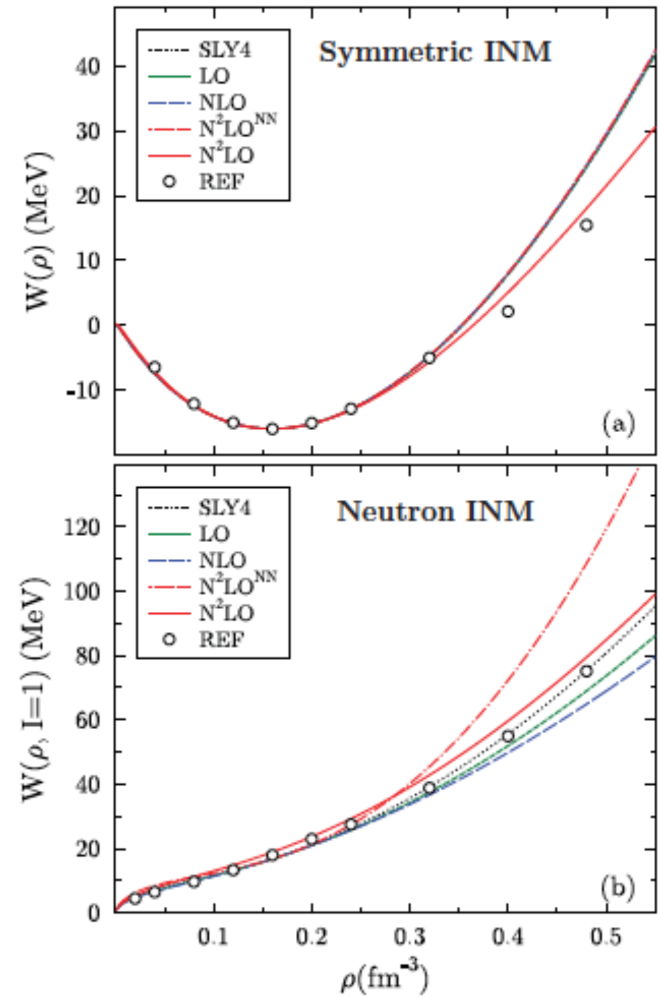
↓

Apply the DME approach + LDA approximation

↓

Leads to skyrme like functional with density-dependent coupling

$$E_x^{NN}[\rho] \approx \sum_{t=0,1} \int d\mathbf{R} \{ g_t^{\rho\rho} \rho_t^2 + g_t^{\rho\tau} \rho_t \tau_t + g_t^{\rho\Delta\rho} \rho_t \Delta \rho_t + g_t^{J\nabla\rho} \boldsymbol{J}_t \cdot \nabla \rho_t + g_t^{JJ} \boldsymbol{J}_t^2 \},$$



Stoitsov et al, PRC 82 (2010)

Ab-initio methods helping nuclear DFT approach

Some illustrations

The Density-Matrix Expansion + (ex) MBPT approach

(Negele, Vautherin, PRC 5 (1972), PRC 11 (1975))

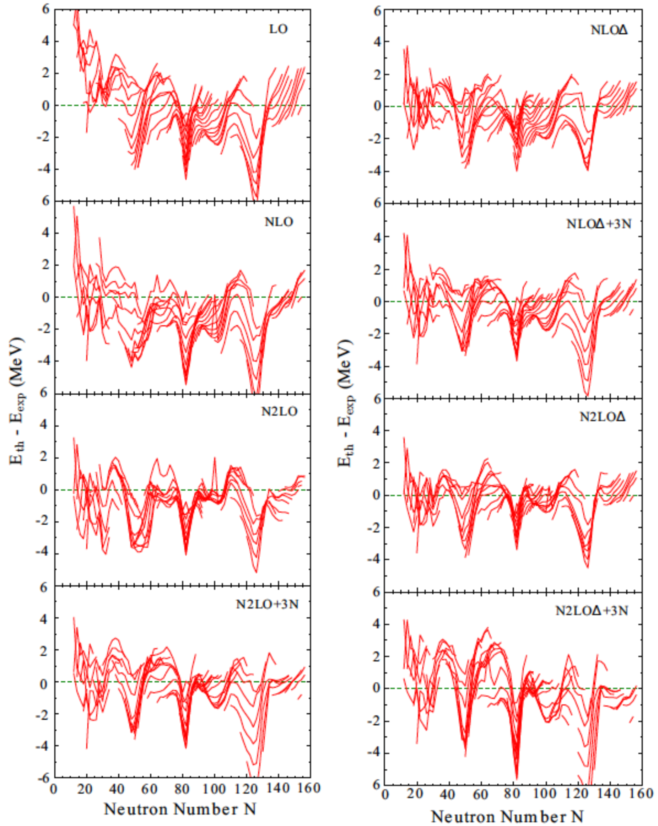
Take your favorite N-body Hamiltonian

Use for instance the HF+MBPT framework

Apply the DME approach + LDA approximation

Leads to skyrme like functional with density-dependent coupling

$$E_x^{NN}[\rho] \approx \sum_{t=0,1} \int d\mathbf{R}\{g_t^{\rho\rho}\rho_t^2 + g_t^{\rho\tau}\rho_t\tau_t + g_t^{\rho\Delta\rho}\rho_t\Delta\rho_t + g_t^{J\nabla\rho}\boldsymbol{J}_t\cdot\nabla\rho_t + g_t^{JJ}\boldsymbol{J}_t^2\},$$



Navarro Pérez, PRC 97 (2018)

- For the moment only at the HF level
- Functional are still fitted
- Looks like Skyrme but much more complicated density dependence.

Some additional challenges/difficulties with our DFT strategy

Mean-Field (MF) versus Beyond Mean-Field (BMF)

Strategy 1

Strategy 2

Take your favorite effective int. → HF like theory → Beyond HF (MBPT, symmetry. Breaking, conf. mixing)

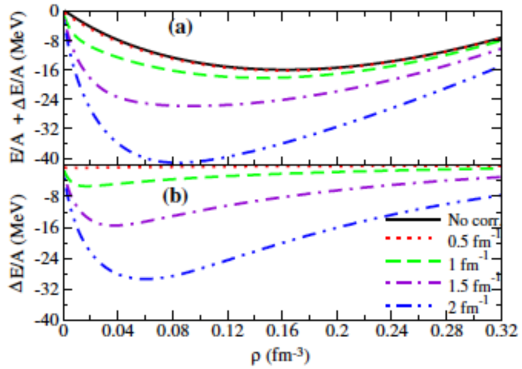
Stick to HF like theory

New aspects with strategy 2

Illustration: Lee-Huang Yang formula

$$\frac{E}{E_{\mathrm{FG}}} = 1 + \underbrace{\frac{10}{9\pi}(\nu-1)(k_F a_s)}_{\text{HF} \quad (\rho^2)} + \underbrace{(\nu-1)\frac{4}{21\pi^2}(11-2\ln 2)(k_F a_s)^2}_{2^{\text{nd}} \text{ order MBPT or HF with DD term} \quad (\rho^{7/3})} + \cdots$$

Using MBPT with contact interaction requires specific attention (EFT)

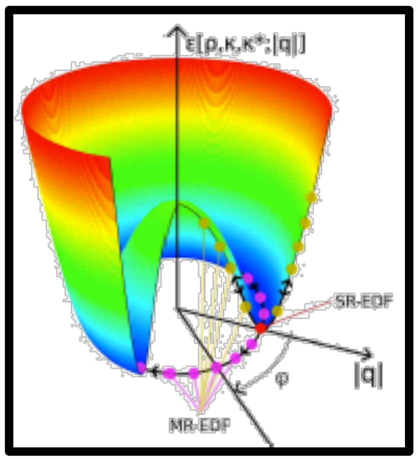


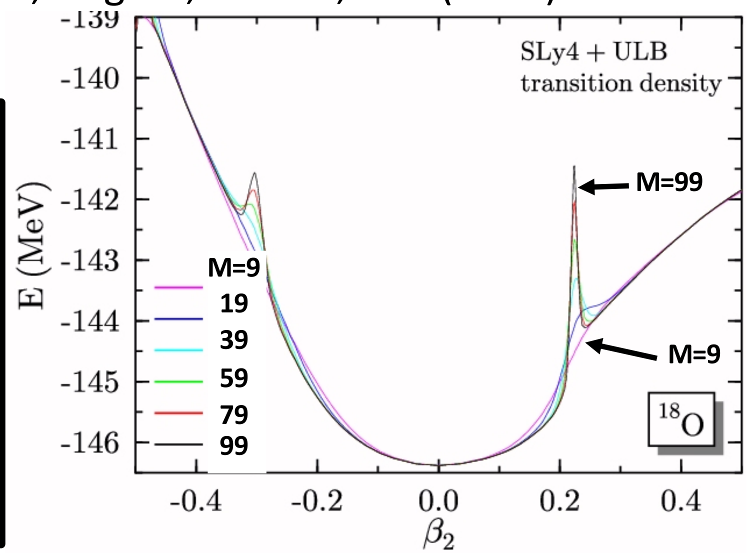
Moghrabi, Grasso et al, PRL 105 (2010), Yang, Grasso et al, PRC 94 (2016)

Density dependent coupling in symmetry restoration?

Lacroix, Duguet, Bender, PRC (2009)

$$P^N = \frac{1}{2\pi}\int_0^{2\pi} d\varphi \; e^{i\varphi(\hat{N}-N)}$$





Take your favorite effective int.

Stick to HF like theory

One solution: avoid DD coupling?

Illustrations

$$\frac{E}{E_{\rm FG}} = 1 + \frac{10}{9\pi}(\nu-1)(k_F a_s) + (\nu-1)\frac{4}{21\pi^2}(11-2\ln 2)(k_F a_s)^2 + \cdots$$

Gezerlis, Bersch, PRL105 (2010)

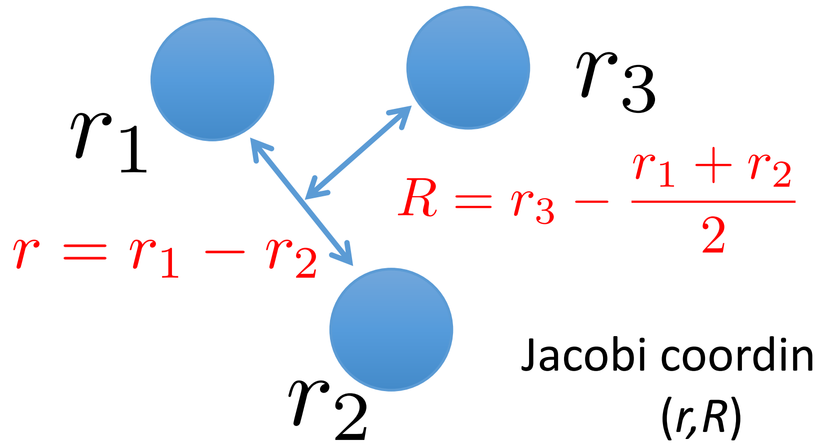
Can be mimic by the HF of a 3-body interaction

$$\hat{H}_3 = f(\mathbf{r},\mathbf{r}')\sum_{\sigma}\psi^\dagger_{\sigma_1\mathbf{r}'}\psi^\dagger_{\sigma_2\mathbf{r}'}\psi^\dagger_{\sigma_3\mathbf{r}}\psi_{\sigma_4\mathbf{r}'}\psi_{\sigma_5\mathbf{r}}\psi_{\sigma_6\mathbf{r}}$$

Valid in low density Fermi gas

with $f(\mathbf{r},\mathbf{r}') = \frac{\hbar^2 a^2}{m}\frac{C}{|\mathbf{r}-\mathbf{r}'|}$

Semi-contact 3-body interaction

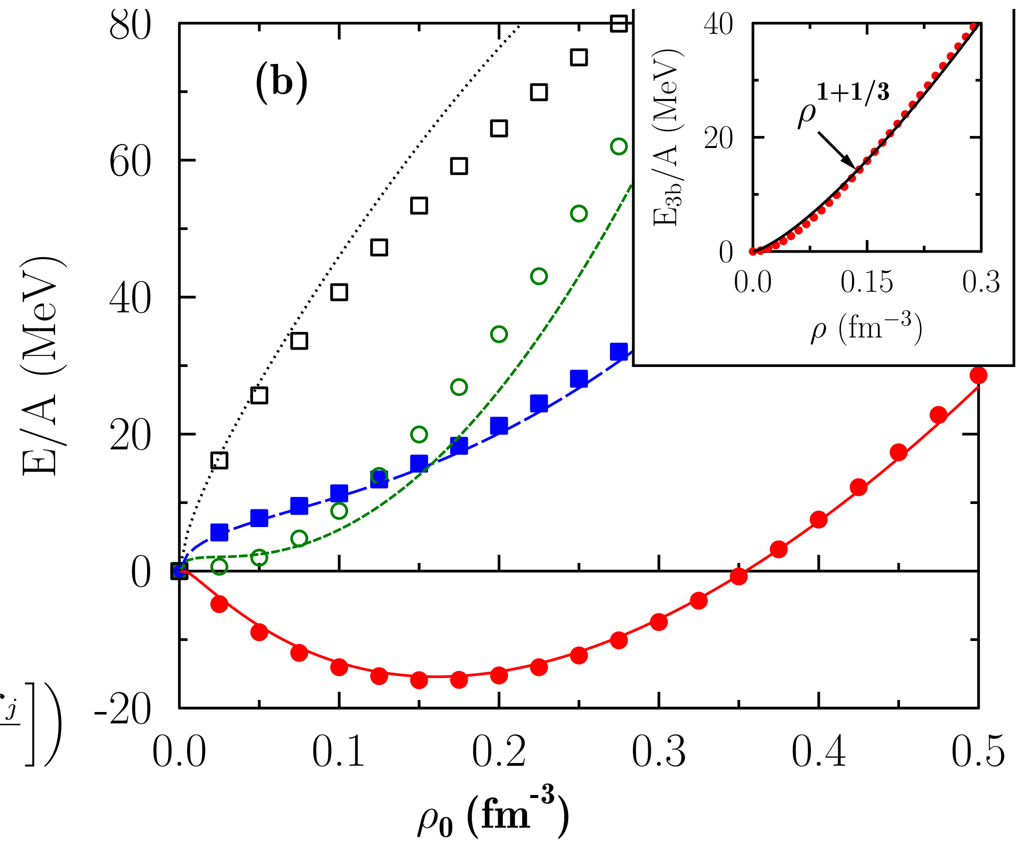


Jacobi coordinate
(r,R)

Idea: take a zero range in *R*

$$v_{ijk} = \left\{V_0(r) + V_\sigma(r)P_\sigma + V_\tau(r)P_\tau + V_{\sigma\tau}(r)P_\sigma P_\tau\right\} \times \delta\left(\mathbf{r}_k - \left[\frac{\mathbf{r}_i + \mathbf{r}_j}{2}\right]\right)$$

Still rather involved



Lacroix, Bennaceur, Phys. Rev. C91 (2015).

One solution: avoid DD coupling?

Illustrations

Take your favorite effective int.

Stick to HF like theory

$$v_C = v^{(0)} + v^{(2)} + v^{(4)} + v^{(6)}$$

with

$$v^{(0)}(\mathbf{r}) = t_0\left(1 + x_0 P_\sigma\right),$$

$$v^{(2)}(\mathbf{r}) = \tfrac{1}{2} t_1\left(1 + x_1 P_\sigma\right)\left[\mathbf{k}'^2 + \mathbf{k}^2\right] + t_2\left(1 + x_2 P_\sigma\right)\mathbf{k}' \cdot \mathbf{k},$$

Systematic expansion of contact interaction

Davesne et al, J. Phys. G90 (2015)

$$v^{(4)}(\mathbf{r}) = \frac{1}{4} t_1^{(4)}\left(1 + x_1^{(4)} P_\sigma\right) \times \left[\left(\mathbf{k}^2 + \mathbf{k}'^2\right)^2 + 4(\mathbf{k}' \cdot \mathbf{k})^2\right] + t_2^{(4)}\left(1 + x_2^{(4)} P_\sigma\right)(\mathbf{k}' \cdot \mathbf{k})\left(\mathbf{k}^2 + \mathbf{k}'^2\right),$$

$$v^{(6)}(\mathbf{r}) = \frac{t_1^{(6)}}{2}\left(1 + x_1^{(6)} P_\sigma\right)\left(\mathbf{k}'^2 + \mathbf{k}^2\right) \times \left[\left(\mathbf{k}'^2 + \mathbf{k}^2\right)^2 + 12(\mathbf{k}' \cdot \mathbf{k})^2\right] + t_2^{(6)}\left(1 + x_2^{(6)} P_\sigma\right)(\mathbf{k}' \cdot \mathbf{k}) \times \left[3\left(\mathbf{k}'^2 + \mathbf{k}^2\right)^2 + 4(\mathbf{k}' \cdot \mathbf{k})^2\right],$$

...

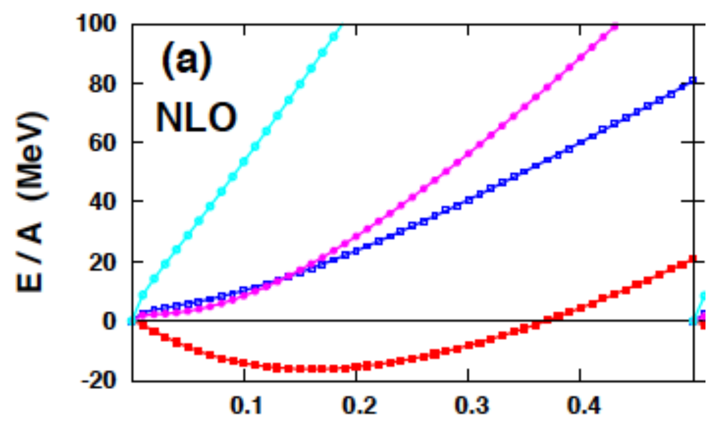
Looks very much like EFT except here only HF

Introduction of non-local effects

Bennaceur et al, J. Phys. G44 (2017)

$$\mathcal{V}_j^{(n)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_3, \mathbf{r}_4) = \left(W_j^{(n)} \hat{1}_\sigma \hat{1}_\tau + B_j^{(n)} \hat{1}_\tau \hat{P}^\sigma - H_j^{(n)} \hat{1}_\sigma \hat{P}^\tau - M_j^{(n)} \hat{P}^\sigma \hat{P}^\tau\right) \times \underbrace{\boxed{\hat{O}_j^{(n)}(\mathbf{k}_{12}, \mathbf{k}_{34})}}_{\text{Non-locality}} \delta(\mathbf{r}_{13}) \delta(\mathbf{r}_{24}) \underbrace{\boxed{g_a(\mathbf{r}_{12})}}_{\text{Gaussian regulator}}.$$

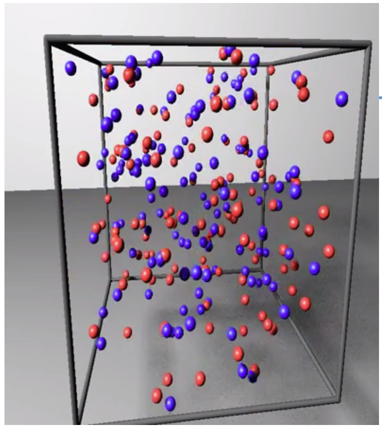
Machleidt, Sammarucca; Phys. Script (2016)



One recurrent difficulty (effective mass)

	$\rho_{\rm sat}$ (fm^{-3})	B (MeV)	K_∞ (MeV)	m^*/m	J (MeV)	L (MeV)
NLO	0.1599	-16.17	229.8	0.4076	31.96	64.04
N^{2}LO	0.1601	-16.09	230.0	0.4061	31.95	64.68

See also discussion in Davesne et al, PRC97 (2018)

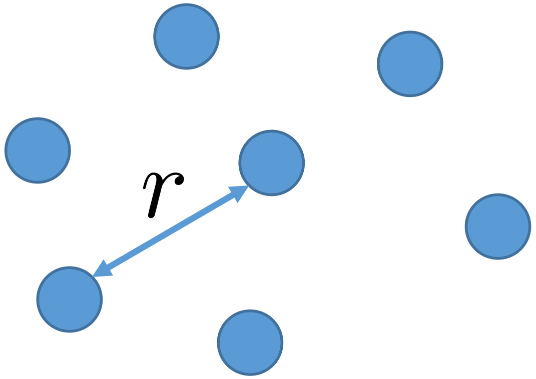


Using EFT techniques/concepts in the nuclear DFT

The low-density Fermi gas limit: the EFT guidance

EFT strategy

See for instance: R. J. Furnstahl, in *Renormalization Group and Effective Field Theory Approaches to Many-Body Systems*, edited by A. Schwenk and J. Polonyi, Lecture Notes in Physics, Vol. 852 (Springer, Berlin, 2012), Chap. 3.



At low density *r* is large

$$\Delta r \Delta k \sim 1$$

→ We only need a low-momentum expansion Of the interaction

$$\langle \mathbf{k}|V_{\mathrm{eft}}|\mathbf{k}'\rangle = C_0 + \frac{1}{2}C_2(\mathbf{k}^2 + \mathbf{k}'^2) + C_2'\,\mathbf{k}\cdot\mathbf{k}' + \cdots$$

Example of the s-wave

C_0, C_2, C'_2 are directly linked to low energy constant

$$\sigma = \frac{4\pi}{k^2}\frac{1}{1+\cot^2\delta_0} = \frac{4\pi a^2}{ak^2 + [1 - ar_{\mathrm{ef}}k^2/2]^2}$$

$$C_0 = \frac{4\pi\hbar^2}{m}a_s,\ C_2 = \frac{2\pi\hbar^2}{m}r_e a_s^2,\ C_2' = \frac{4\pi\hbar^2}{m}a_p^3.$$

Constructive many-body perturbative approach

$$E = E^{\mathrm{HF}} + E^{2^{\mathrm{nd}}} + E^{3^{\mathrm{rd}}} + \ldots$$

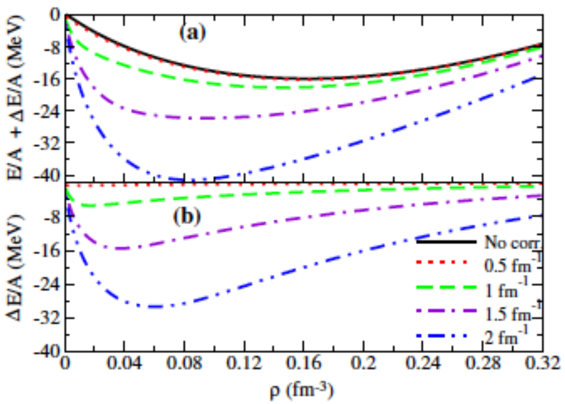
H.W. Hammer and R.J. Furnstahl, NPA678 (2000)

Using EFT techniques/concepts in the nuclear DFT

Take your favorite effective int. → HF like theory → Beyond HF (MBPT, symmetry. Breaking, conf. mixing)

Use of EFT methods to regularize the MBPT

Moghrabi, Grasso et al, PRL 105 (2010); Yang, Grasso et al, PRC 94 (2016)



Cutoff regularization

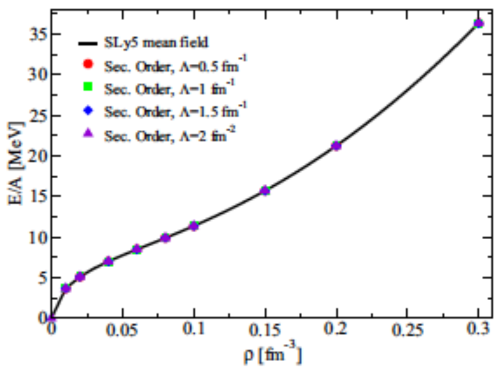
$$E = E^{\mathrm{HF}} + E^{2^{\mathrm{nd}}} + \ldots$$

E_{HF} → Skyrme functional

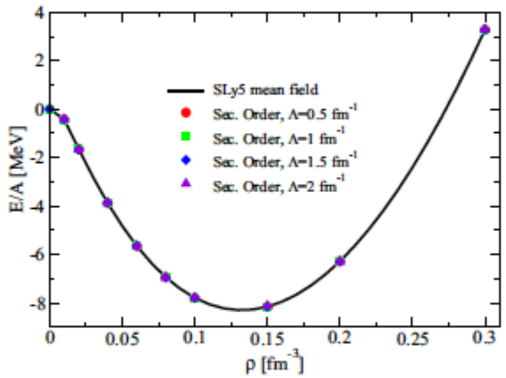
$$E^{2nd} = E^{2nd}_{\mathrm{Non-div}} + \cancel{E^{2nd}}(\Lambda)$$

Minimal subtraction + refitting

Neutron matter



Symmetric matter



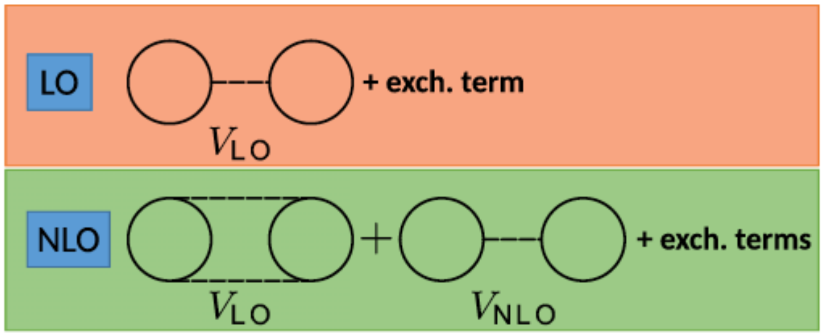
Other EFT technique can be employed

See also coming review by M. Grasso, arXiv:1811.01039, to be published PPNP

- dimensional Regularization was also used in Yang, Grasso et al, PRC 94 (2016)
- Renormalization: some divergence can be absorbed (for certain density dependence) by using cut-off dependent coupling constants Yang, Grasso, Moghrabi, van Kolck et al, PRC 95 (2017)

$$E^{2nd} = E^{2nd}_{\mathrm{Non-div}} + E^{2nd}(\Lambda)$$

- A first step towards a systematic approach to design new DFTs inspired from MBPT: the counter-term technique Yang, Grasso, Lacroix, PRC 96 (2017)



$$V_{\mathrm{LO}} = t_0(1 + x_0 P_\sigma) + \frac{t_3}{6}(1 + x_3 P_\sigma)\rho^\alpha$$

$$E_{\mathrm{LO}} = E_{HF}(t_0, t_3)$$

$$V_{\mathrm{NLO}}\colon t_1(1 + x_1 P_\sigma)(\mathbf{k}'^2 + \mathbf{k}^2)$$

$$V_{\mathrm{NLO}}\colon t_2(1 + x_2 P_\sigma)\mathbf{k}' \cdot \mathbf{k}$$

$$E_{\mathrm{NLO}} = E_{HF}(t_1, t_2) + E^{2nd}(t_0, t_3) + E_{HF}(\text{counter term})$$

...

Counter terms

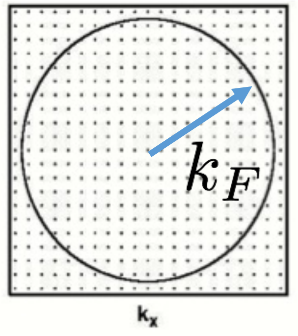
$$V^{(a)}_{\mathrm{NLO}} = a(1 + P_\sigma x_a) f_a[(\vec{k} - \vec{k}')^{-3v_a}, \rho^{v_a}],$$

$$V^{(b)}_{\mathrm{NLO}} = b(1 + P_\sigma x_b) f_b[(\vec{k} - \vec{k}')^{3\alpha-3v_b}, \rho^{v_b}]$$

$$V^{(c)}_{\mathrm{NLO}} = c(1 + P_\sigma x_c) f_b[(\vec{k} - \vec{k}')^{6\alpha-3v_c}, \rho^{v_c}]$$

k_F expansion

Back to the problem of DFT linked to Low energy constants (LEC)



$$E = E^{\mathrm{HF}} + E^{2^{\mathrm{nd}}} + E^{3^{\mathrm{rd}}} + \ldots$$

$\rho = \frac{\nu}{6\pi^2} k_F^2$ with ν degeneracy

Many-body Perturbation Theory

E^{HF} $E^{2^{\mathrm{nd}}}$ $E^{3^{\mathrm{rd}}}$ $+ \cdots$ [MBPT]

Expansion as polynomial of LEC

$(a_s k_F)$ $(r_e k_F)$ $\cdots$

Functionals of increasing complexity

$$E \equiv \mathcal{E}(\rho)$$

Difficulty

valid for $a_s k_F < 1$

For neutron matter $a_s = -18.9 \text{ fm}$

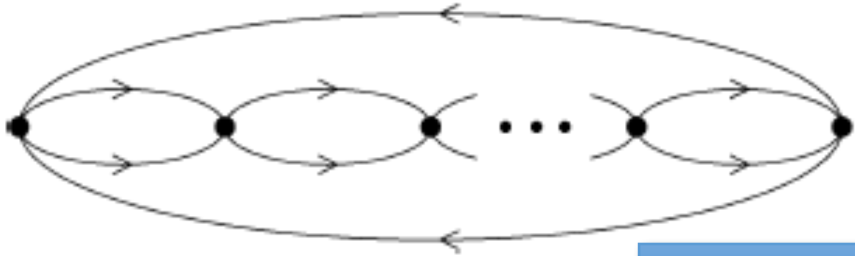
$r_e = 2.7 \text{ fm}$

Valid for $\rho < 10^{-6} \text{ fm}^{-3}$

Highlighting work

Schaefer, Kao, Cotanch, NPA 762 (2005)

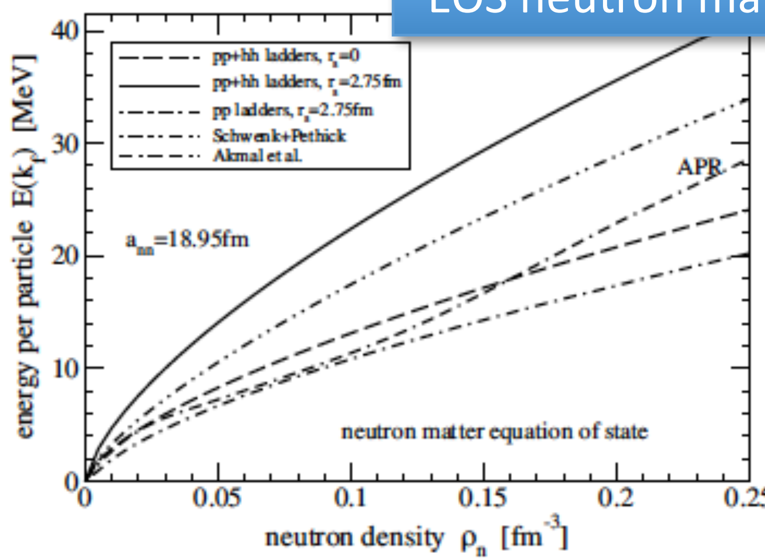
Resummation of particle-particle diagrams



$$\frac{E_{PP}}{A} = \frac{3(g-1)\pi^2}{k_F^3}\int \frac{d^3P}{(2\pi)^3}\frac{d^3k}{(2\pi)^3}\theta_k^- \frac{4\pi a/M}{1-\frac{k_F a}{\pi} f_{PP}(\kappa, s)}.$$

- Contains terms to all order in $(a_s k_F)$
- Results strongly depends on selected diagram

EOS neutron matter



Kaiser, EPJA 48 (2012)

The pragmatic approach

$$E \sim \frac{3}{5}\frac{\hbar^2 k_F^2}{2m}\frac{\frac{10}{9\pi}(a_s k_F)}{1-\frac{6}{35\pi}(11-2\ln 2)(a_s k_F)} \sim \langle f_{PP}\rangle$$

Interpretations:

-Minimal Padé approximation
-Phase-space average
-asymptotic values
-...

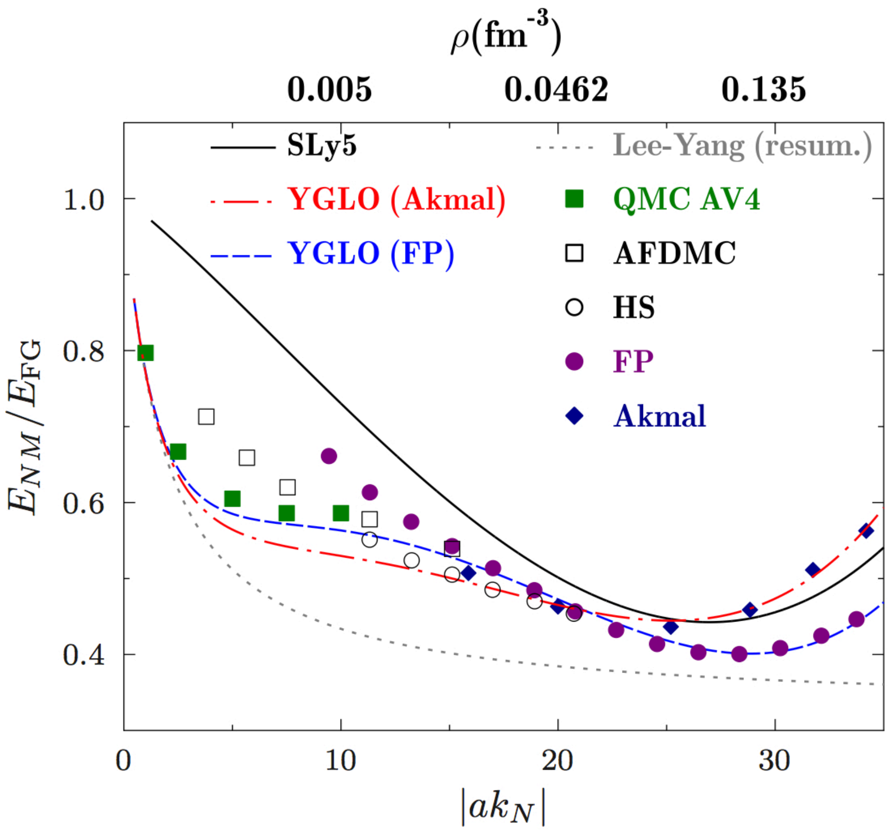
First illustration of an EFT guided EDF: the YGLO* hybrid functional

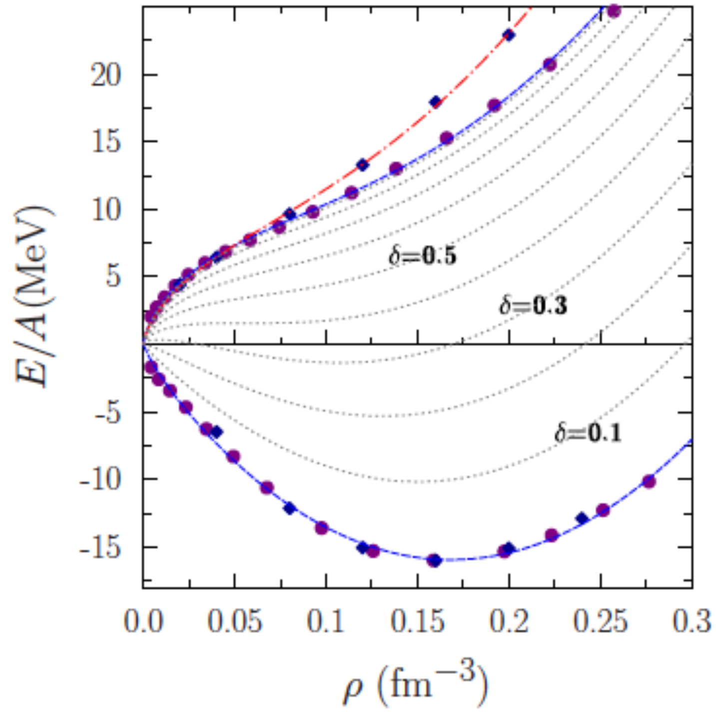
Yang, Grasso, Lacroix PRC94 (2016)

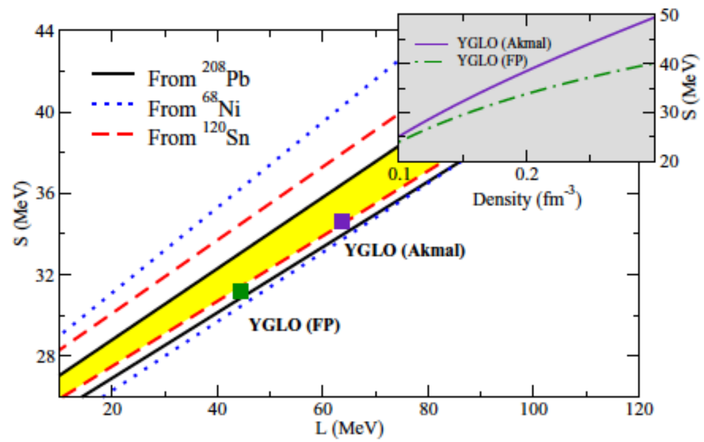
Functional form

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

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







*YGLO: Yang-Grasso-Lacroix Orsay

Alternative method for density dependent constants

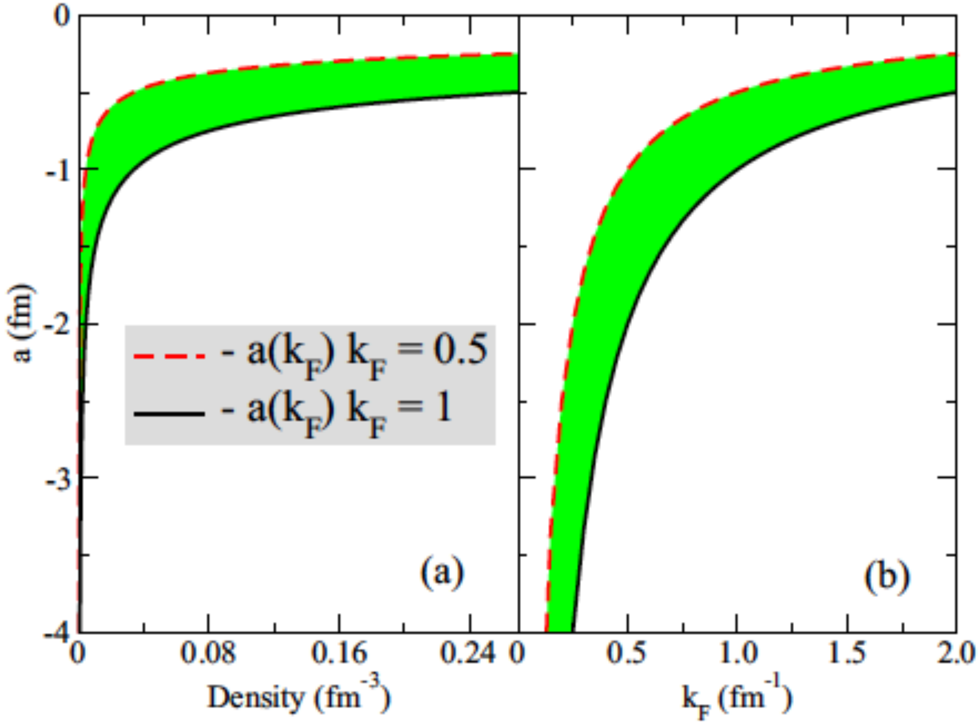
The Lee-Yang inspired functional (ELYO* functionals)

Grasso, Lacroix, Yang, PRC 95 (2017)

$$\frac{E}{N} = \frac{\hbar^2 k_F^2}{2m}\left[\frac{3}{5} + \frac{2}{3\pi}(k_F a) + \frac{4}{35\pi^2}(11 - 2\ln 2)(k_F a)^2 + \frac{1}{10\pi}(k_F r_s)(k_F a)^2 + 0.019(k_F a)^3\right],$$

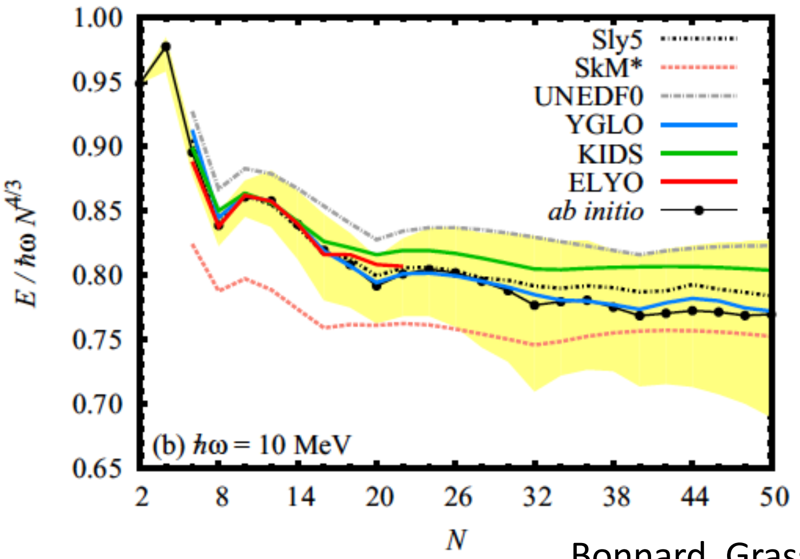
Assume

$$|a_s k_F| < \alpha_{\rm th}$$



*ELYO : Extended Lee-Yang Orsay

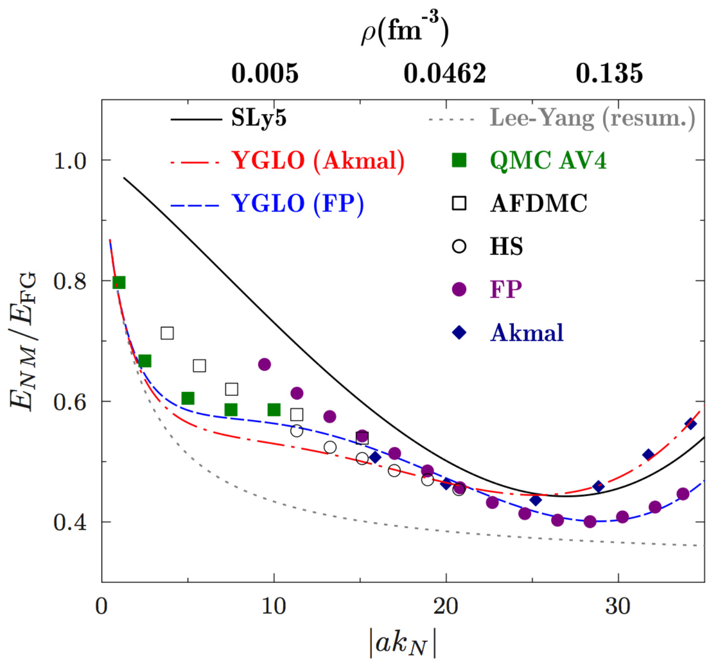
Recent application to neutron drop



Bonnard, Grasso, Lacroix, PRC 98(2018)

Brainstorming after YGLO

From the YGLO work



Lee-Yang guided functional

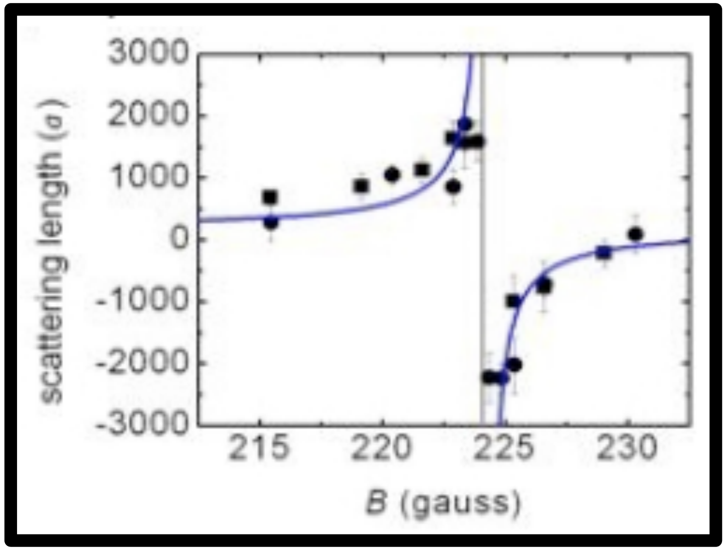
Grasso, Lacroix, Yang, PRC95 (2017)

$$\frac{E}{N} = \frac{\hbar^2 k_F^2}{2m}\left[\frac{3}{5} + \frac{2}{3\pi}(k_F a) + \frac{4}{35\pi^2}(11 - 2\ln 2)(k_F a)^2 + \frac{1}{10\pi}(k_F r_s)(k_F a)^2 + 0.019(k_F a)^3\right],$$

In neutron matter a_s is very large

Physics might be close to the unitary gas regime:

- -low density system
- $a_s \to +\infty$



Most important for us, it has the simplest DFT ever !

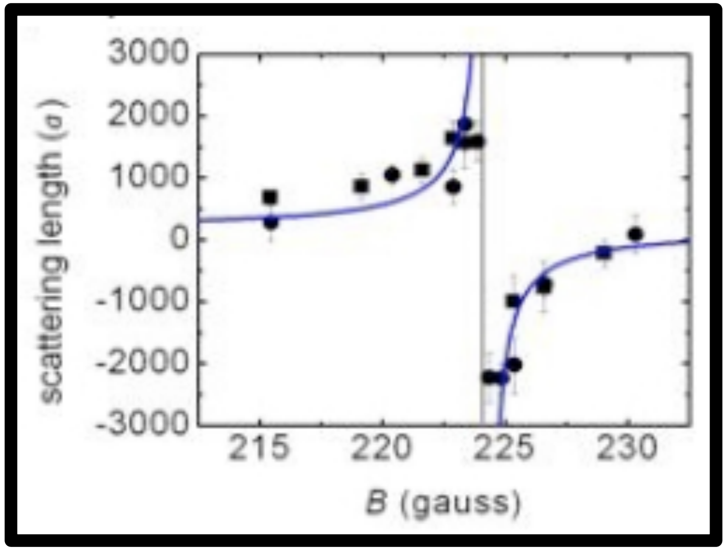
$$\mathcal{E}[\rho] = \xi \times \mathcal{E}_{\rm FG}[\rho]$$

$\xi = 0.37$ Berstch parameter is universal

Idea: develop the theory starting from the unitary gas

DFT: Lacroix, PRA 94 (2016)
EFT: Konig, Griesshamer, Hammer, van Kolck, PRL 118 (2017)

Great interest of resummed expression:
It has a finite limit for Unitary gas



For unitary gas:

- low density system
- $a_s \to +\infty$

$$\frac{3}{5}\frac{\hbar^2 k_F^2}{2m}\frac{\frac{10}{9\pi}(a_s k_F)}{1-\underbrace{\frac{6}{35\pi}(11-2\ln 2)}_{=\langle f\rangle}(a_s k_F)} \longrightarrow 0.32\ \frac{3}{5}\frac{\hbar^2 k_F^2}{2m}$$

$$\frac{E}{A} = \left(\frac{3}{5} + \frac{2k_F a_s/3}{\pi - 2k_F a_s}\right)\frac{k_F^2}{2M} \longrightarrow 0.4\ \frac{3}{5}\frac{\hbar^2 k_F^2}{2m}$$

Not so far from the "admitted" value of the Bertsch parameter for unitary gas (0.37)

Important remark for us, unitary gas has the simplest DFT ever !

$$\mathcal{E}[\rho] = \xi \times \mathcal{E}_{\rm FG}[\rho]$$

$$\xi = 0.37$$

The interest for us is that in neutron matter a_s is very large

Density Functional Theory for system at or close to unitarity

A very pragmatic approach

Lacroix, PRA 94 (2016)

Minimal DFT for unitary gas

$$\frac{E}{E_{\rm FG}} = \left\{1 + \frac{(ak_F)A_0}{1 - A_1(ak_F)}\right\}$$

$|a_s k_F| \ll 1$ $\longrightarrow$ $|a_s k_F| \gg 1$

$$\frac{E}{E_{\rm FG}} = 1 + \frac{10}{9\pi}(\nu - 1)(k_F a_s) + \cancel{(\nu - 1)\frac{4}{21\pi^2}(11 - 2\ln 2)(k_F a_s)^2 + \cdots}$$

$$\frac{E}{E_{\rm FG}} = \xi_0$$

Adjusting only on low density

$$A_0 = \frac{10}{9\pi}(\nu - 1)$$

$$A_0 A_1 = (\nu - 1)\frac{4}{21\pi^2}(11 - 2\ln 2)$$

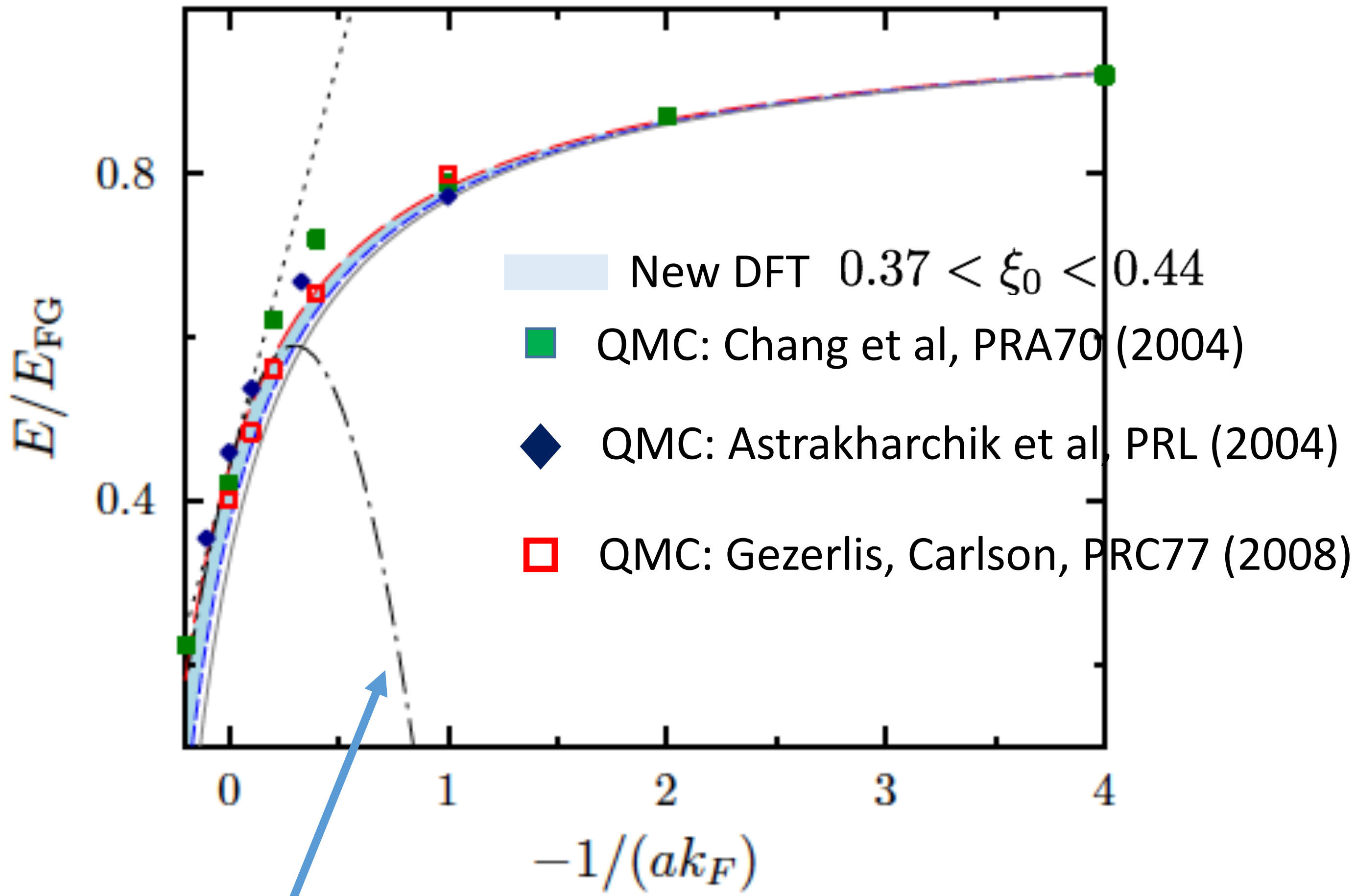
Adding the unitarity constraint

$$A_0 = \frac{10}{9\pi}(\nu - 1)$$

$$1 - \frac{A_0}{A_1} = \xi_0$$

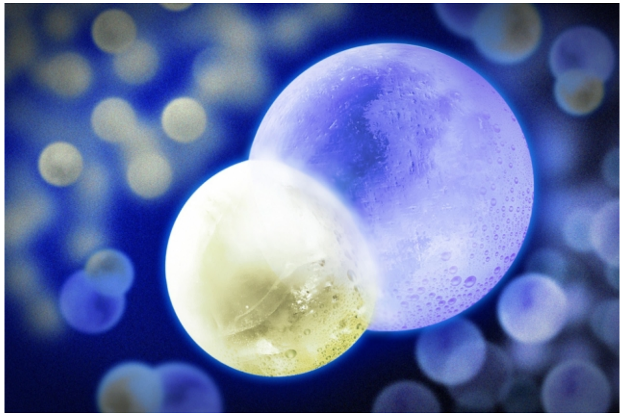
Result of the DFT for at or close to unitarity

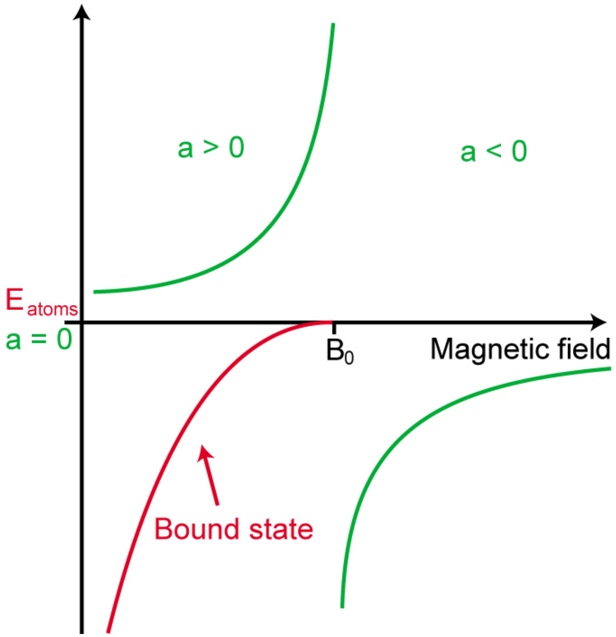
Lacroix, PRA 94 (2016)

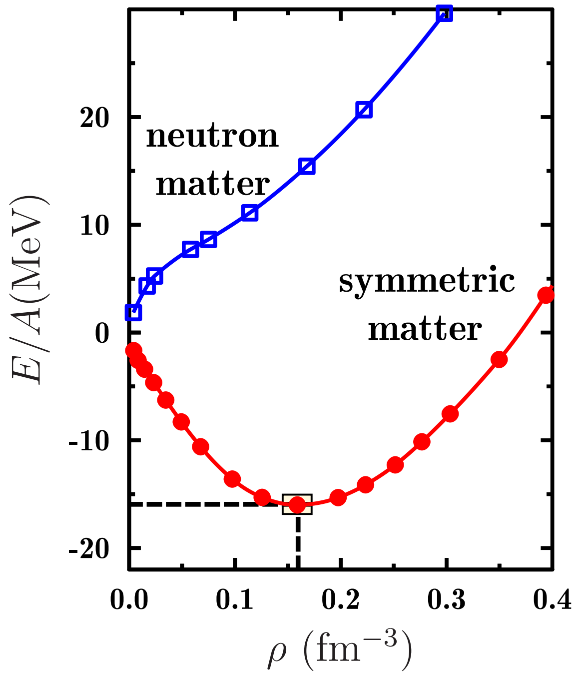


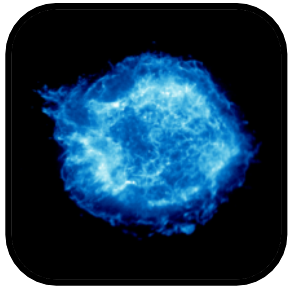
$$\frac{E}{E_{\mathrm{FG}}} \simeq \xi_0 - \frac{\zeta}{(ak_F)} - \frac{5}{3}\frac{\nu}{(ak_F)^2} + \cdots \qquad \zeta \simeq \nu \simeq 1$$

Taylor expansion in $(a_s k_F)^{-1}$: Bulgac and Bertsch, PRL 94 (2005)









Most often, only a_s matter

$$a_s = -18.9 \text{ fm}$$

$$r_e = 2.7 \text{ fm}$$

$$a_p^3 = 0.2 - 0.6 \text{ fm}^3$$

There is a hierarchy of scales $a_p \ll r_e \ll a_s$

but $r_e, \; a_p \cdots$ could not be neglected

and k_F is not small

From cold atom to neutron matter: inclusion of effective range

Lacroix, PRA 94 (2016)

$$\frac{E}{E_{\rm FG}} = 1 - \frac{U_0}{1-(a_s k_F)^{-1}U_1} + \frac{R_0(r_e k_F)}{[1-R_1(a_s k_F)^{-1}][1-R_1(a_s k_F)^{-1}+R_2(r_e k_F)]}$$

Effective range part
(form obtained by resumming
effective range effects
in HF theory)

New constraints

$|a_s k_F| \ll 1$

$|a_s k_F| \gg 1$

$$\frac{E}{E_{\rm FG}} 1 + \frac{10}{9\pi}(\nu-1)(k_F a_s) + (\nu-1)\frac{1}{6\pi}(k_F r_e)(k_F a_s)^2 + \cdots$$

$$\xi(+\infty, r_e k_F) \equiv \xi_0 + (r_e k_F)\eta_e + (r_e k_F)^2\delta_e$$

Forbes, Gandolfi, Gezerlis, PRA86 (2012)

$$\begin{cases} U_0 = (1-\xi_0) = 0.62400, \\ U_1 = \frac{9\pi}{10}(1-\xi_0) = 1.76432, \\ R_0 = \eta_e = 0.12700, \\ R_1 = \sqrt{\frac{6\pi\eta_e}{(\nu-1)}} = 1.54722, \\ R_2 = -\delta_e/\eta_e = 0.43307. \end{cases}$$

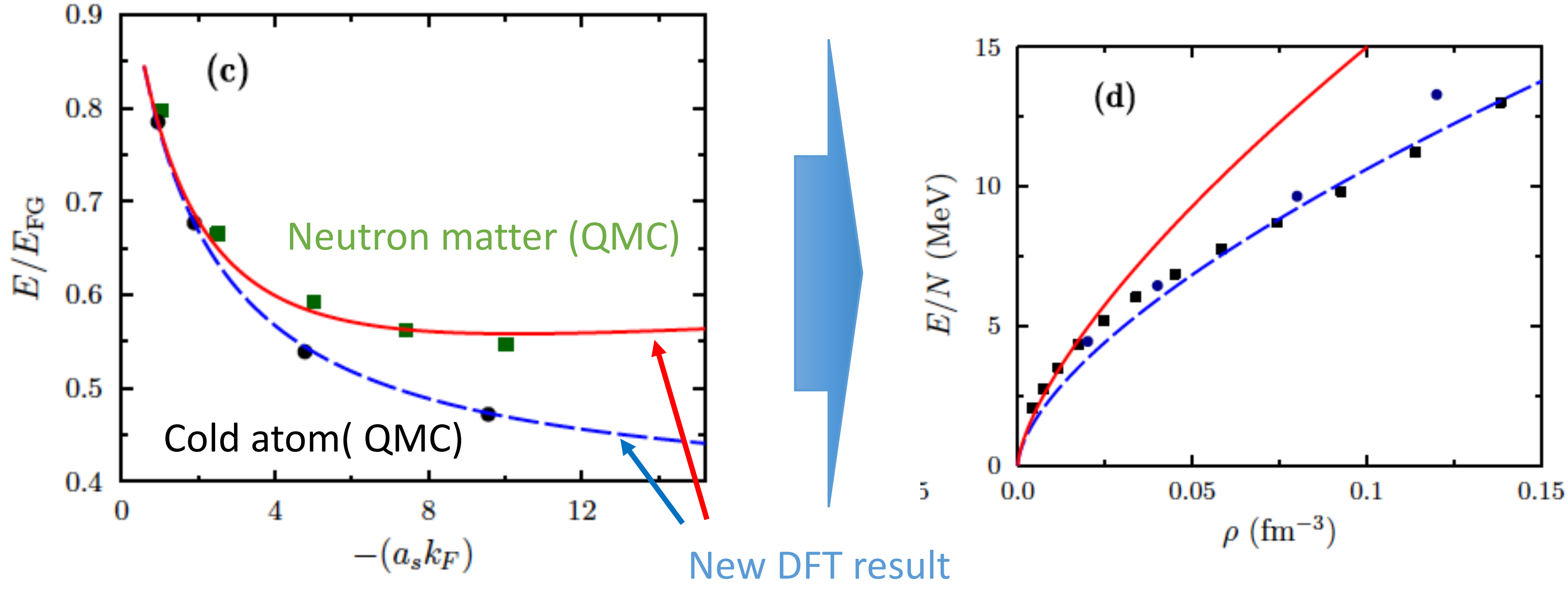
$\xi_0 = 0.376,$

$\eta_e = 0.127$

$\delta_e = -0.055$

EDF with no-free parameters: Predictive power for neutron matter

Lacroix, Boulet, Grasso, Yang, PRC 95 (2017)



[QMC: Gezerlis, Carlson, PRC81 (2010)]

Range of validity

Lee-Yang $\rho < 10^{-6}\ \mathrm{fm}^{-3}$

New DFT $\rho < 0.01\ \mathrm{fm}^{-3}$

Yang, Grasso, Lacroix PRC94 (2016)

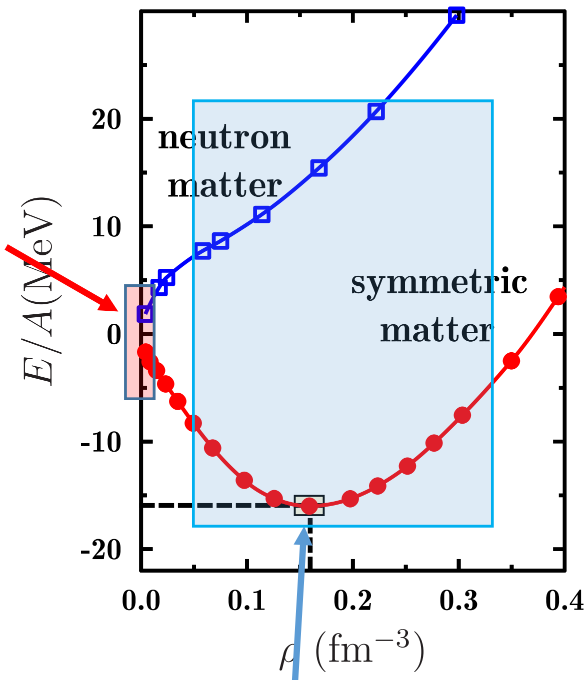
Skyrme functional

$$
\begin{aligned}
v(\mathbf{r}_1-\mathbf{r}_2) \; &= t_0\,(1+x_0\hat{P}_\sigma)\,\delta(\mathbf{r}) \\
&+\tfrac{1}{2}t_1\,(1+x_1\hat{P}_\sigma)\left[\mathbf{P}'^2\,\delta(\mathbf{r})+\delta(\mathbf{r})\,\mathbf{P}^2\right] \\
&+t_2\,(1+x_2\hat{P}_\sigma)\,\mathbf{P}'\cdot\delta(\mathbf{r})\,\mathbf{P}
\end{aligned}
$$

MBPT + expansion in LEC is valid here

is very close to the EFT starting point

$$\langle \mathbf{k}|V_{\text{eft}}|\mathbf{k}'\rangle = C_0 + \frac{1}{2}C_2(\mathbf{k}^2+\mathbf{k}'^2) + C_2'\,\mathbf{k}\cdot\mathbf{k}' + \cdots$$



But Skyrme works because it has been adjusted here !!!

Additional remarks on traditional Skyrme

Lacroix, Boulet, Yang, Grasso, PRC94 (2016)

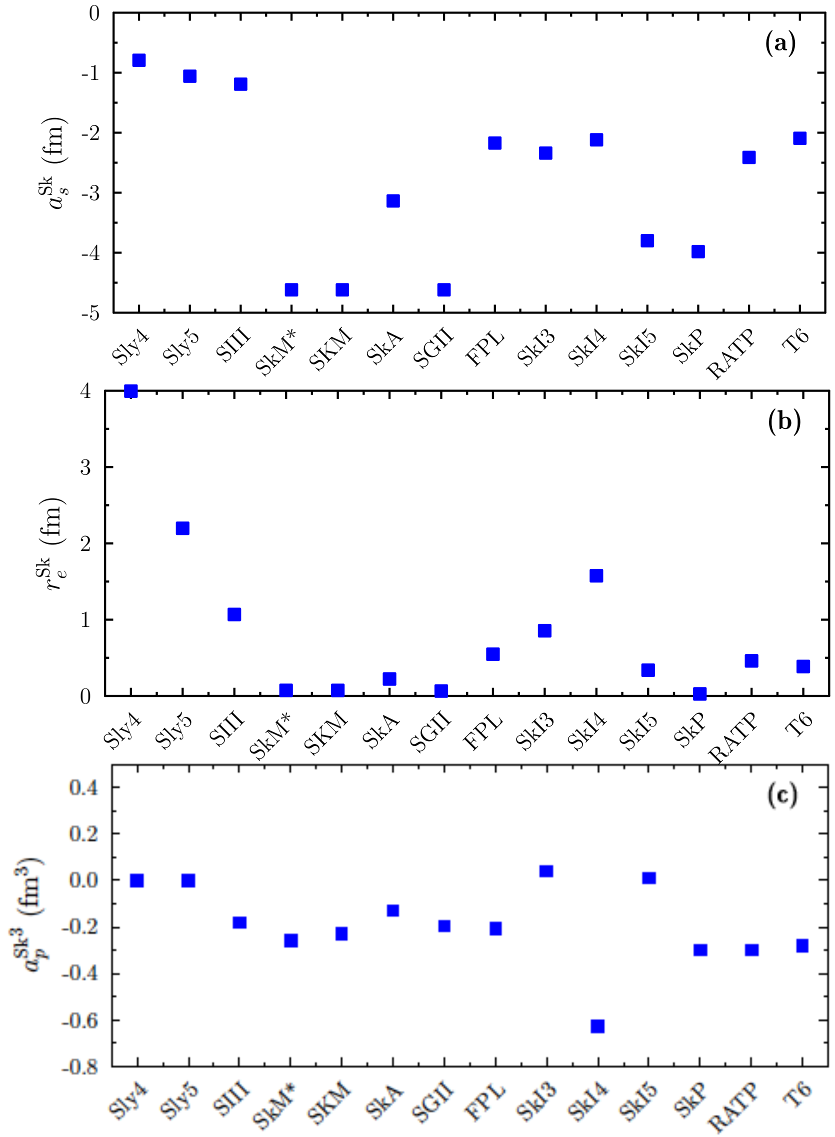
Due to the analogy, one can define equivalent low energy constant

$$C_0 = t_0(1 - x_0) = \frac{4\pi\hbar^2}{m} a_s,$$

$$C_2 = t_1(1 - x_1) = \frac{2\pi\hbar^2}{m} r_e a_s^2,$$

$$C_2' = t_2(1 + x_2) = \frac{4\pi\hbar^2}{m} a_p^3.$$

See discussion in Furnstahl, EFT for DFT (2007)



Very far from
$a_s = -18.9$ fm

Can we make contact with Skyrme like empirical functional ?

Lacroix, Boulet, Grasso, Yang, PRC 95 (2017)

Starting point

$$\frac{E}{E_{\rm FG}} = 1 - \frac{U_0}{1-(a_s k_F)^{-1}U_1} + \frac{R_0(r_e k_F)}{[1-R_1(a_s k_F)^{-1}][1-R_1(a_s k_F)^{-1}+R_2(r_e k_F)]}$$

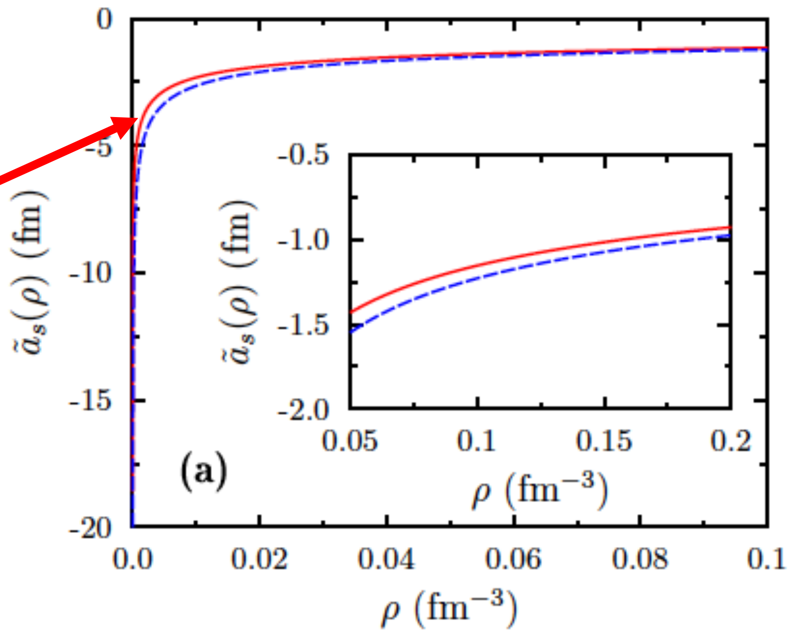
Rewrite it as

$$\frac{E}{E_{\rm FG}} = 1 + \frac{k_F^3}{4\pi^2 E_{\rm FG}}\left\{\frac{\widetilde{C}_0(k_F)}{3} + \frac{k_F^2}{10}[(\nu-1)\widetilde{C}_2(k_F)+(\nu+1)\widetilde{C}_2'(k_F)]\right\}$$

Define density dependent scattering length and range

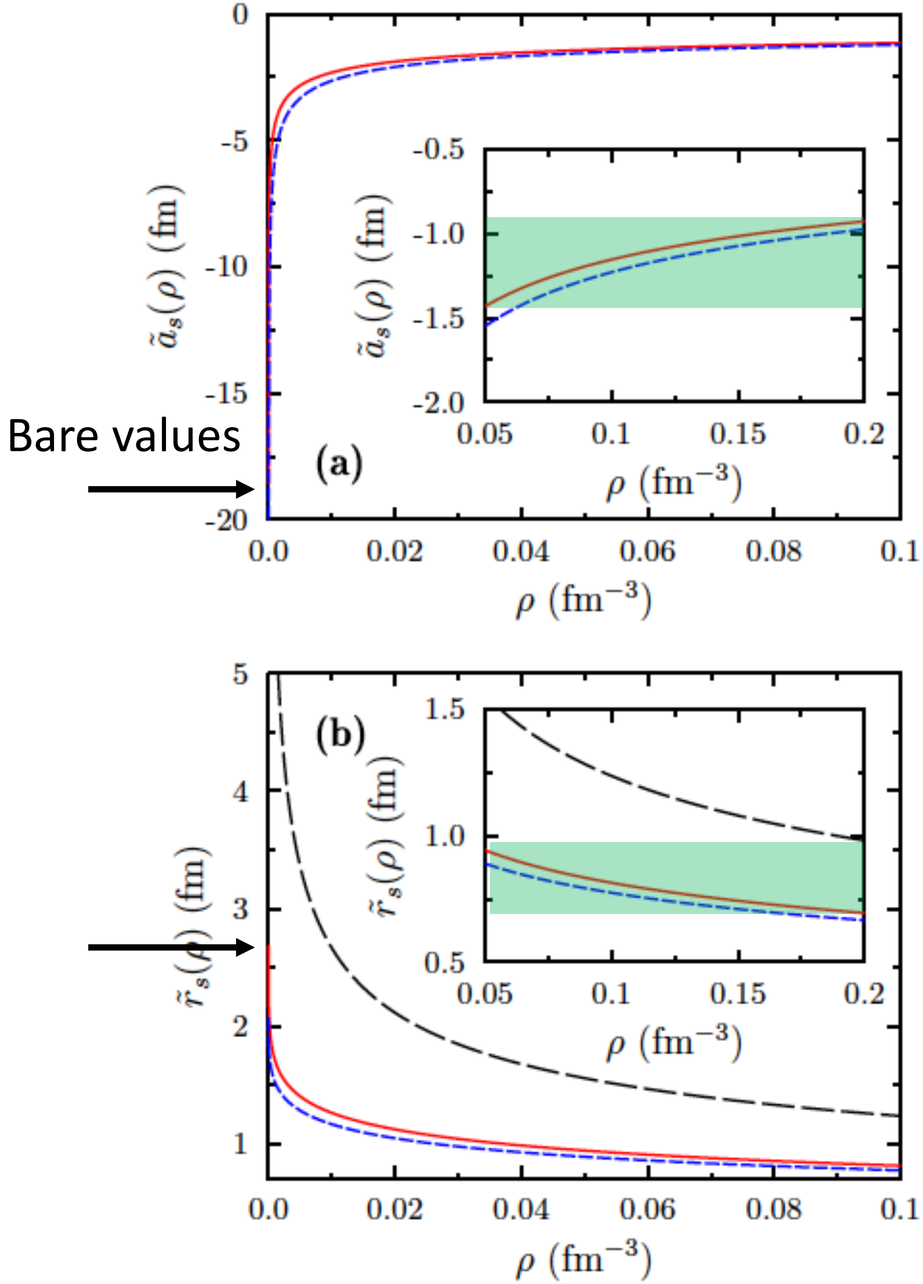
$$\tilde{C}_0(k_F) = \frac{4\pi\hbar^2}{m}\tilde{a}_s(k_F)$$

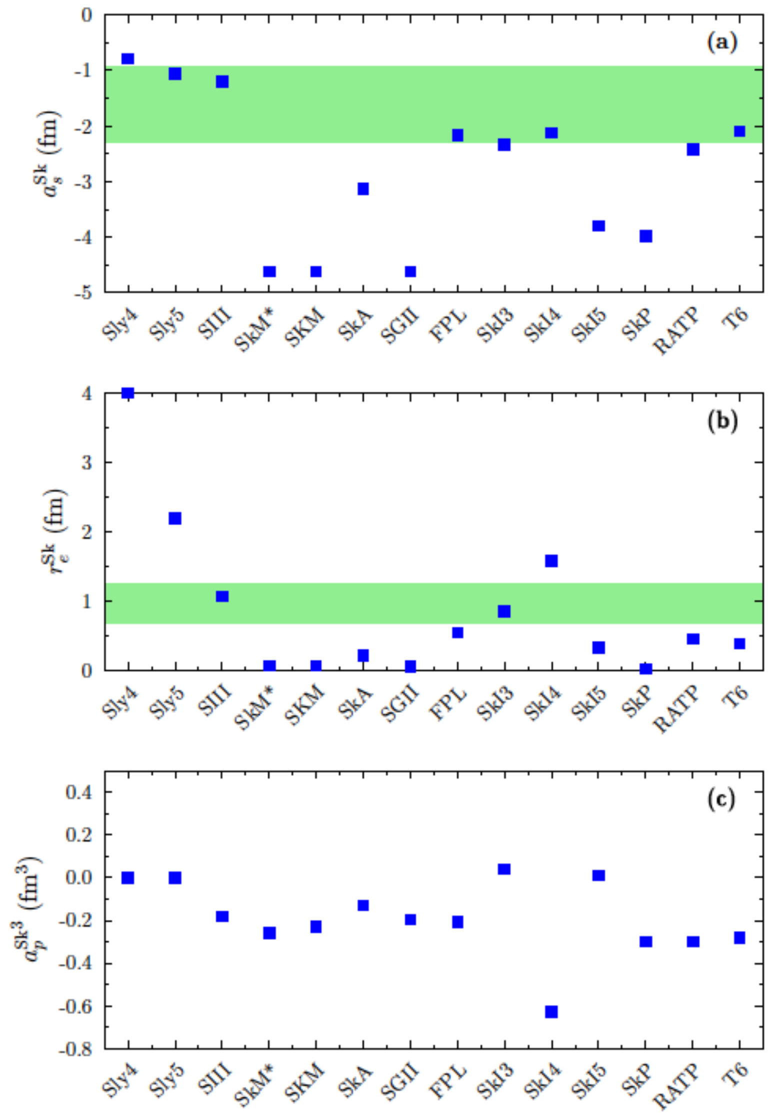
$$\tilde{C}_2(k_F) = \frac{2\pi\hbar^2}{m}\tilde{r}_e(k_F)\tilde{a}_s^2(k_F)$$



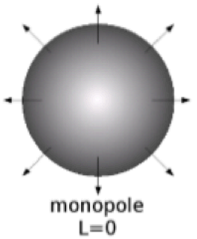
Can we make contact with empirical functional ?

Lacroix, Boulet, Grasso, Yang, PRC 95 (2017)





Gives an empirical explanation of the Skyrme success

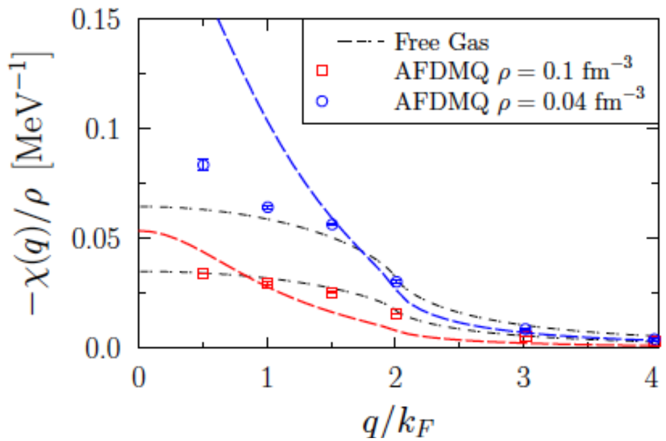


Ongoing work along this line

Static response of neutron matter DFT/EDF

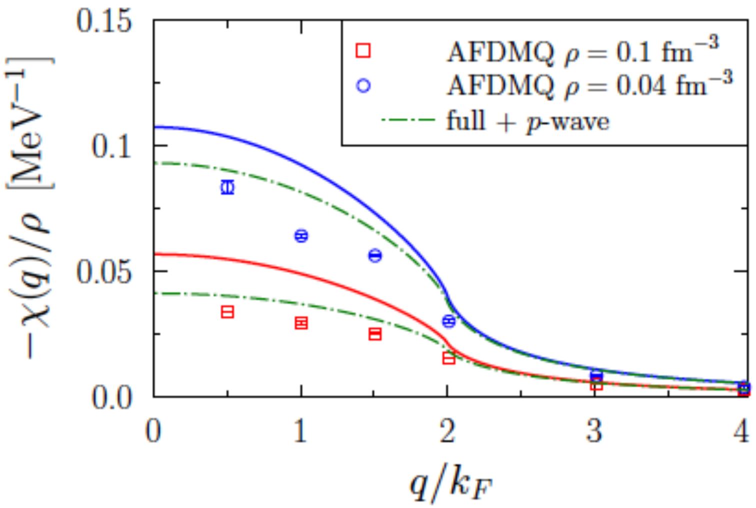
Boulet, Lacroix, PRC 97 (2018)

Empirical functional (Sly5)



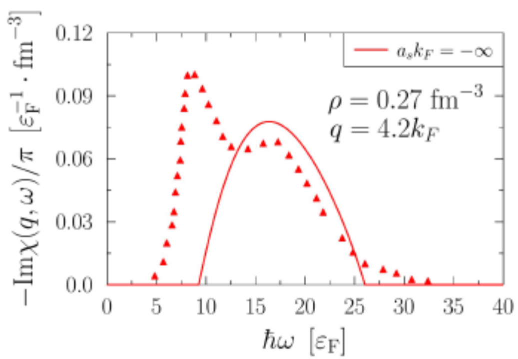
[Buraczynski and Gezerlis, PRL **116** (2016)]

Non-empirical functional + p-wave



$$\frac{E_p}{E_{FG}} = \frac{1}{\pi}(a_p k_F)^3$$

Dynamical response



[P. Zou *et al.*, New J. Phys. **18**, 113044 (2016)]

There is a need to have quasi-particle properties directly

Resummed self-energies (A. Boulet PhD thesis)

There is a need to include superfluidity

Summary and further discussion

Conclusions

- Ab-initio methods although not really precise can provide strong guidance to DFT
- EFT methods can be exported also to DFT
- This has led to a novel generation of DFT and maybe to the possibility to connect DFT with The bare interaction in a simple way.
- Still remains many problems: power counting (if any), symmetry breaking and true interactions …

Some other interesting/interdisciplinary issues

- Quasi-particles properties at anomalously large (but not infinite) scattering length
- Systems with multi-body interactions
- Quantum droplets (stabilized by quantum fluctuations)