Nuclear density functional theory from low energy constants: application to cold atoms and neutron matter

Denis Lacroix

INSTITUT DE PHYSIQUE NUCLÉAIRE ORSAY

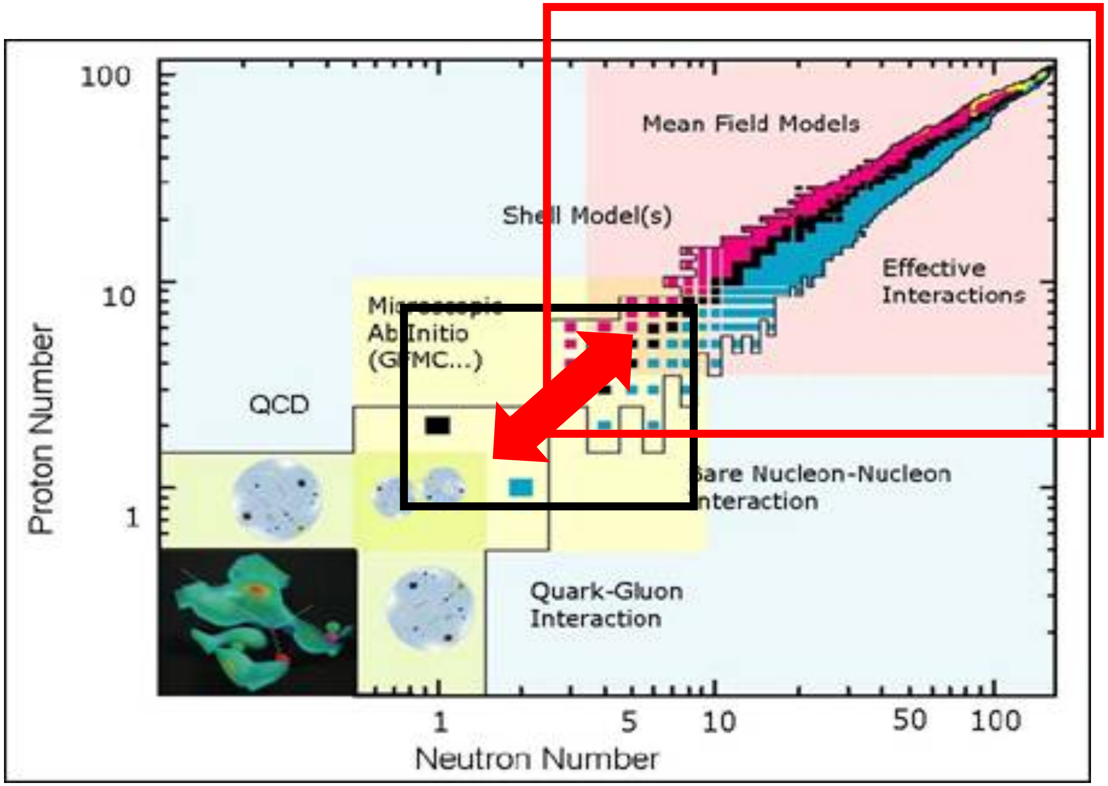
ENSAR2

Outline:

- Brief historical overview of DFT for nuclei
- EFT guiding the construction of DFT/EDF
- Illustration: the YGLO functional
- Unitary gas guidance: role of large but finite s-wave scattering length
- Applications: equation of states, collective modes.

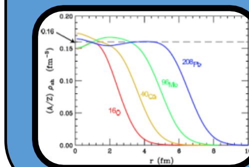
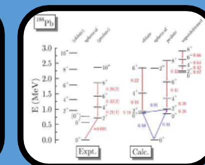
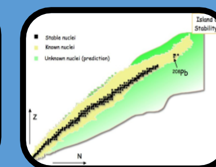
Coll: J. Bonnard, A. Boulet, M. Grasso and C.J. Yang

So why we need to do something else?

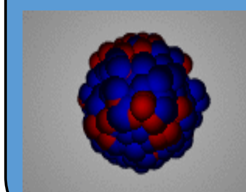
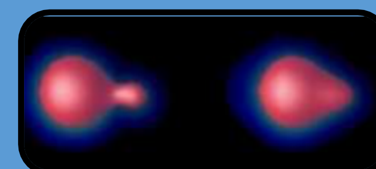


But we want to do a little bit more…

GROUND STATE-STRUCTURE OF THE ATOMIC NUCLEUS

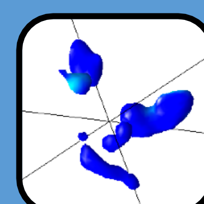
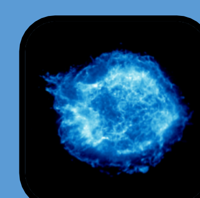




SMALL AND LARGE AMPLITUDE DYNAMICS

Nuclear Thermodynamic

(from finite or infinite systems)

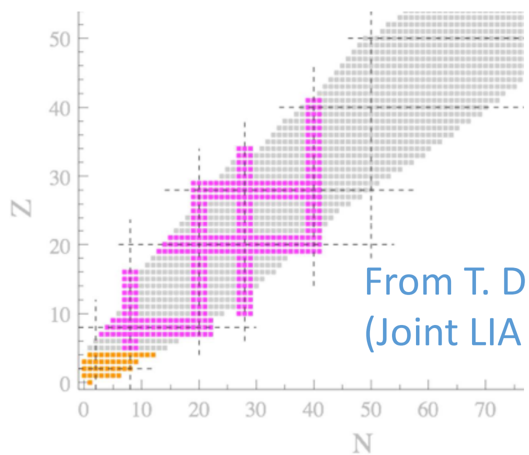



State of the art
ab-initio calculation
in 2016

New generation

Ex: pionless EFT

- -LO : 2 parameters
- -NLO + 7 parameters
- -N^3LO + 15 parameters
- -N^5LO +26 parameters
- ….



From T. Duguet
(Joint LIA talk)

Nuclear Energy Density Functional based on effective interaction

Constraining the functional

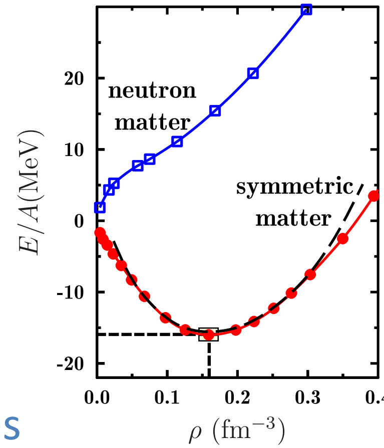
Static

Vautherin, Brink, PRC (1972)

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

See for instance, Meyer EJC1997

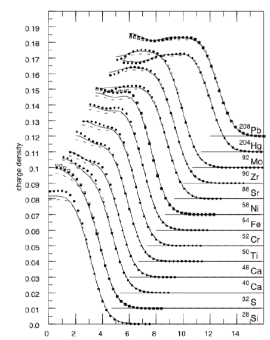
Infinite nuclear matter and Nuclear Masses



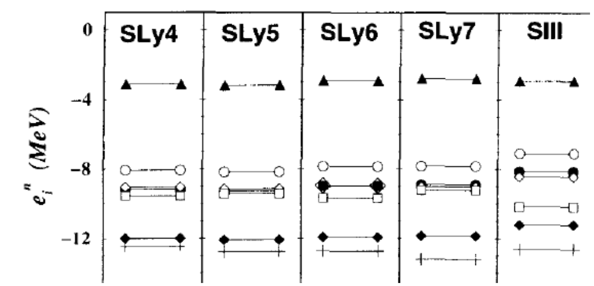
$$E_0,\ \left.\frac{\partial E}{\partial \rho}\right|_{\rho_0},\ \left.\frac{\partial^2 E}{\partial \rho^2}\right|_{\rho_0}$$

The ρ^α term
Is a trick to get
the curvature right!

Densities



Shell effect

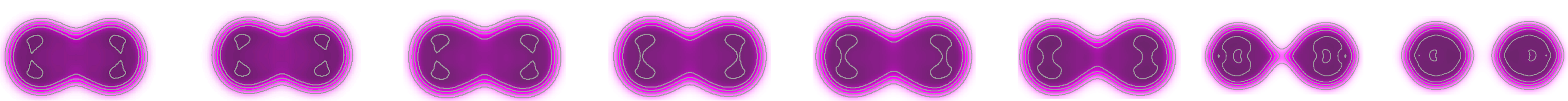


Chabanat et al, NPA (1998)

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

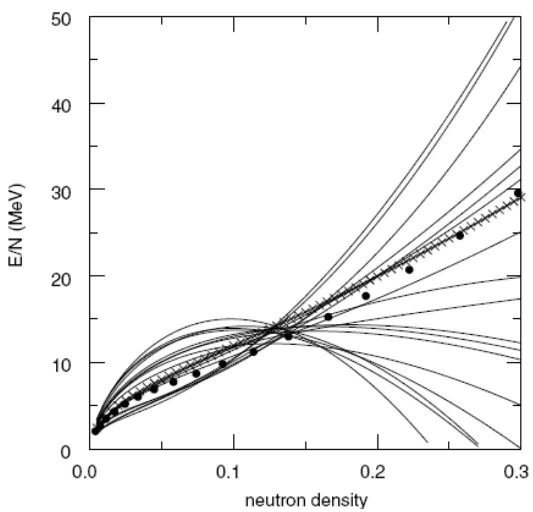
Limitation and drawback

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

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

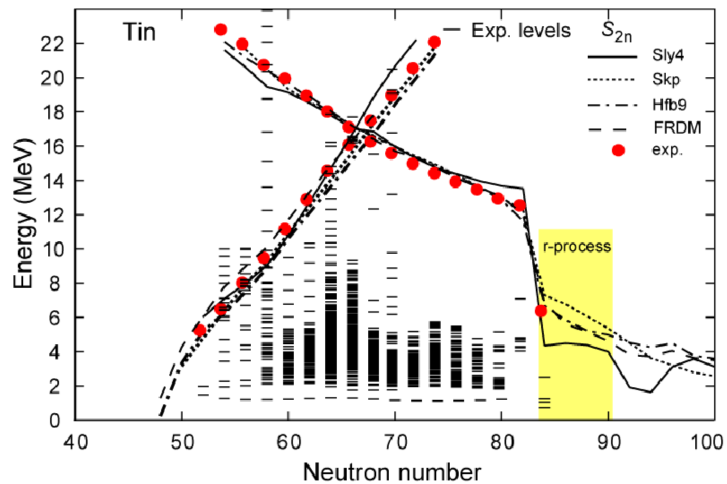
Since we directly fit on experiments there is no more link with the interaction and associated low energy constants…

EOS of pure neutron matter



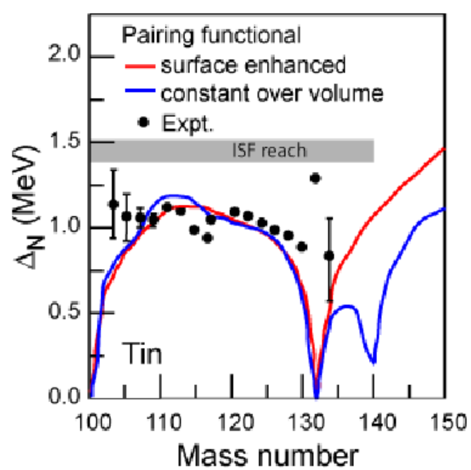
Brown, PRL85 (2000).

S_{2n} and S_{2p} in Tin isotopic chain

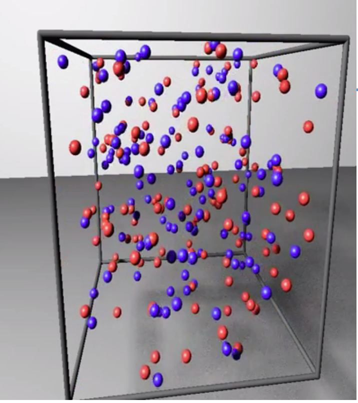


http://www.nscl.msu.edu/future/isf

Pairing gap



Can we link the energy density functional to the low energy constants of the bare interaction?
and render it less empirical?

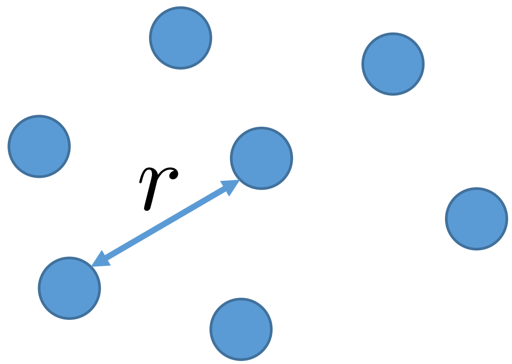


Towards a constructive approach for DFT

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

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

Example of the s-wave

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

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

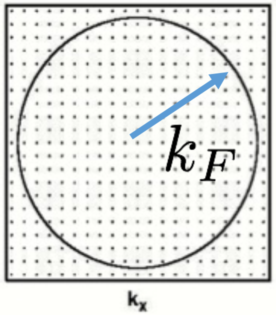
$$C_0 = \frac{4\pi\hbar^2}{m}a_s,\ C_2 = \frac{2\pi\hbar^2}{m}r_e a_s^2,\ C_2' = \frac{4\pi\hbar^2}{m}a_p^3.$$

Constructive many-body perturbative approach

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

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

Leads to the Lee-Yang functional (valid at low density) with possible higher order term



The Lee-Yang *density functional theory (infinite system)*

$$\frac{E}{E_{\rm FG}} = 1 + \frac{E^{(1)}}{E_{\rm FG}} + \frac{E^{(2)}}{E_{\rm FG}} + \cdots \quad \text{with} \qquad \frac{E_{\rm FG}}{N} = \frac{3\hbar^2 k_F^2}{10m}$$

Hartree-Fock contribution

$$\frac{E^{(1)}}{E_{\rm FG}} = \frac{10}{9\pi}(\nu-1)(k_F a_s) + (\nu-1)\frac{1}{6\pi}(k_F r_e)(k_F a_s)^2 + (\nu+1)\frac{1}{3\pi}(k_F a_p)^3 + \cdots$$

Second order

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

ν Degeneracy and from $\rho = \frac{\nu}{6\pi^2} k_F^2$

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

Could be extended to any order with some efforts

Difficulty in nuclear systems

Yang, Grasso, Lacroix PRC94 (2016)

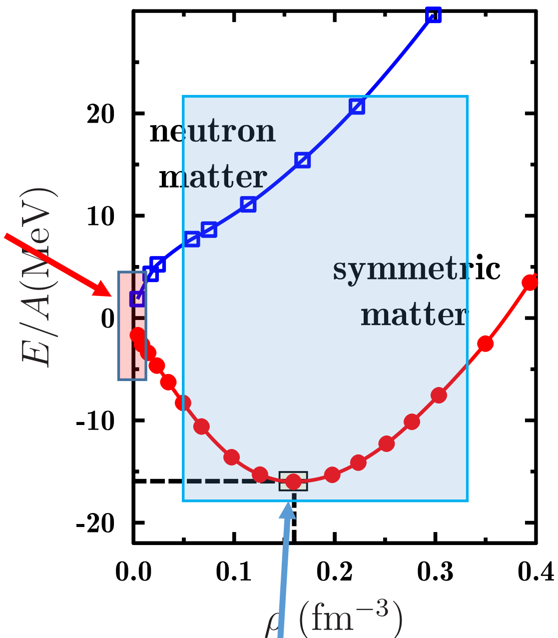
The Taylor expansion valid for $a_s k_F < 1$

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

$r_e = 2.7 \text{ fm}$

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

Lee Yang is valid here



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

Side remark 1: on Skyrme interaction

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

is equivalent to

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

The analogy between Skyrme interaction and EFT has been recently used to provide a systematic constructive framework for EDF

C. J. Yang, M. Grasso,et al, PRC 94 (2016); C. J. Yang, M. Grasso,et al PRC in press

Additional remarks on traditional Skyrme

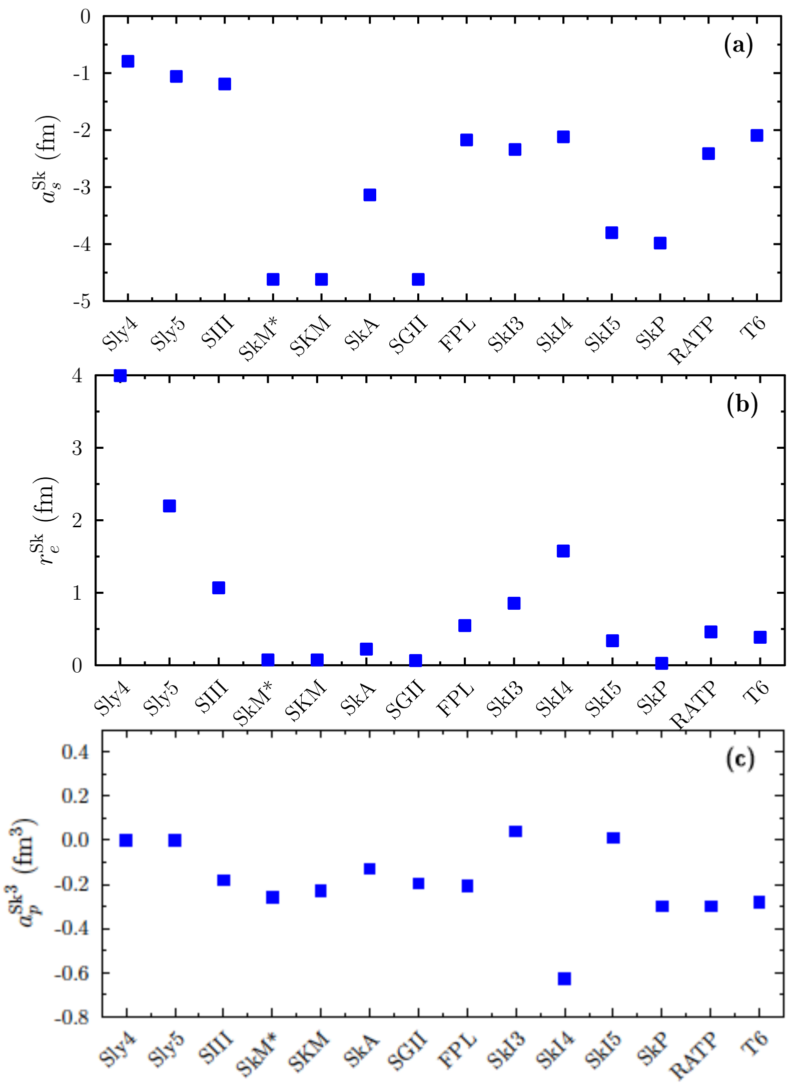
Lacroix, Boulet, Yang, Grasso, PRC94 (2016)

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

$$C_0 = t_0(1-x_0) = v_0 - v_\sigma = \frac{4\pi\hbar^2}{m}a_s,$$

$$C_2 = t_1(1-x_1) = -\frac{\mu^2}{2}(v_0 - v_\sigma) = \frac{2\pi\hbar^2}{m}r_e a_s^2,$$

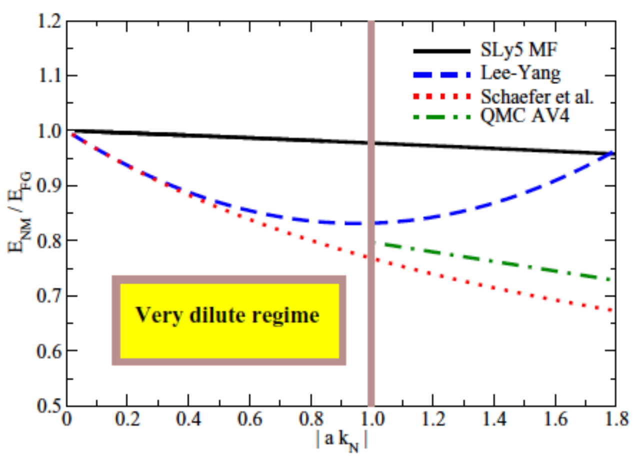
$$C_2' = t_2(1+x_2) = \frac{\mu^2}{2}(v_0 + v_\sigma) = \frac{4\pi\hbar^2}{m}a_p^3.$$



Very far from
$a_s = -18.9$ fm

Consequence: failure of EDF at low density

Yang, Grasso, Lacroix PRC94 (2016)



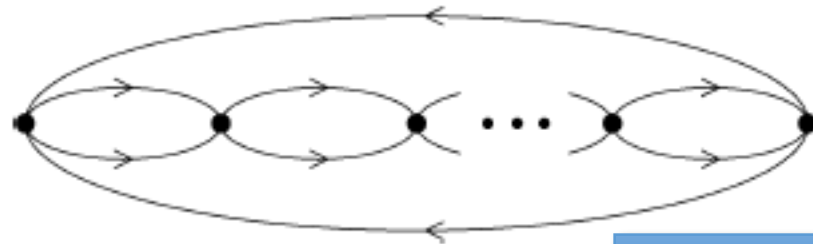
Does if have any consequence?

Can we have EDF linked to low energy constant

The magic technique: resummation

Highlighting work Schaefer, Kao, Cotanch, NPA 762 (2005)

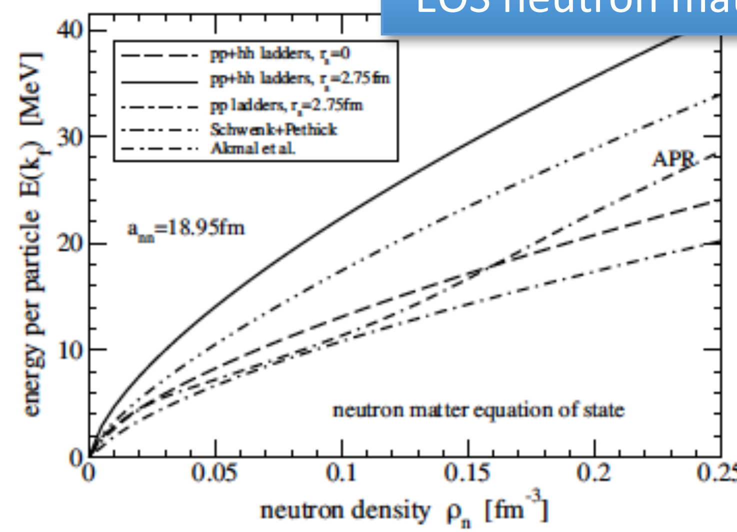
Resummation of particle-particle latter



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

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

EOS neutron matter



Kaiser, EPJA 48 (2012)

Our pragmatic approach

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

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

Interpretations:
- Minimal Padé approximation
- Phase-space average

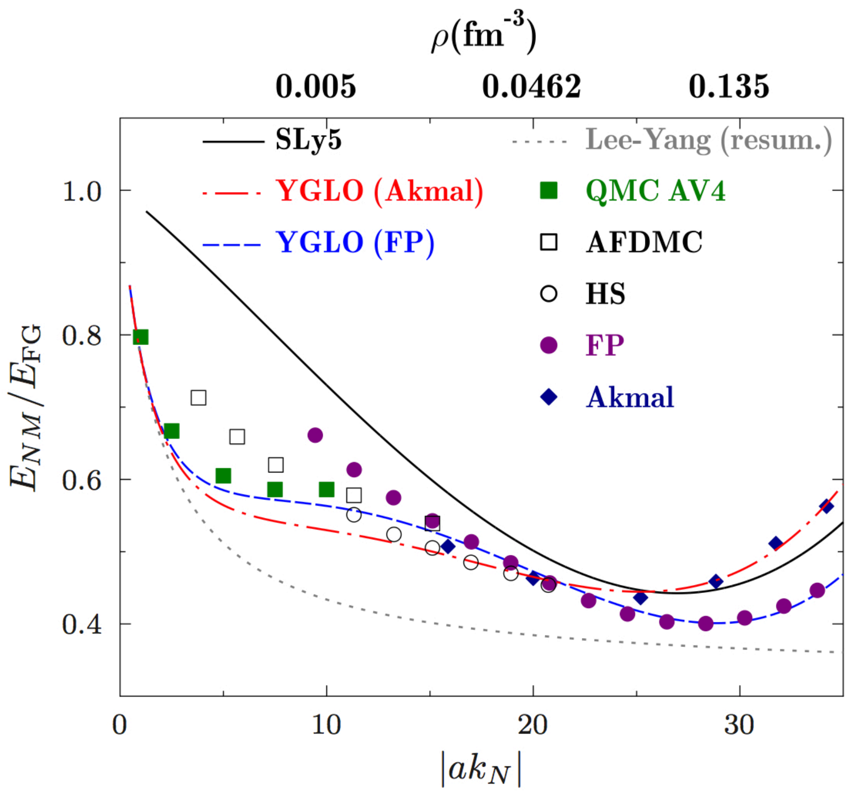
First illustration of an EFT guided EDF: the YGLO* functional

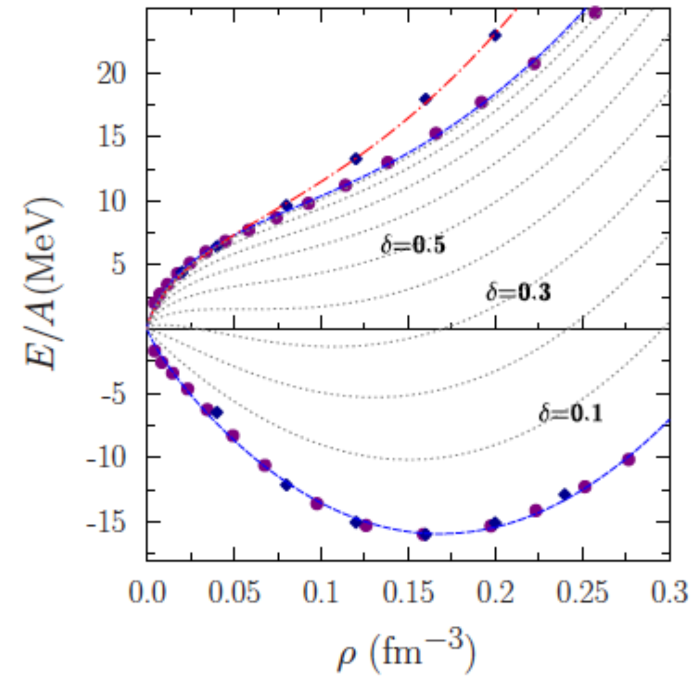
Yang, Grasso, Lacroix PRC94 (2016)

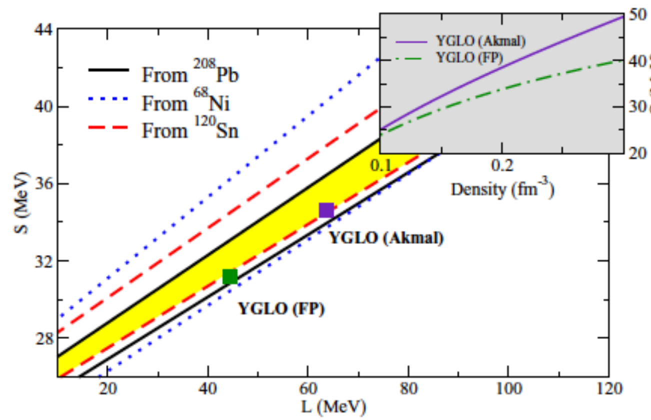
Functional form

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

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



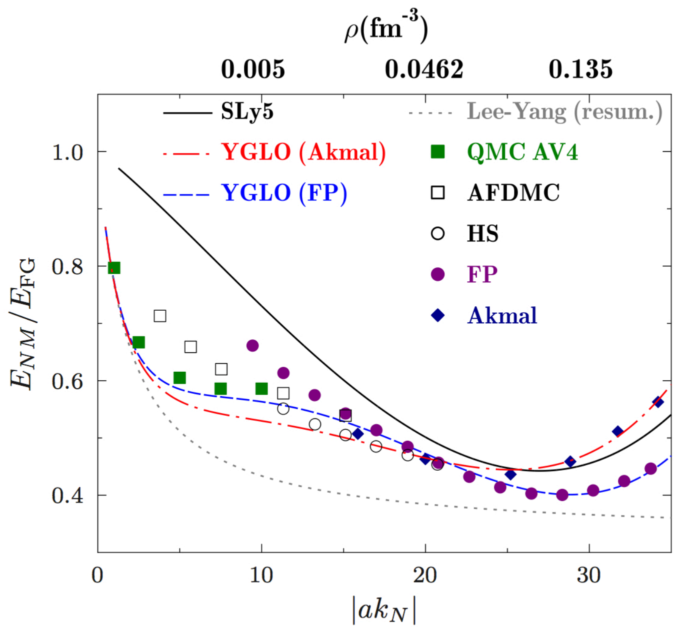




*YGLO: Yang-Grasso-Lacroix Orsay

Brainstorming after YGLO

From the YGLO work



Lee-Yang guided functional

Grasso, Lacroix, Yang, PRC95 (2017)

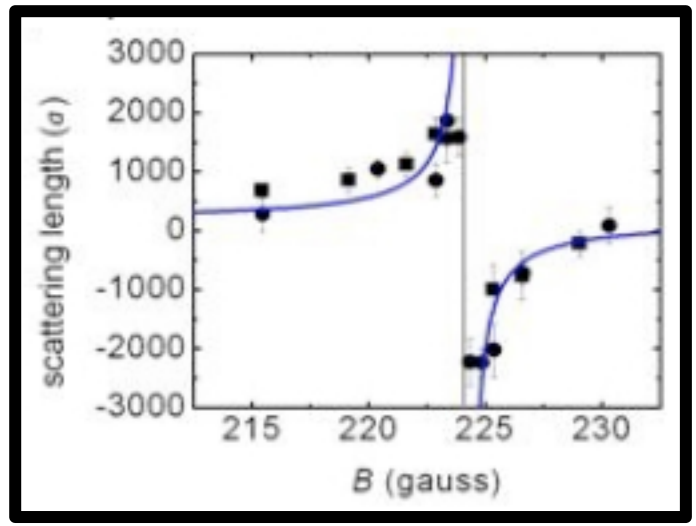
$$\frac{E}{N} = \frac{\hbar^2 k_F^2}{2m}\left[\frac{3}{5} + \frac{2}{3\pi}(k_F a) + \frac{4}{35\pi^2}(11 - 2\ln 2)(k_F a)^2 + \frac{1}{10\pi}(k_F r_s)(k_F a)^2 + 0.019(k_F a)^3\right],$$

In neutron matter a_s is very large

Physics might be close to the unitary gas regime:

-low density system

- $a_s \rightarrow +\infty$



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

Density Functional Theory for system at or close to unitarity

A very pragmatic approach

Minimal DFT for unitary gas

Lacroix, PRA 94 (2016)

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

$|a_s k_F| \ll 1$ → $|a_s k_F| \gg 1$

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

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

Adjusting only on low density

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

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

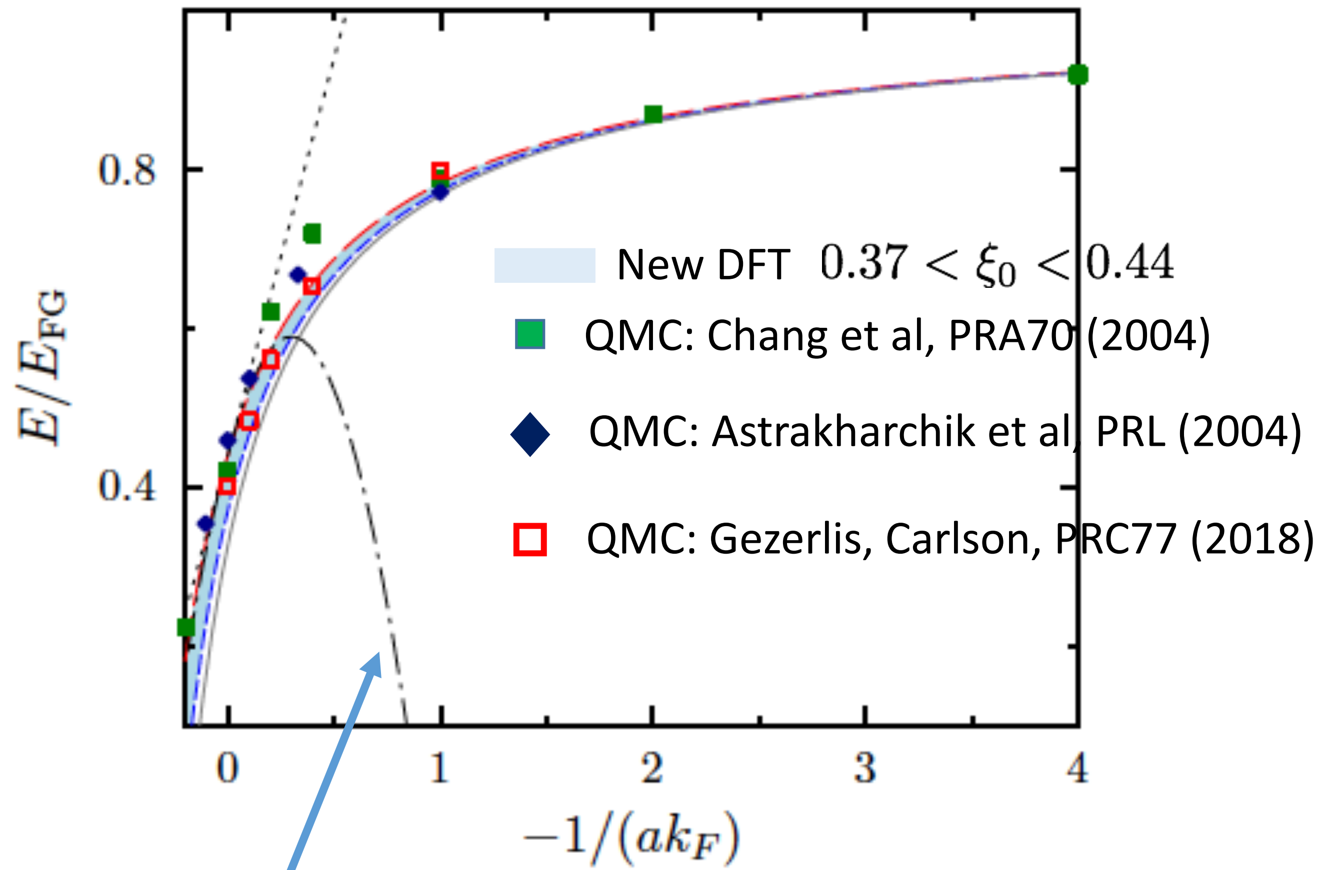
Adding the unitarity constraint

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

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

Result of the DFT for unitary systems

Lacroix, PRA 94 (2016)



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

Bulgac and Bertsch, PRL 94 (2005)

Example of applications

Lacroix, PRA 94 (2016)

$$\frac{E}{E_{\rm FG}} = \mathcal{F}(a_s, k_F) \equiv \mathcal{F}(a_s, \rho)$$

Any quantity that could be obtained through partial derivatives of the energy with respect to a_s or k_F or ρ is straightforward to obtain

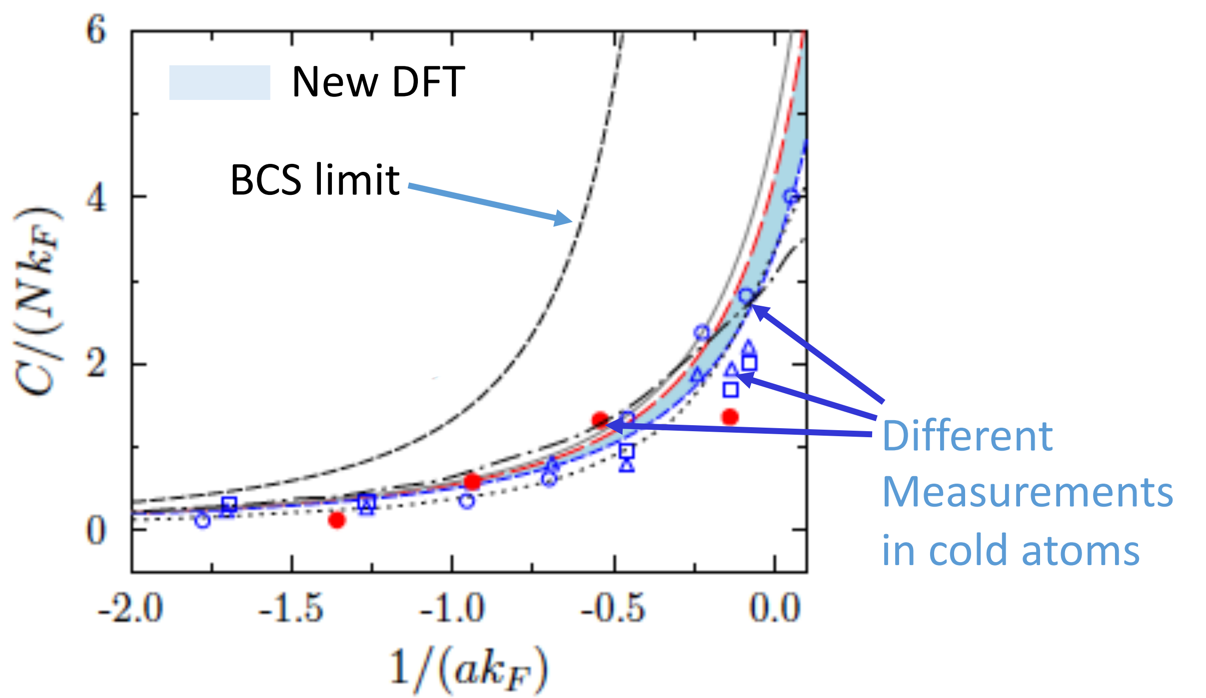
Estimate of the density dependence of the Tan contact parameter

E. Braaten, Lect. Not. Phys. 836 (2011).

$$\frac{C}{Nk_F} = \frac{(3\pi^2)}{k_F^4}\mathcal{C}$$

$$\mathcal{C} = \frac{4\pi m a_s^2}{\hbar^2}\left(\frac{d\mathcal{E}}{da_s}\right)$$

$$\mathcal{E} = \frac{k_F^3 E}{3\pi^2 N}$$



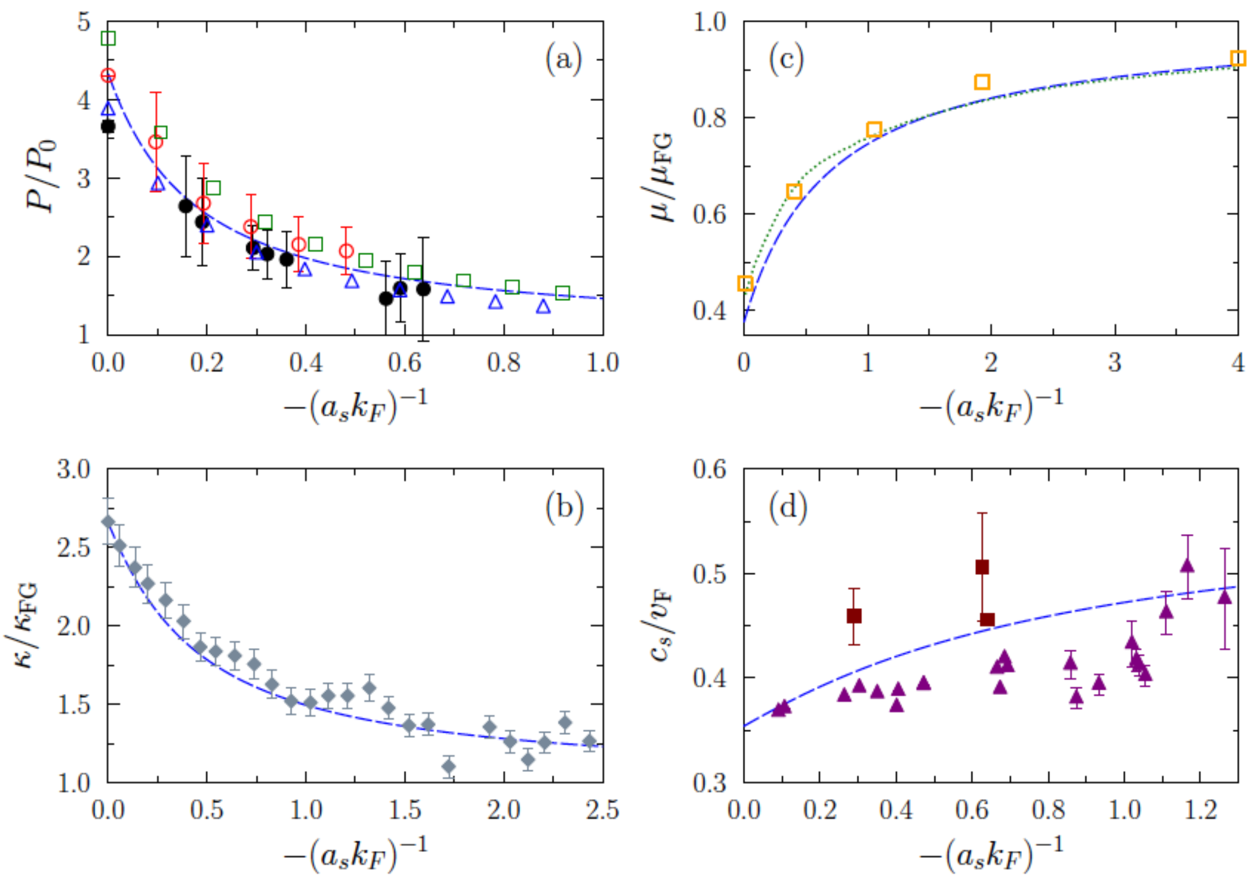
Example of applications: thermodynamical quantities around unitarity

Boulet, Lacroix, submitted to PRC

Pressure

Chemical potential

$$P = \rho_n^2 \frac{\partial E/N}{\partial \rho_n}\Big|_N$$



$$\mu = \frac{\partial E}{\partial N}\Big|_V = \frac{\partial \rho_n E/N}{\partial \rho_n}\Big|_V$$

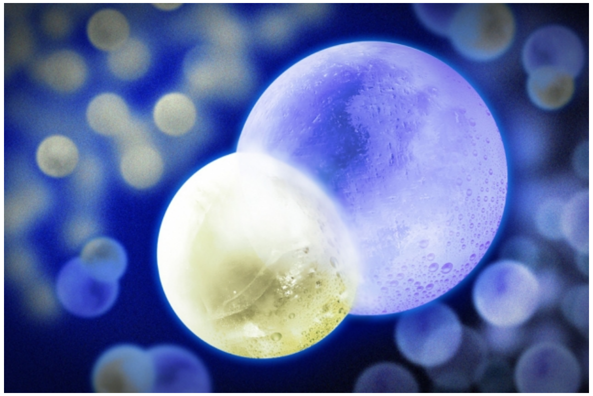
$$\kappa = \frac{1}{\rho_n}\left(\frac{\partial P}{\partial \rho_n}\Big|_N\right)^{-1}$$

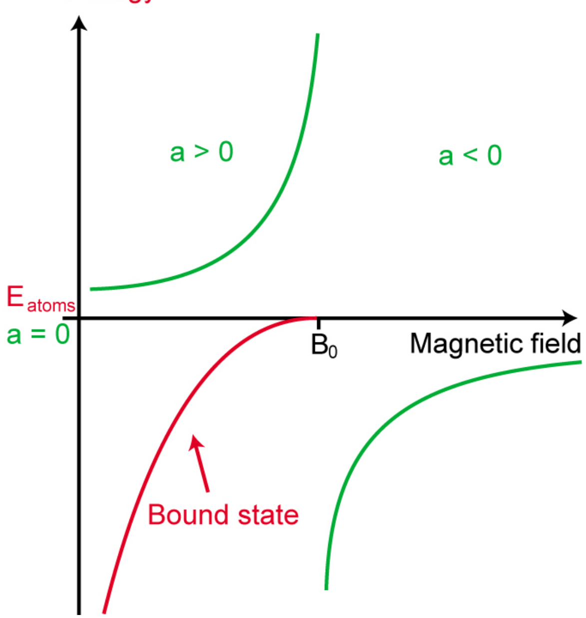
$$c_s^2 = \frac{1}{m \rho_n \kappa}$$

Compressibility

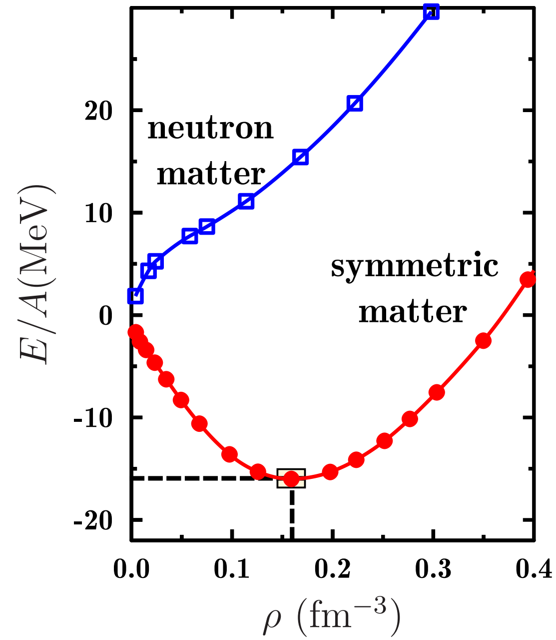
Sound velocity

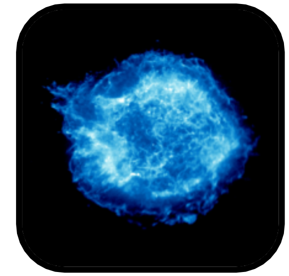
From cold atom to neutron matter





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

$|a_s k_F| \ll 1$ → $|a_s k_F| \gg 1$

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

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

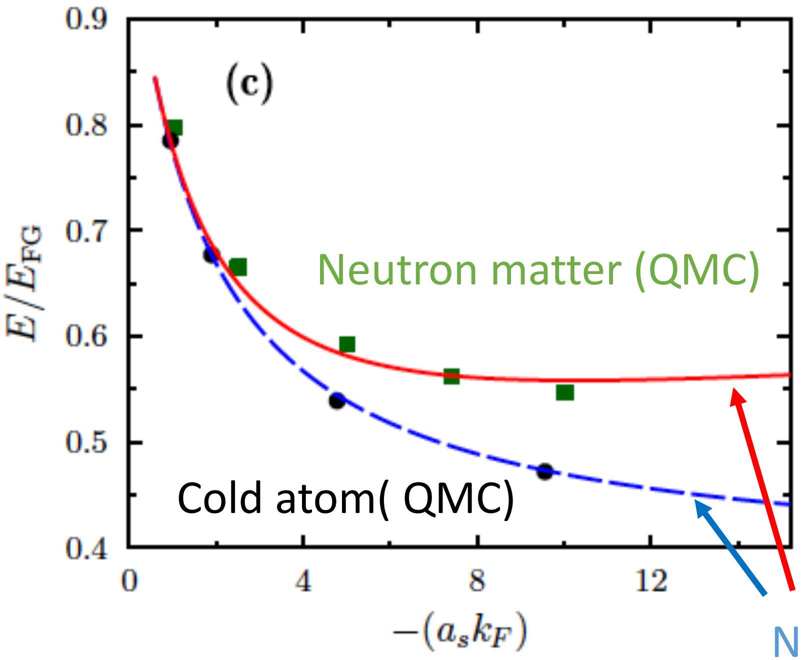
Forbes, Gandolfi, Gezerlis, PRA86 (2012)

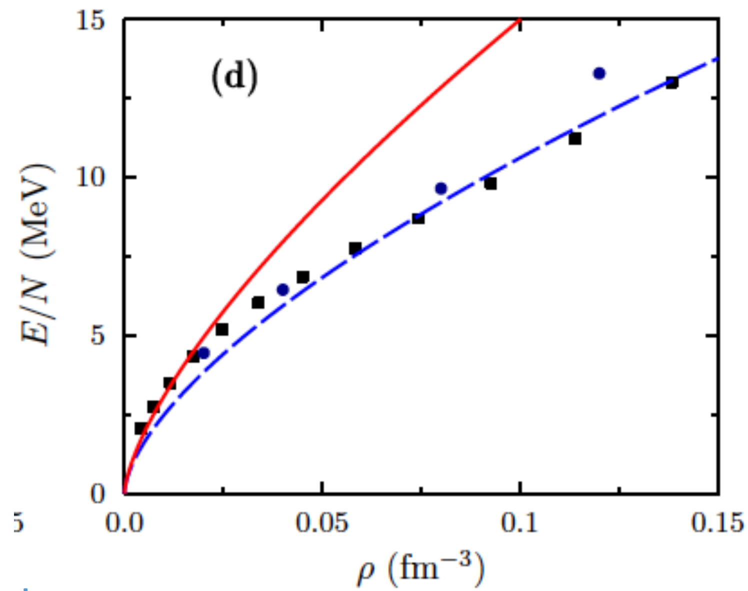
$$\begin{cases} U_0 = (1-\xi_0) = 0.62400, \\ U_1 = \frac{9\pi}{10}(1-\xi_0) = 1.76432, \\ R_0 = \eta_e = 0.12700, \\ R_1 = \sqrt{\frac{6\pi\eta_e}{(\nu-1)}} = 1.54722, \\ R_2 = -\delta_e/\eta_e = 0.43307. \end{cases}$$

$\xi_0 = 0.376,$
$\eta_e = 0.127$
$\delta_e = -0.055$

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

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





New DFT result

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

Range of validity

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

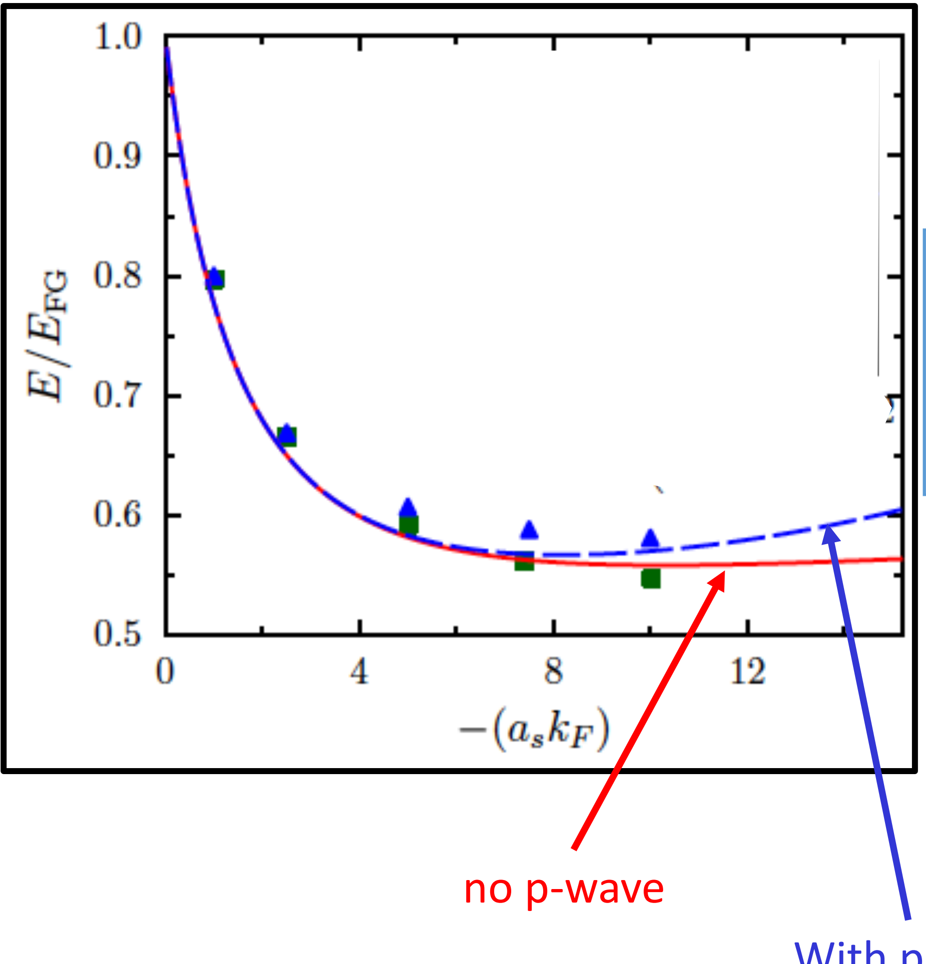
New DFT $\rho < 0.01$ fm^{-3}

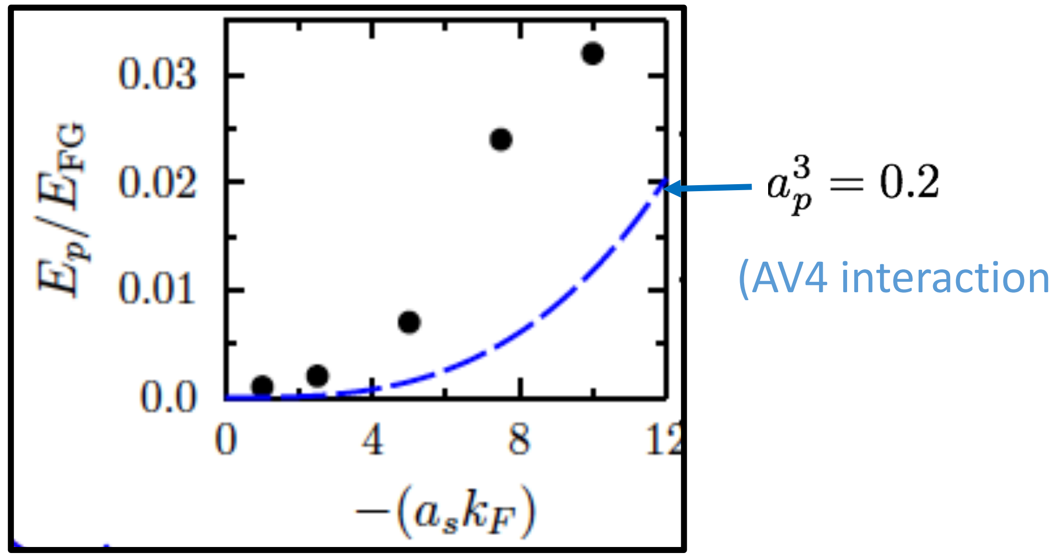
Including the p-wave ?

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

Remember $a_p \ll r_e \ll a_s$

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





$$(\nu + 1)\frac{1}{3\pi}(k_F a_p)^3$$

Can we make contact with Skyrme like empirical functional ?

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

Starting point

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

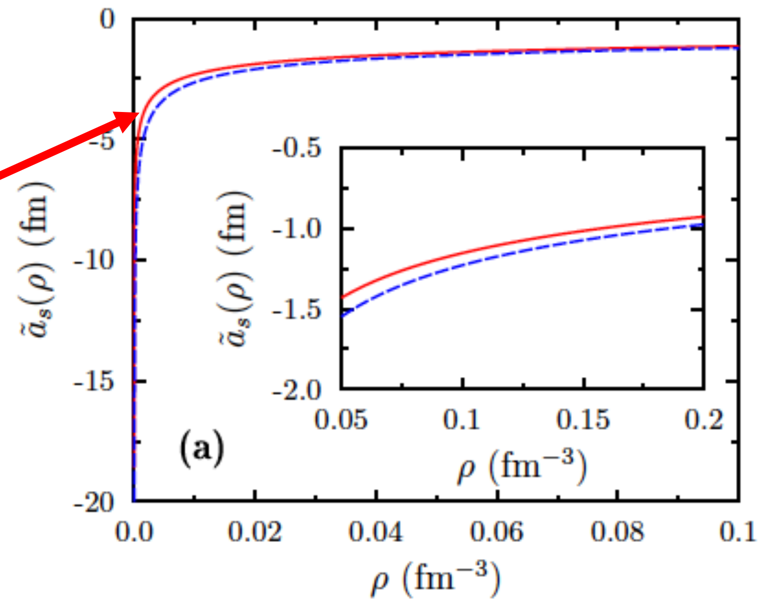
Rewrite it as

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

Define density dependent scattering length and range

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

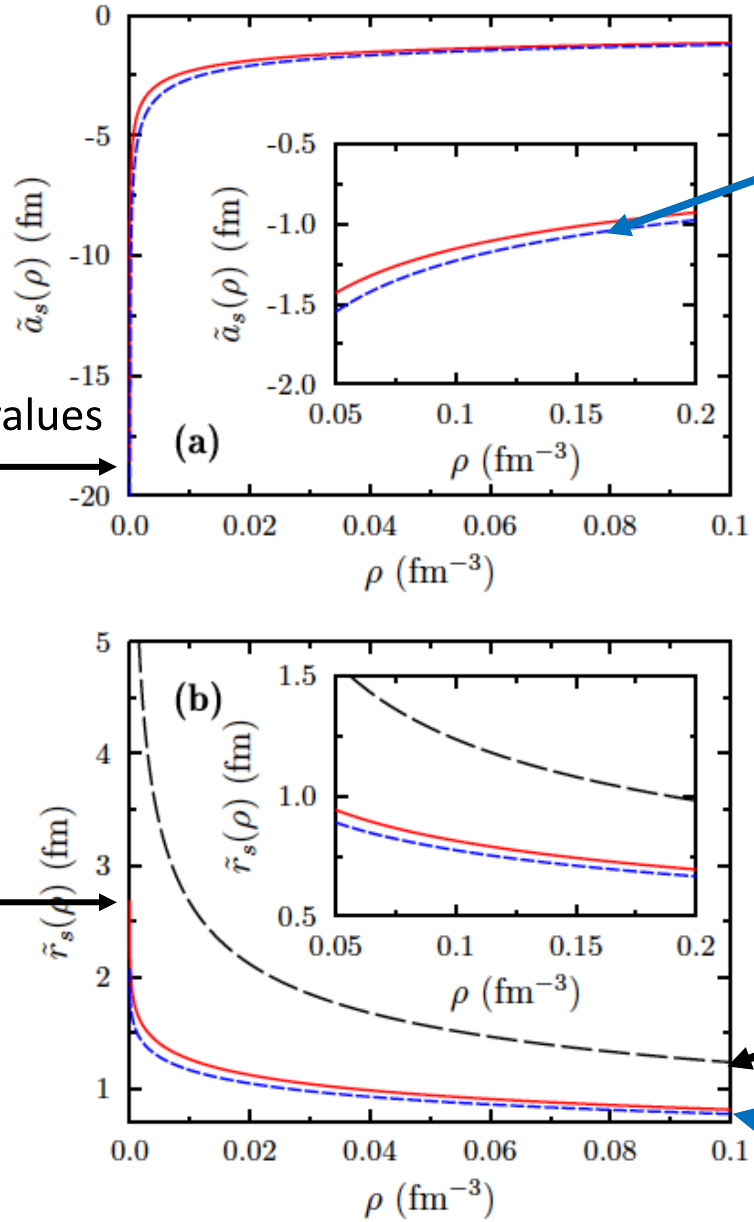
$$\tilde{C}_2(k_F) = \frac{2\pi\hbar^2}{m}\tilde{r}_e(k_F)\tilde{a}_s^2(k_F)$$



Can we make contact with empirical functional ?

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

Bare values



$$\widetilde{a}_s(k_F) \simeq -\frac{9\pi}{10k_F}(1-\xi_0)$$

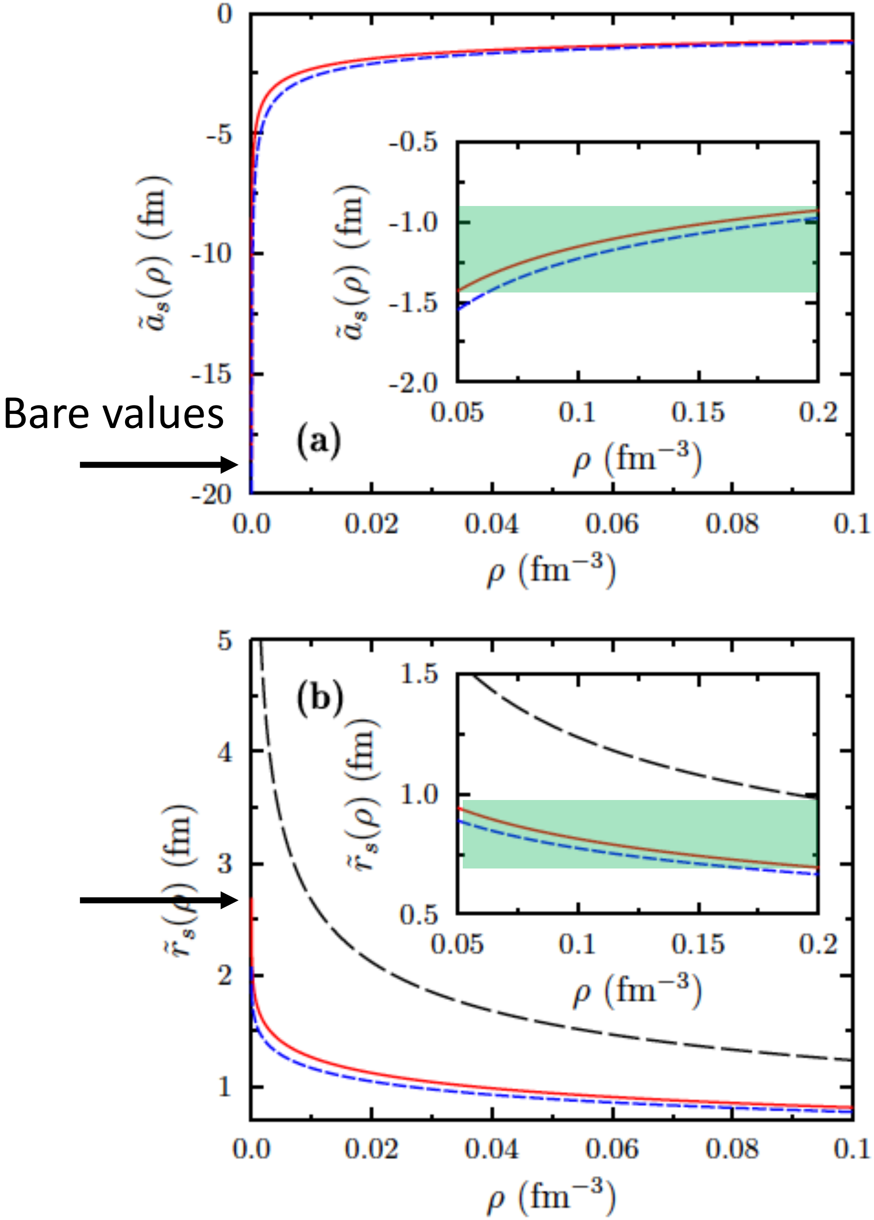
- Fast evolution at low density followed by a slower evolution around saturation density
- Around normal density, a_s dominated by the unitary constraint
- At normal density, a_s is washed out
- Finite r_s plays a non-negligible role

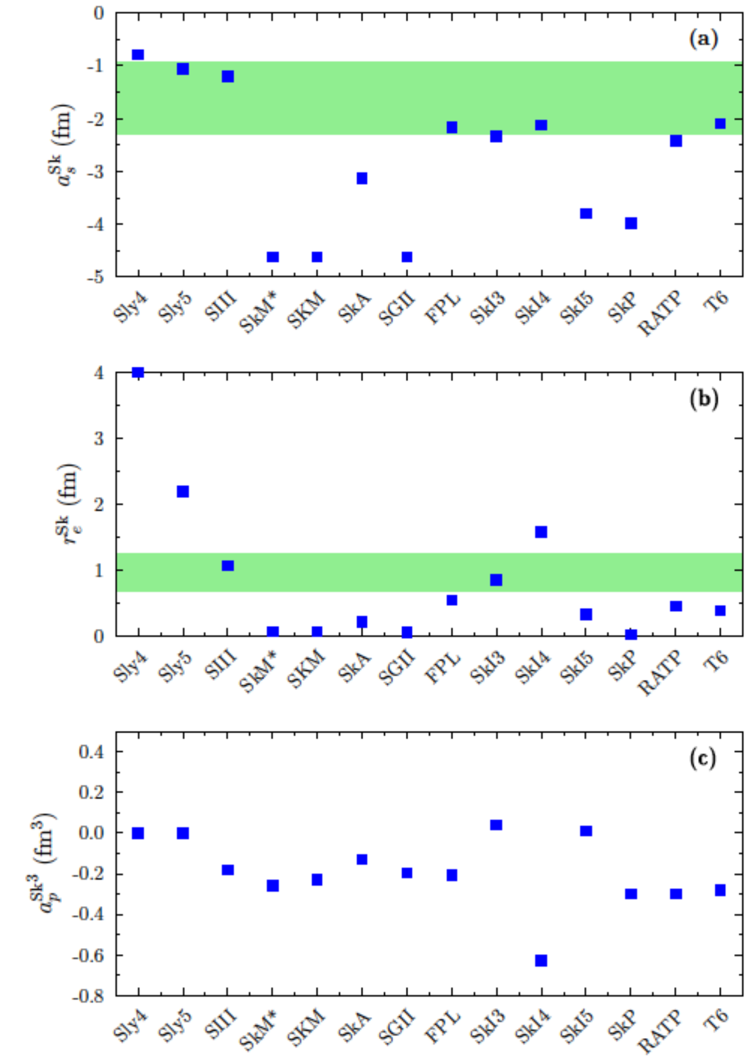
$$\widetilde{r}_e(k_F) \simeq \frac{200}{27(\nu-1)} \frac{\eta_e^2}{(1-\xi_0)^2\delta_e k_F}$$

$$\widetilde{r}_e(k_F) \simeq \frac{200}{27(\nu-1)} \frac{\eta_e}{(1-\xi_0)^2} \frac{r_e}{[1+\delta_e(r_e k_F)/\eta_e]}$$

Can we make contact with empirical functional ?

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





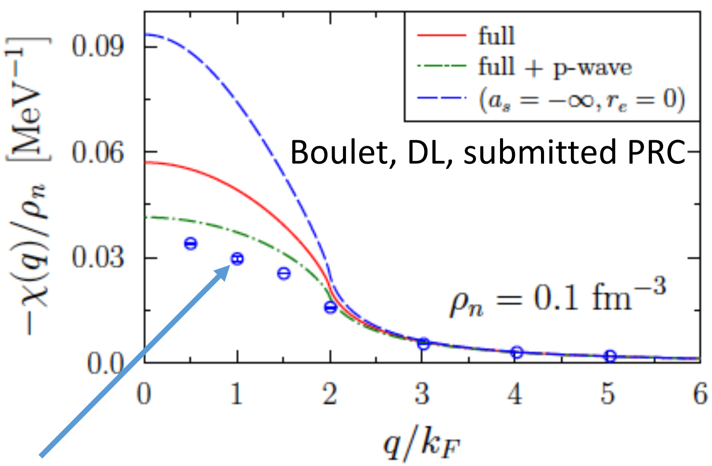
Gives an empirical explanation of the Skyrme success

Conclusions

- We propose a new way design the nuclear (cold atom) DFT to parameters of the interaction
  - Low energy constants becomes the only “non-freely” adjustable parameters
  - Validity $\rho < 0.01\ \mathrm{fm}^{-3}$
- The new DFT reproduces ab-initio results in cold atoms and neutron matter
- Transition from s-wave driven (low density) to unitary gas driven (Bertsch parameter) regime
- Explain in some ways why Skyrme works so well

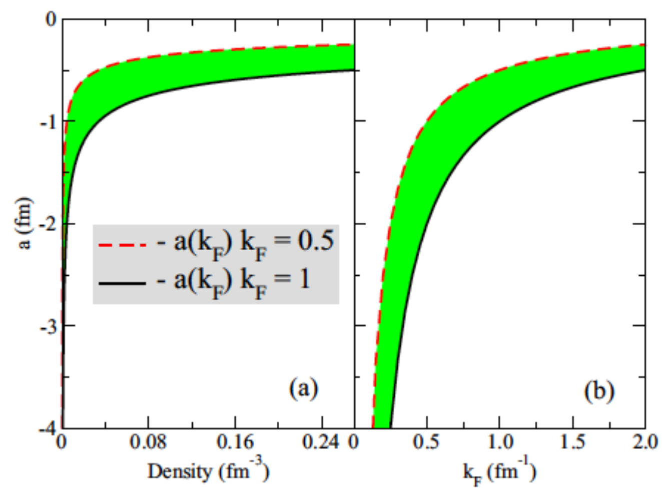
Applications and on-going work

Static response in neutron matter



AFDMC: Buraczynski,Gezerlis, PRL 116 (2016)]

Extension to symmetric matter:Lee-Yang with density dependent LEC



Grasso, DL, Yang, PRC 95 (2017)