Density Functional for cold atoms and neutron matter with no free parameters.

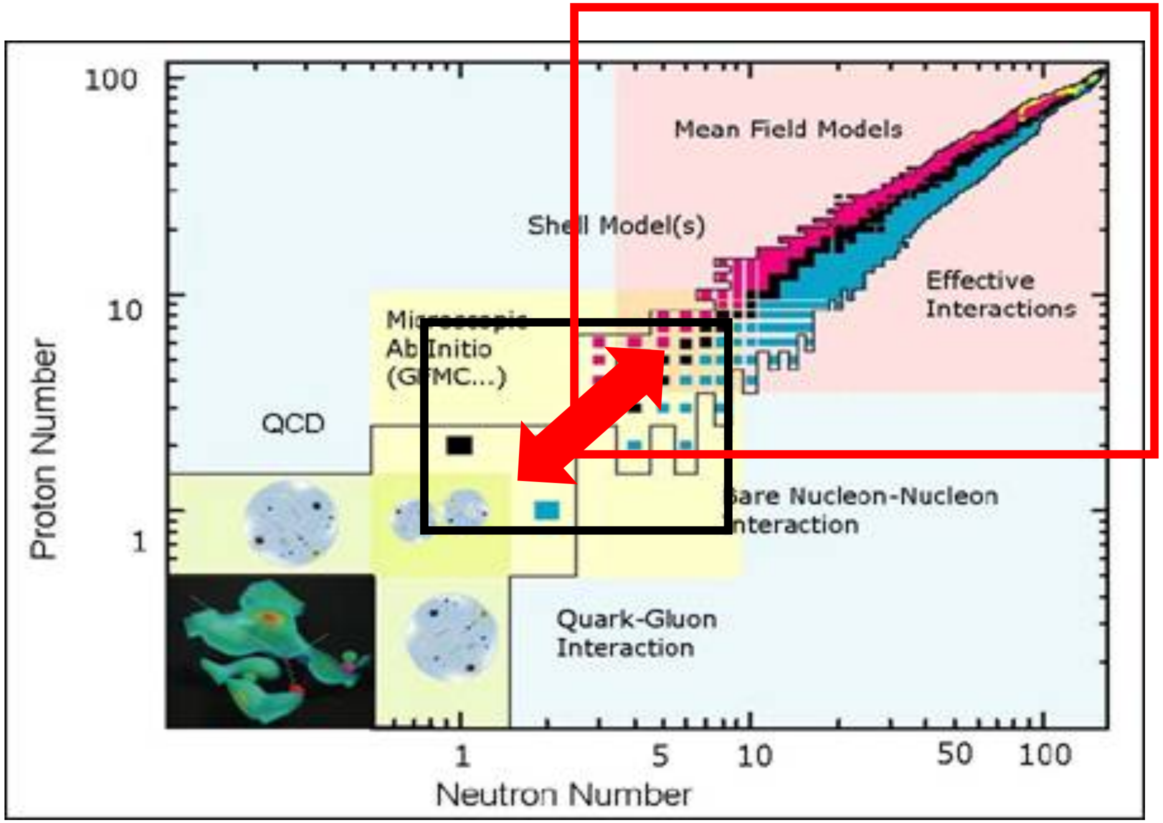
Denis Lacroix

INSTITUT DE PHYSIQUE NUCLÉAIRE ORSAY

Outline:

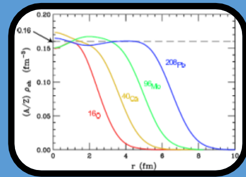
- Brief discussion on DFT for nuclei
- EFT guiding the construction of DFT/EDF: resummation
- Unitary gas guidance: role of large but finite s-wave scattering length
- Applications:cold atoms and neutron matter.

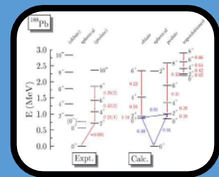
Coll: J. Bonnard, A. Boulet, M. Grasso and C.J. Yang

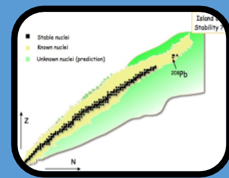


But we want to do a little bit more…

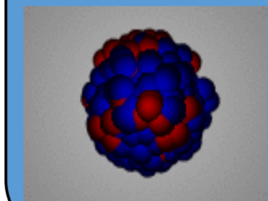
GROUND STATE-STRUCTURE OF THE ATOMIC NUCLEUS

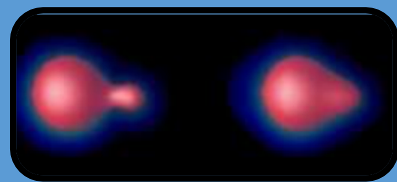






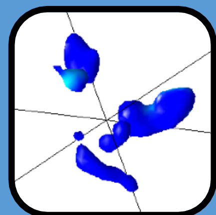
SMALL AND LARGE AMPLITUDE DYNAMICS

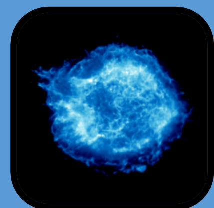




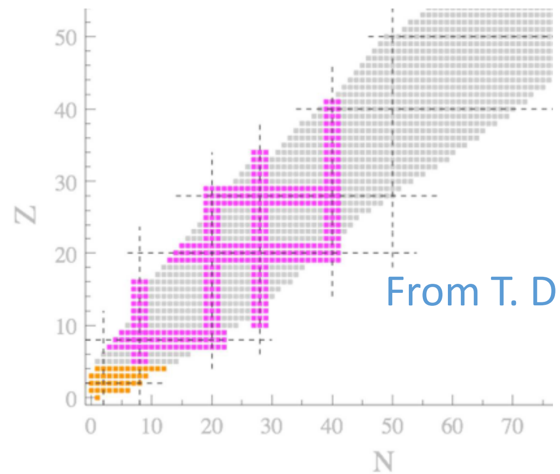
Nuclear Thermodynamic

(from finite or infinite systems)





State of the art ab-initio calculation in 2016



From T. Duguet

Nuclear Energy Density Functional based on effective interaction

Constraining the functional

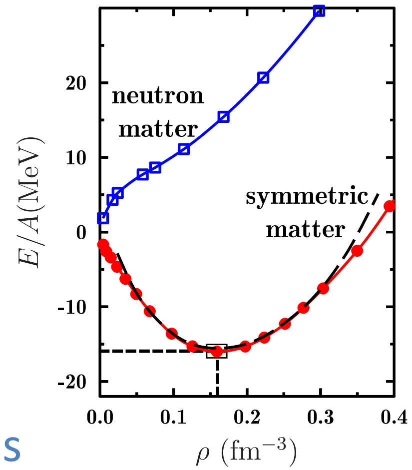
Static

See for instance, Meyer EJC1997

Vautherin, Brink, PRC (1972)

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

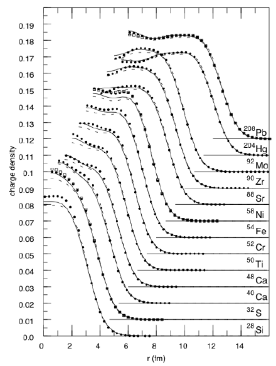
Infinite nuclear matter and Nuclear Masses



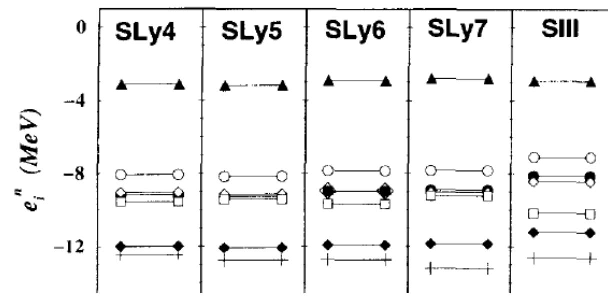
$$E_0,\ \left.\frac{\partial E}{\partial \rho}\right|_{\rho_0},\ \left.\frac{\partial^2 E}{\partial \rho^2}\right|_{\rho_0}$$

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

Densities



Shell effect

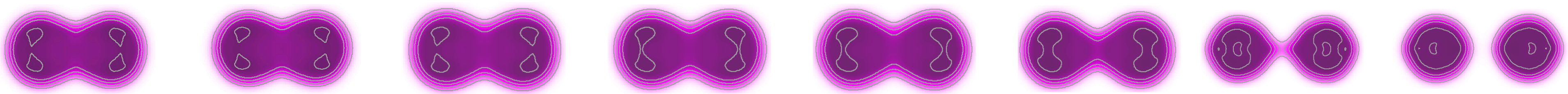


Chabanat et al, NPA (1998)

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

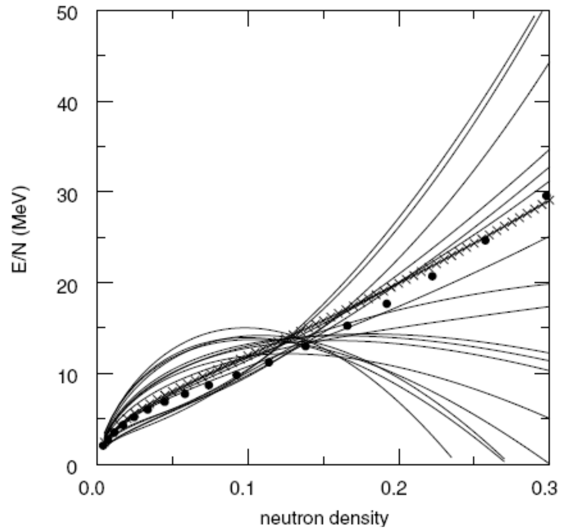
Limitation and drawback

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

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

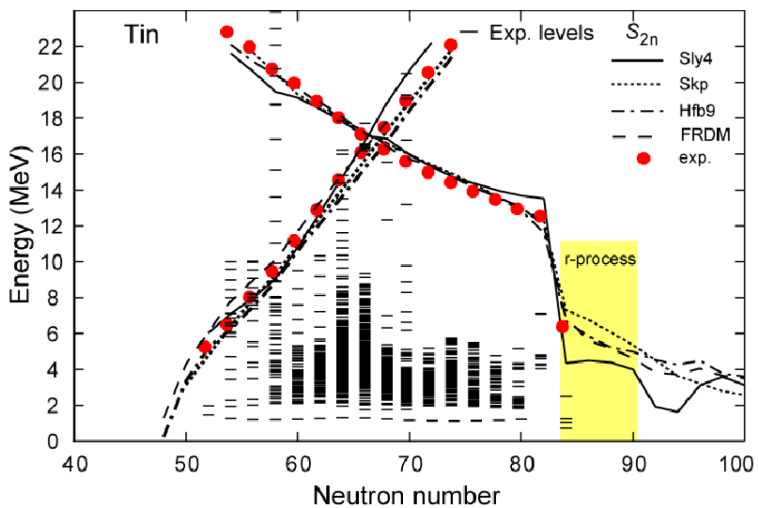
Since we directly fit on experiments there is no more link with the interaction and associated low energy constants…

EOS of pure neutron matter



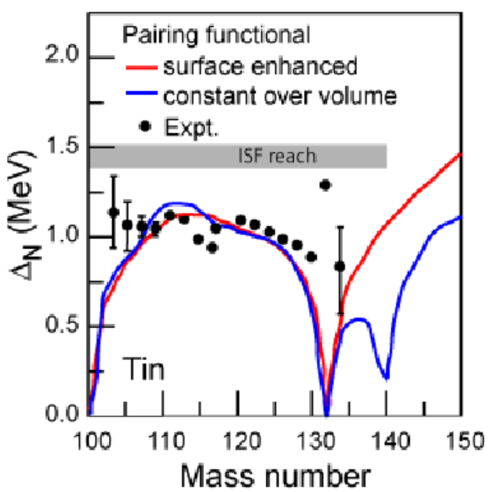
Brown, PRL85 (2000).

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

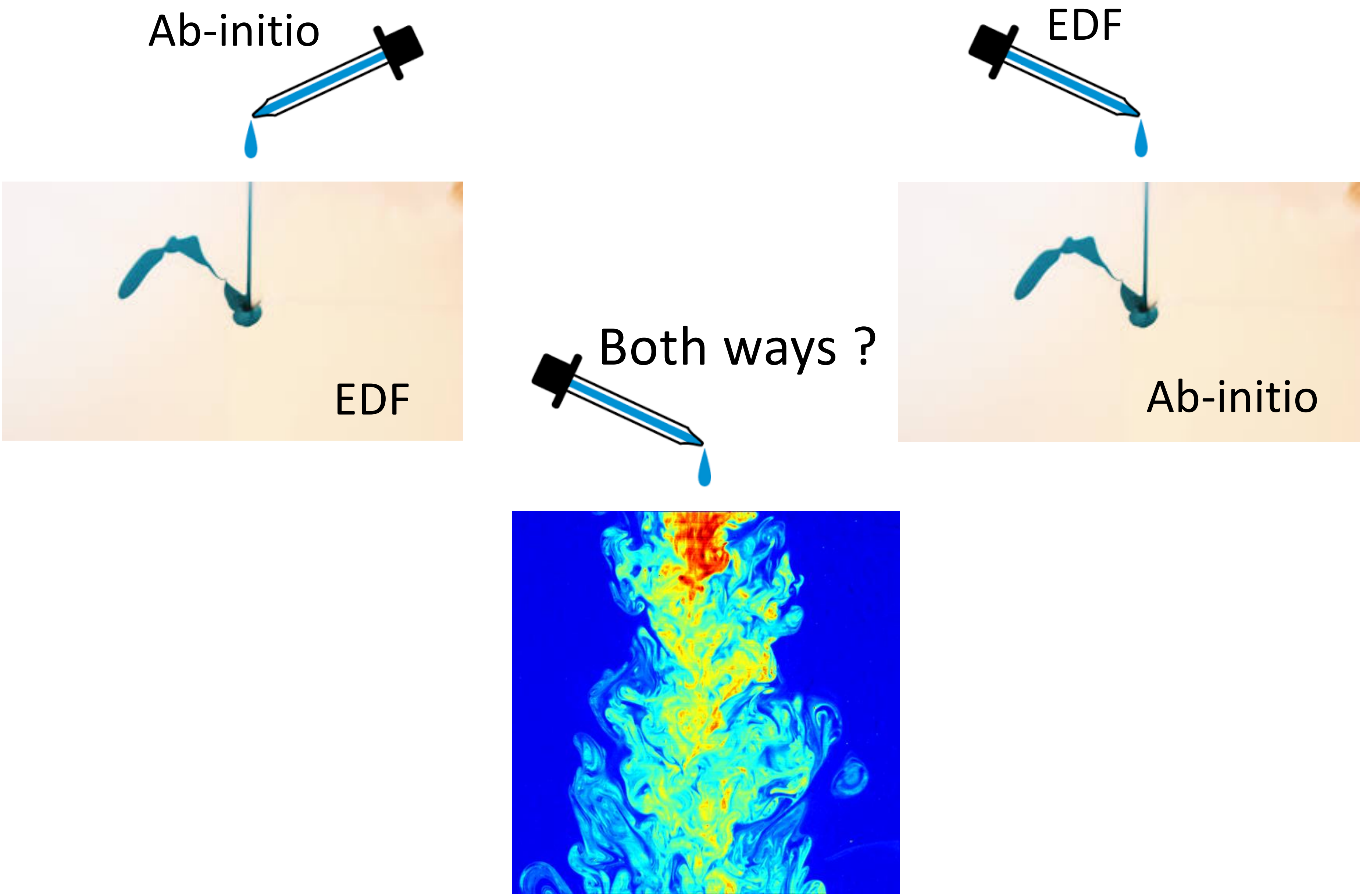


http://www.nscl.msu.edu/future/isf

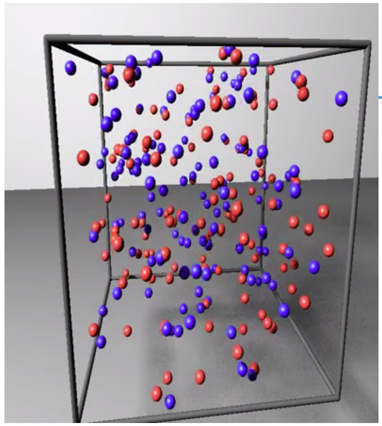
Pairing gap



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



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

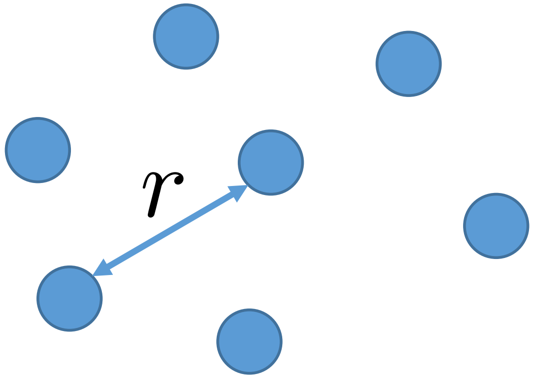


Towards a constructive approach for DFT

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

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

Example of the s-wave

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

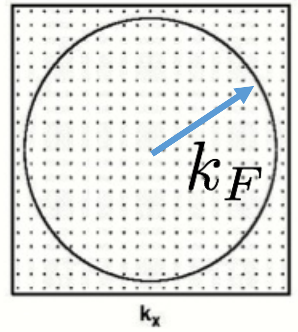
C_0, C_2, C'_2 are directly linked to low energy constant

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

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)



General strategy: infinite systems

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

$\rho = \frac{\nu}{6\pi^2} k_F^2$ 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 $a_s = -18.9$ fm

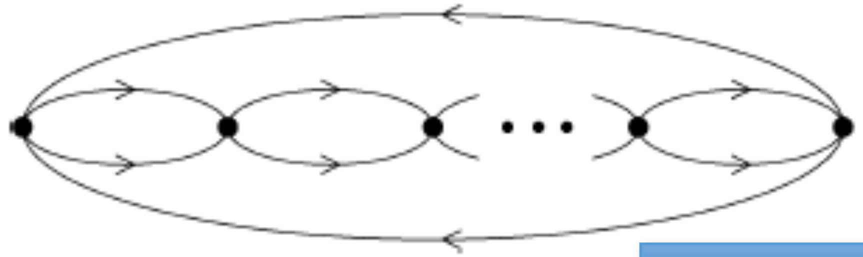
$r_e = 2.7$ fm

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

The “magic” technique: resummation

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

Resummation of particle-particle diagrams

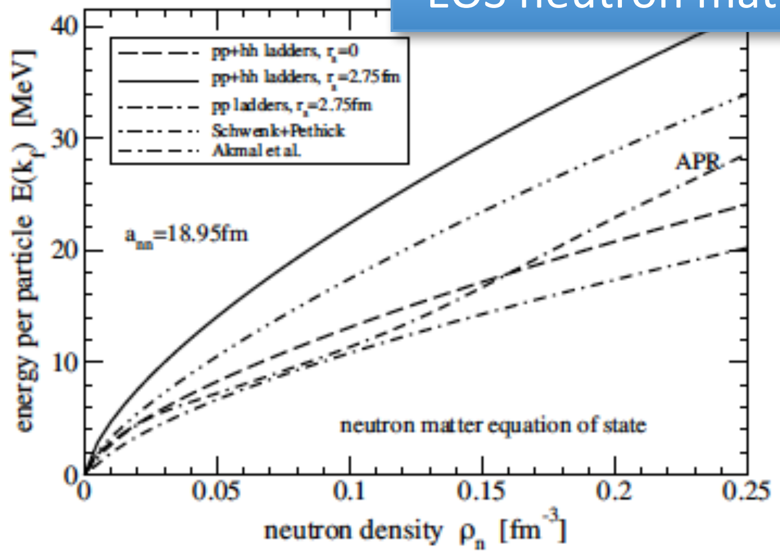


$$\frac{E_{\rm PP}}{A} = \frac{3(g-1)\pi^2}{k_F^3}\int \frac{d^3P}{(2\pi)^3}\frac{d^3k}{(2\pi)^3}\theta_k^- \frac{4\pi a/M}{1-\frac{k_F a}{\pi} f_{\rm PP}(\kappa,s)}.$$

Contains terms to all order in $(a_s k_F)$

Results strongly depends on selected diagram

EOS neutron matter



Kaiser, EPJA 48 (2012)

The pragmatic approach

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

$$\frac{E}{A} = \left(\frac{3}{5}+\frac{2k_F a_s/3}{\pi - 2k_F a_s}\right)\frac{k_F^2}{2M} \qquad \langle f_{\rm PP}\rangle \underset{+\infty}{\rightarrow} 2$$

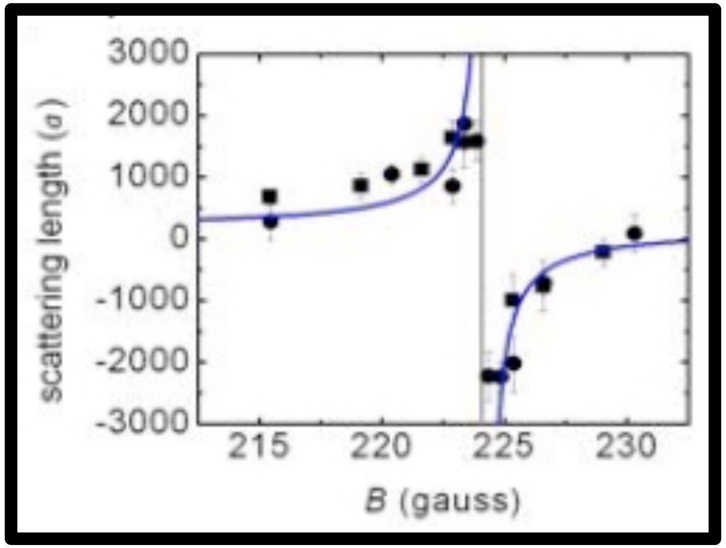
Steele, nucl-th-0010066v2

Interpretations:

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

Resummed formula for Unitary gas

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

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

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

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

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

Adjusting only on low density

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

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

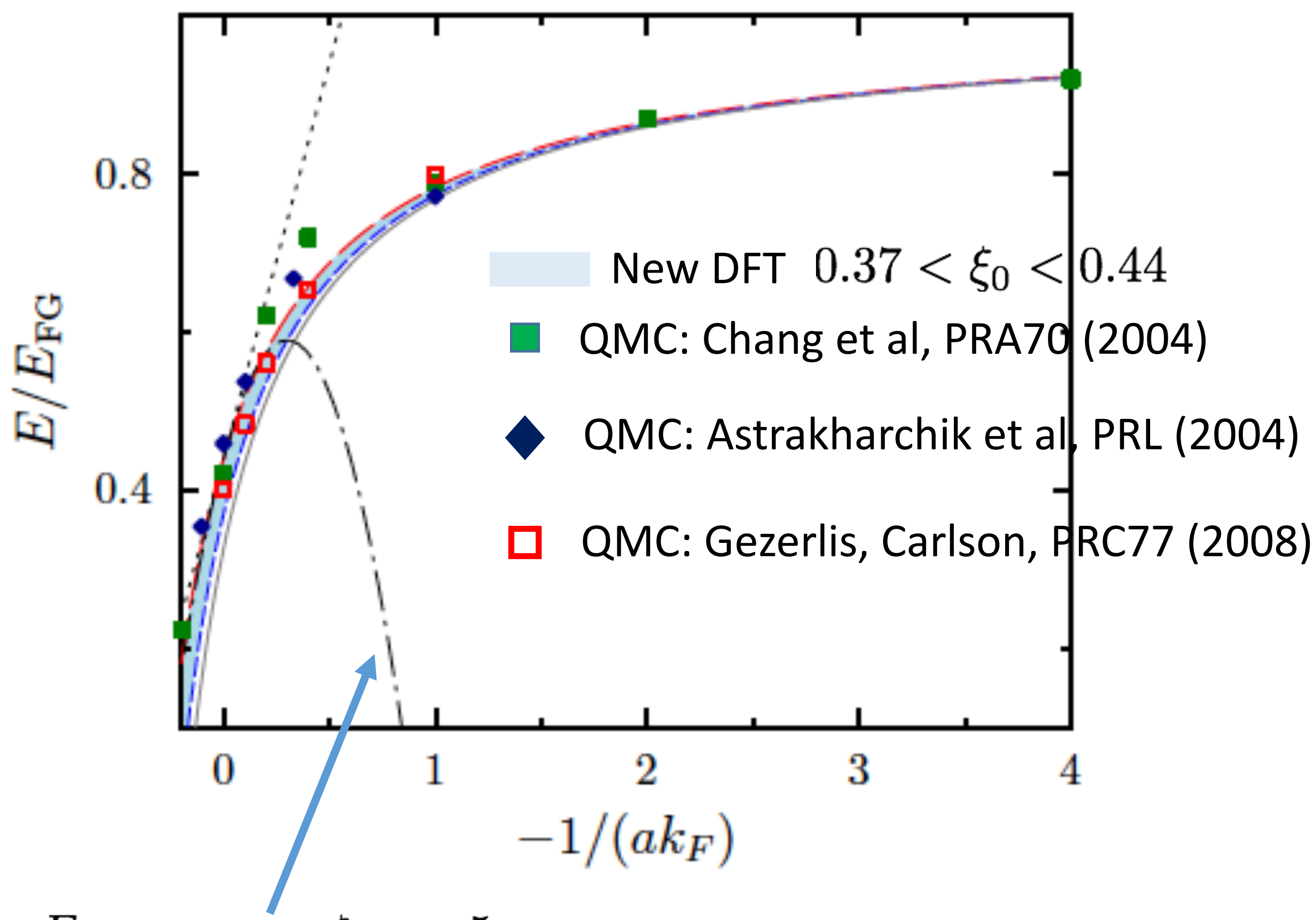
Adding the unitarity constraint

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

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

Result of the DFT for at or close to unitarity

Lacroix, PRA 94 (2016)



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

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

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

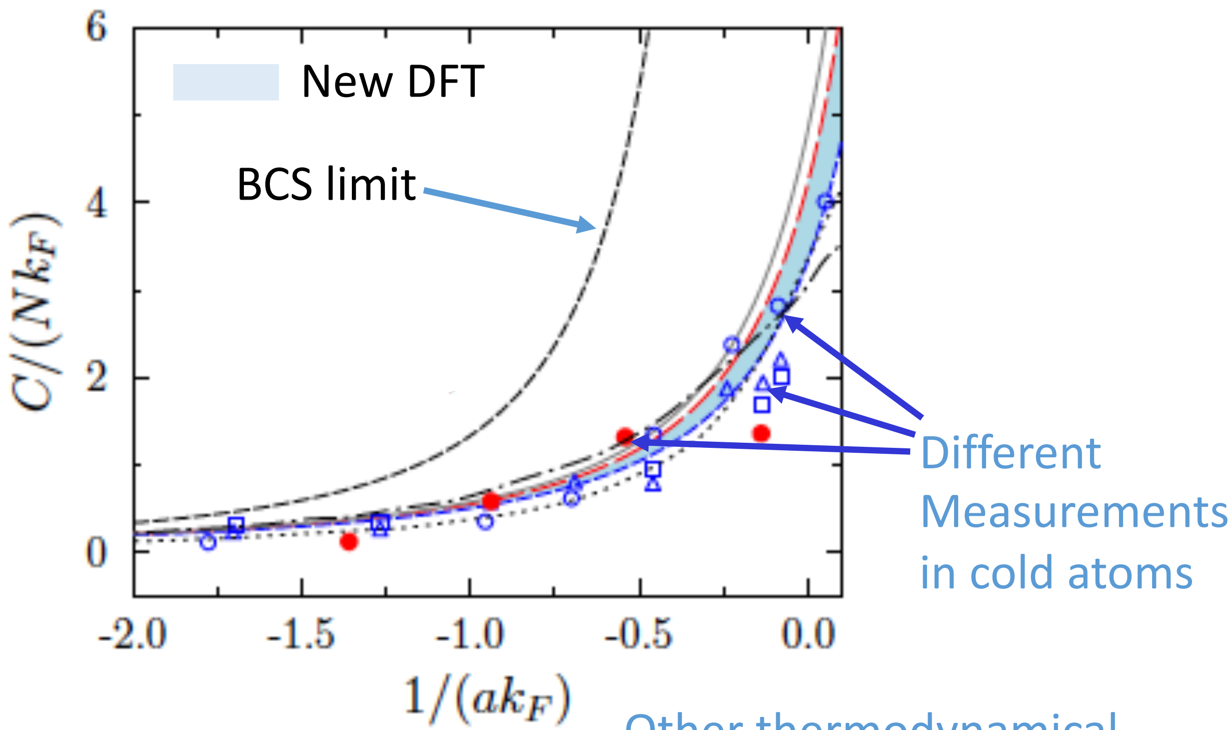
Estimate of the density dependence of the Tan contact parameter

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

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

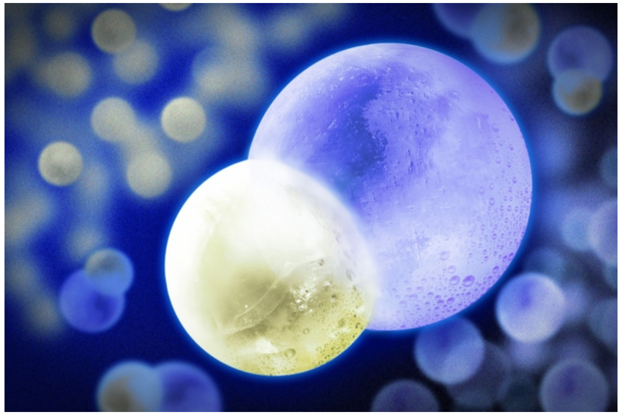
$$\mathcal{C} = \frac{4\pi m a_s^2}{\hbar^2}\left(\frac{d\mathcal{E}}{da_s}\right)$$

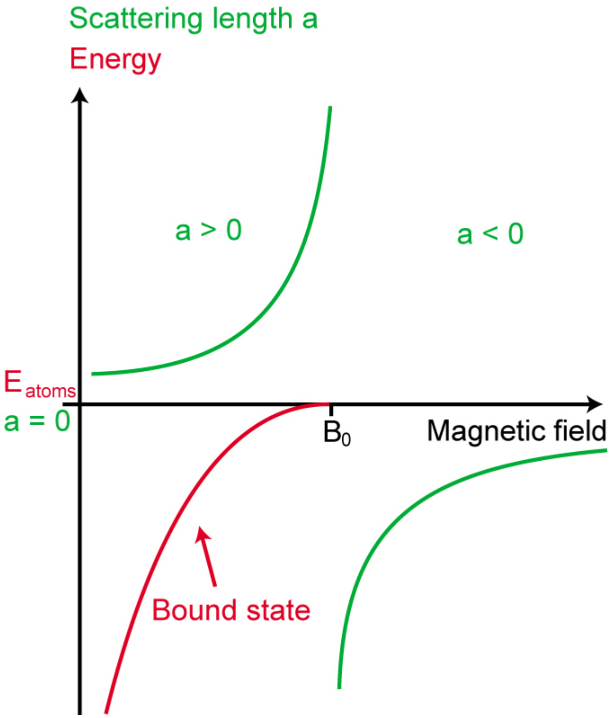
$$\mathcal{E} = \frac{k_F^3 E}{3\pi^2 N}$$



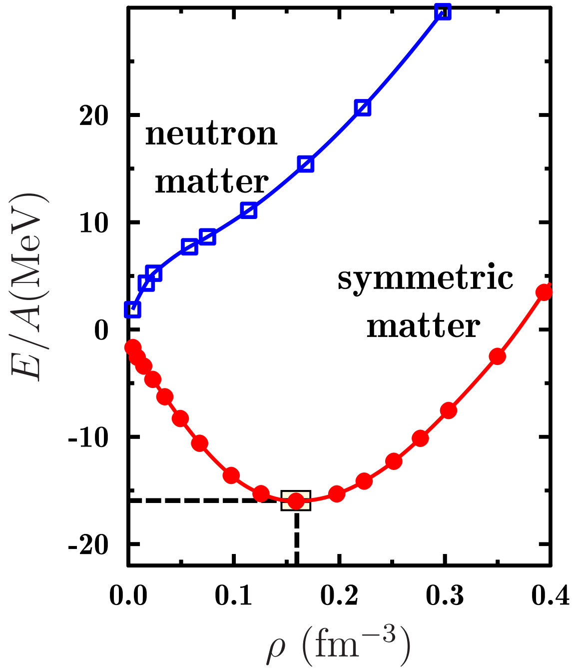
Other thermodynamical Quantities (See A. Boulet talk)

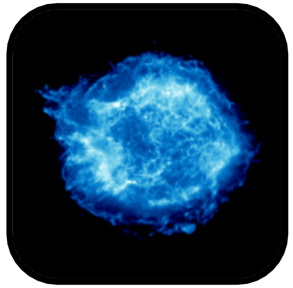
From cold atom to neutron matter





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

$|a_s k_F| \ll 1$

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

$|a_s k_F| \gg 1$

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

Forbes, Gandolfi, Gezerlis, PRA86 (2012)

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

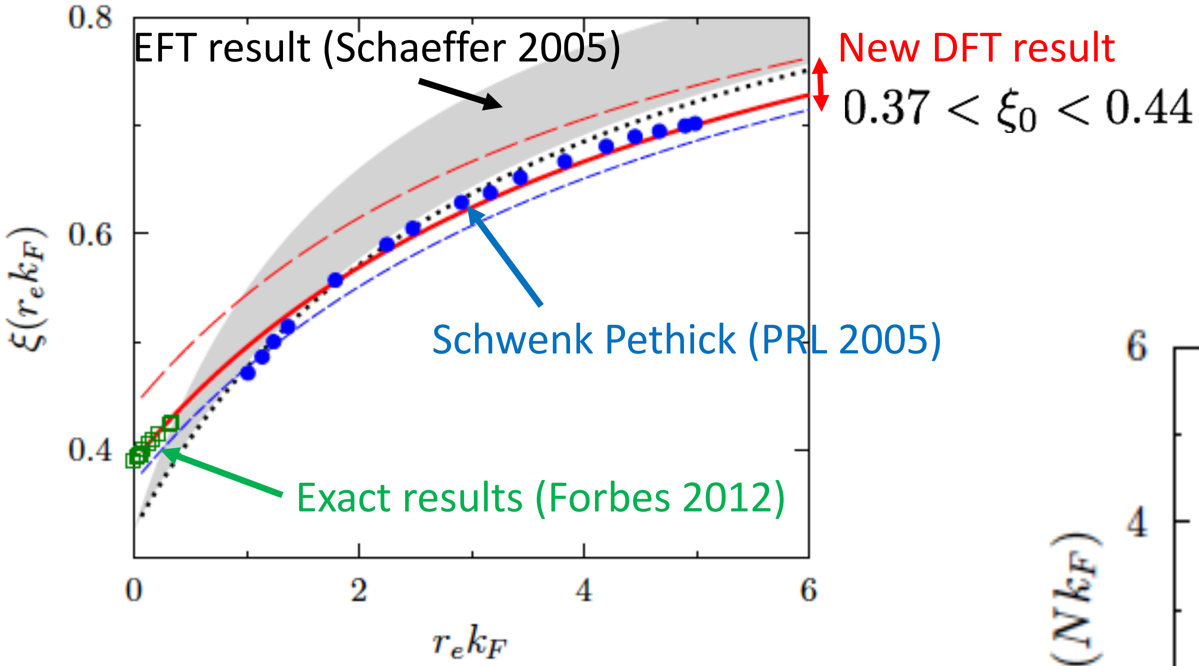
$\xi_0 = 0.376,$
$\eta_e = 0.127$
$\delta_e = -0.055$

Inclusion of effective range effects in cold atoms

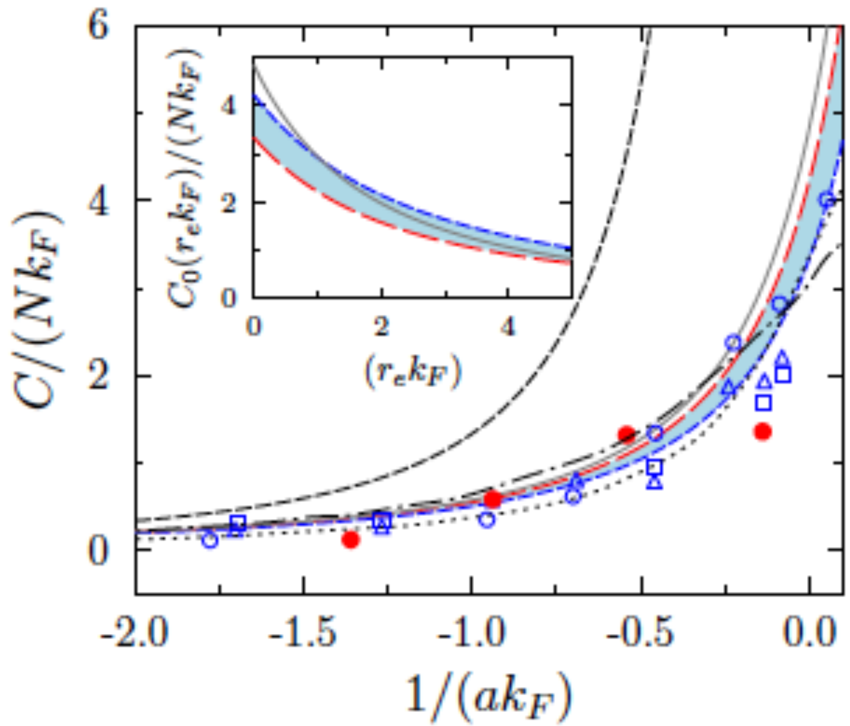
At unitarity

Lacroix, PRA 94 (2016)

$$\frac{E}{E_{\rm FG}} = \xi(r_e k_F)$$

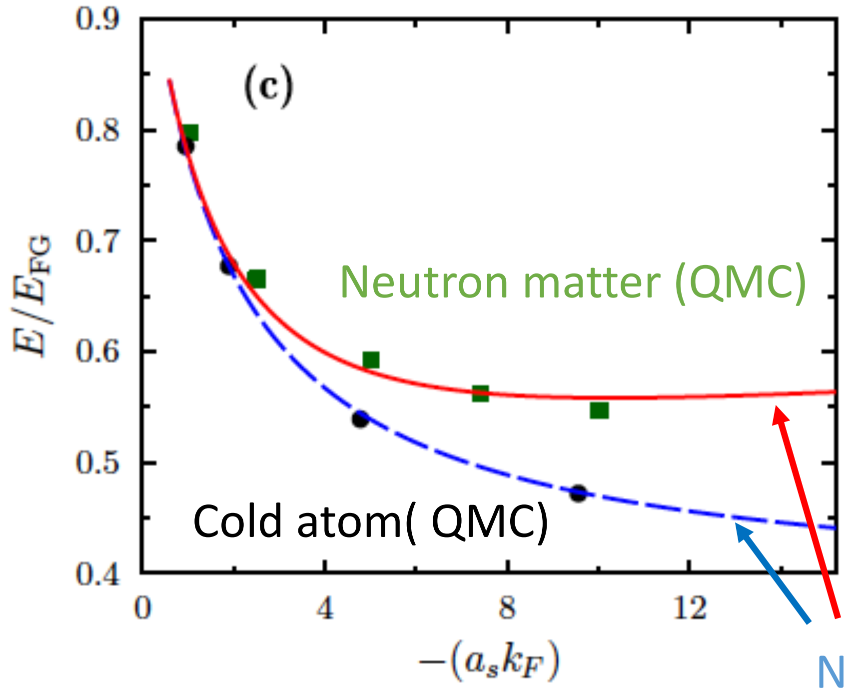


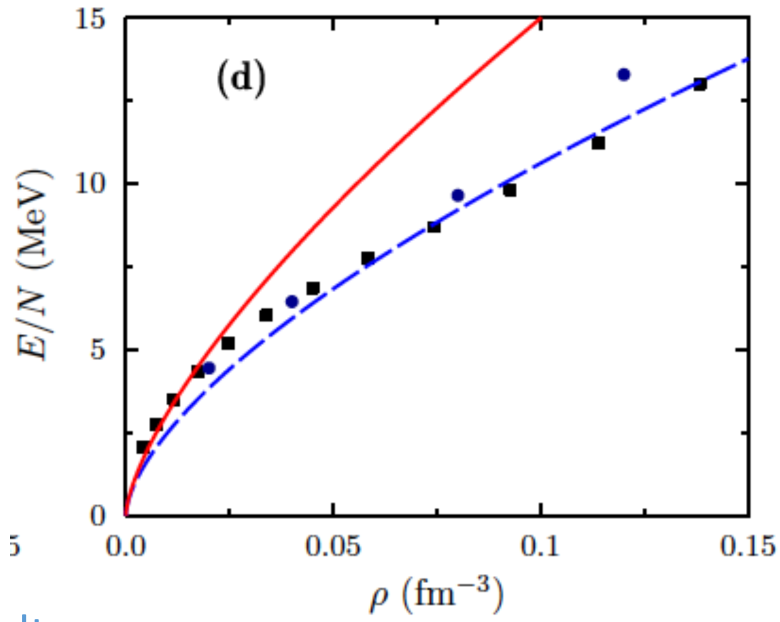
Contact with r_e effects



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

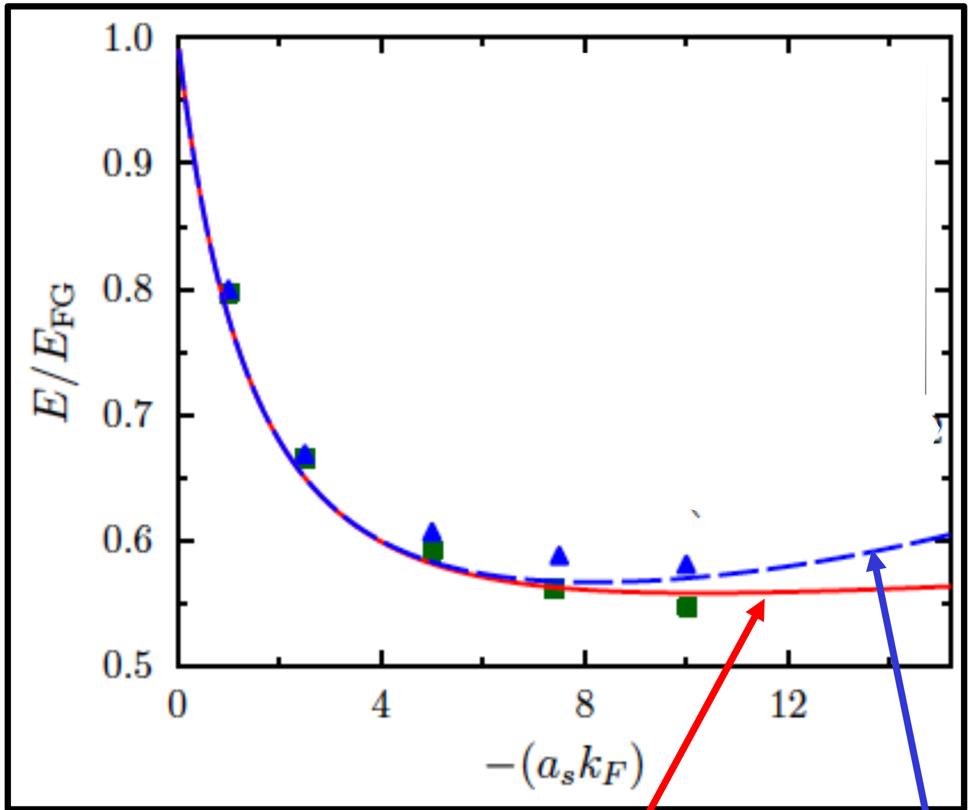
New DFT $\rho < 0.01\ \mathrm{fm}^{-3}$

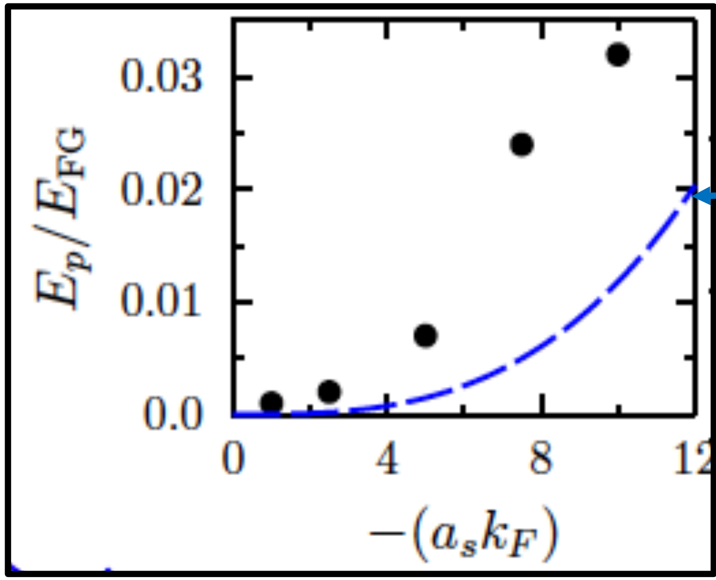
Including the p-wave ?

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

Remember $a_p \ll r_e \ll a_s$

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





$a_p^3 = 0.2$

(AV4 interaction)

no p-wave

With p-wave (LO only)

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

Can we conceal this functional with the Skyrme functionals?

Difficulty in nuclear systems

Yang, Grasso, Lacroix PRC94 (2016)

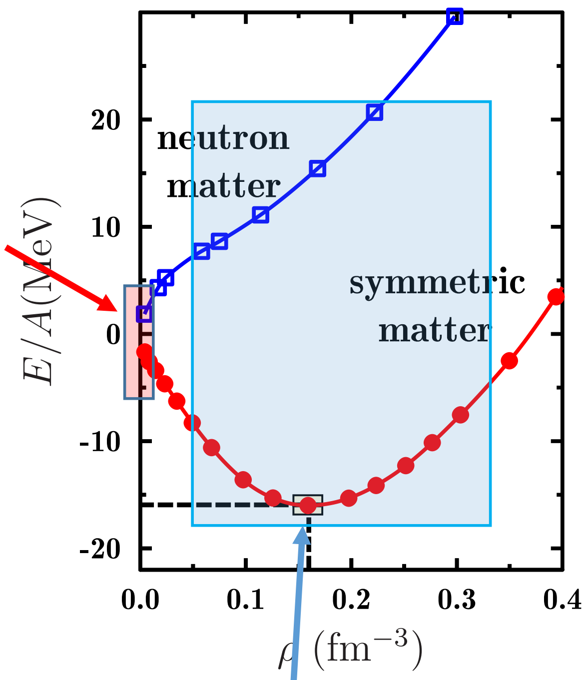
Skyrme functional

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

MBPT + expansion in LEC is valid here

is very close to the EFT starting point

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



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

Additional remarks on traditional Skyrme

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

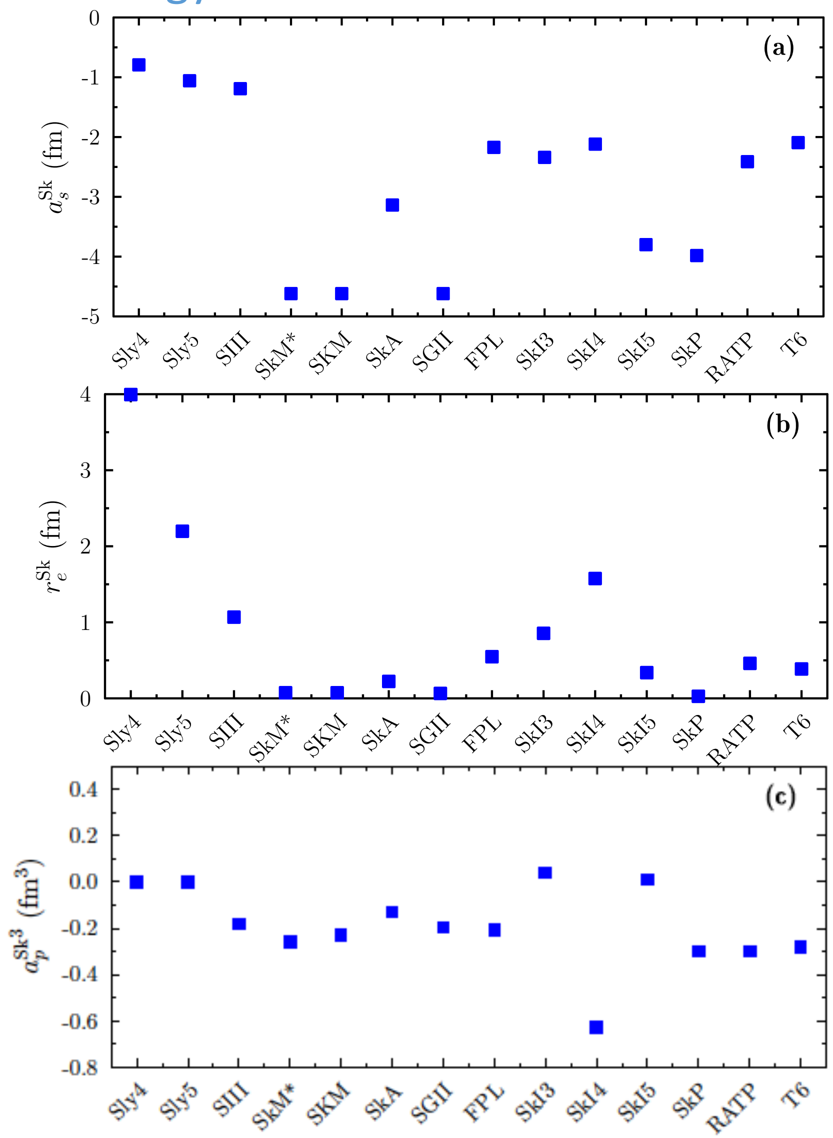
Due to the analogy, one can define equivalent low energy constant

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

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

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

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

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

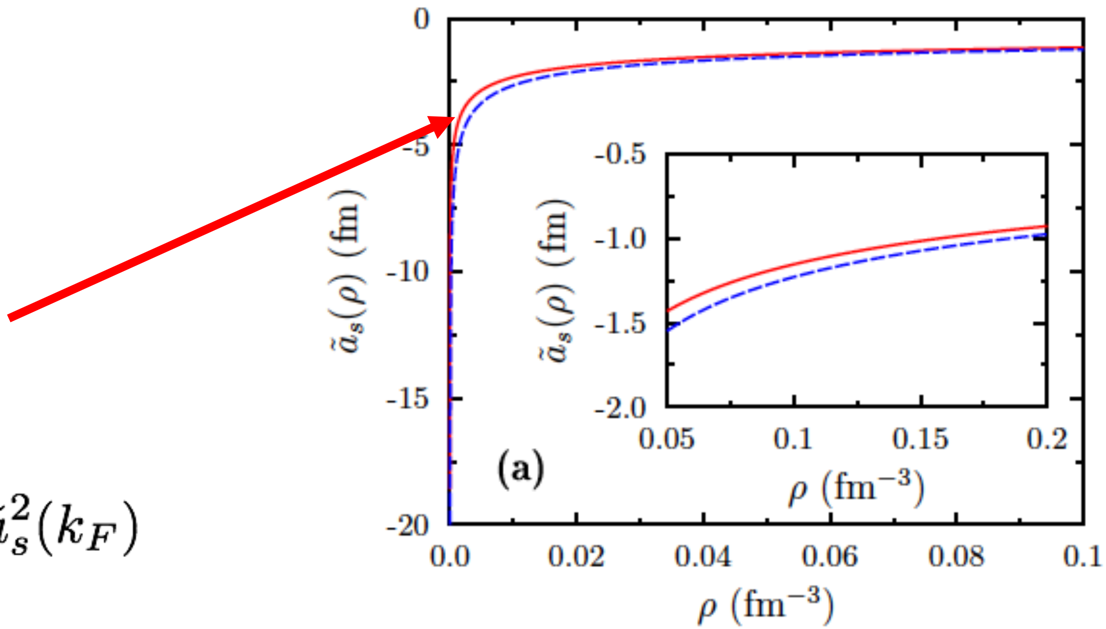
Rewrite it as

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

Define density dependent scattering length and range

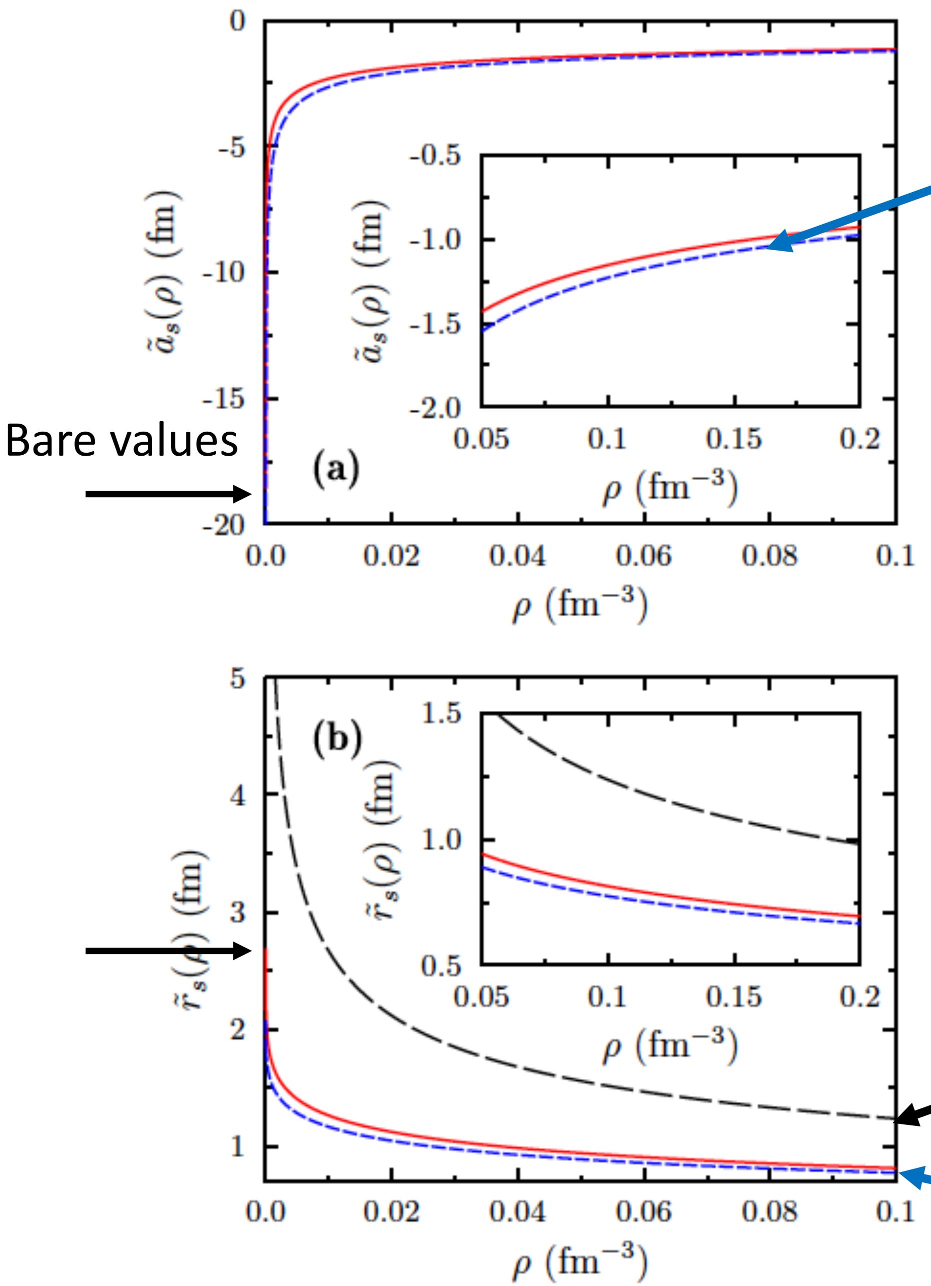
$$\tilde{C}_0(k_F) = \frac{4\pi\hbar^2}{m}\tilde{a}_s(k_F)$$

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



Can we make contact with empirical functional ?

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



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

- 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

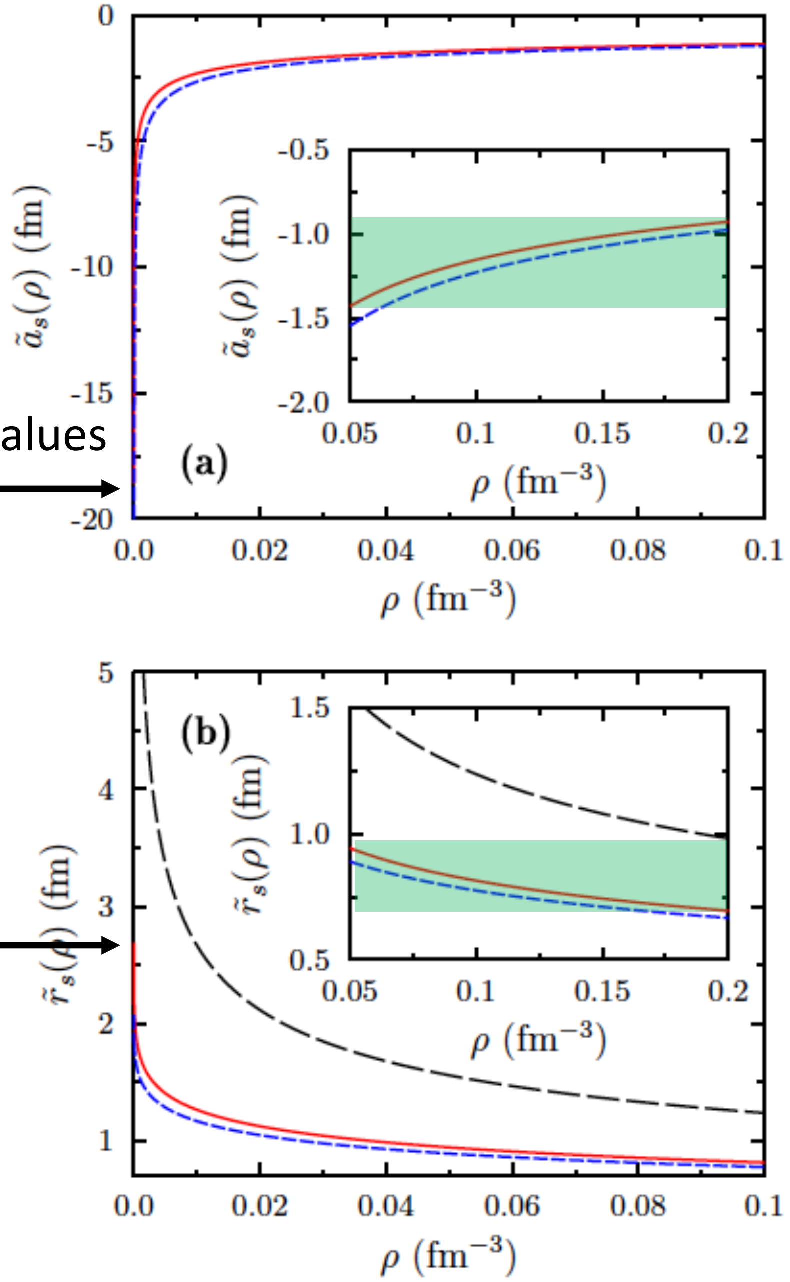
$$\tilde{r}_e(k_F) \simeq \frac{200}{27(\nu-1)}\frac{\eta_e^2}{(1-\xi_0)^2\delta_e k_F}$$

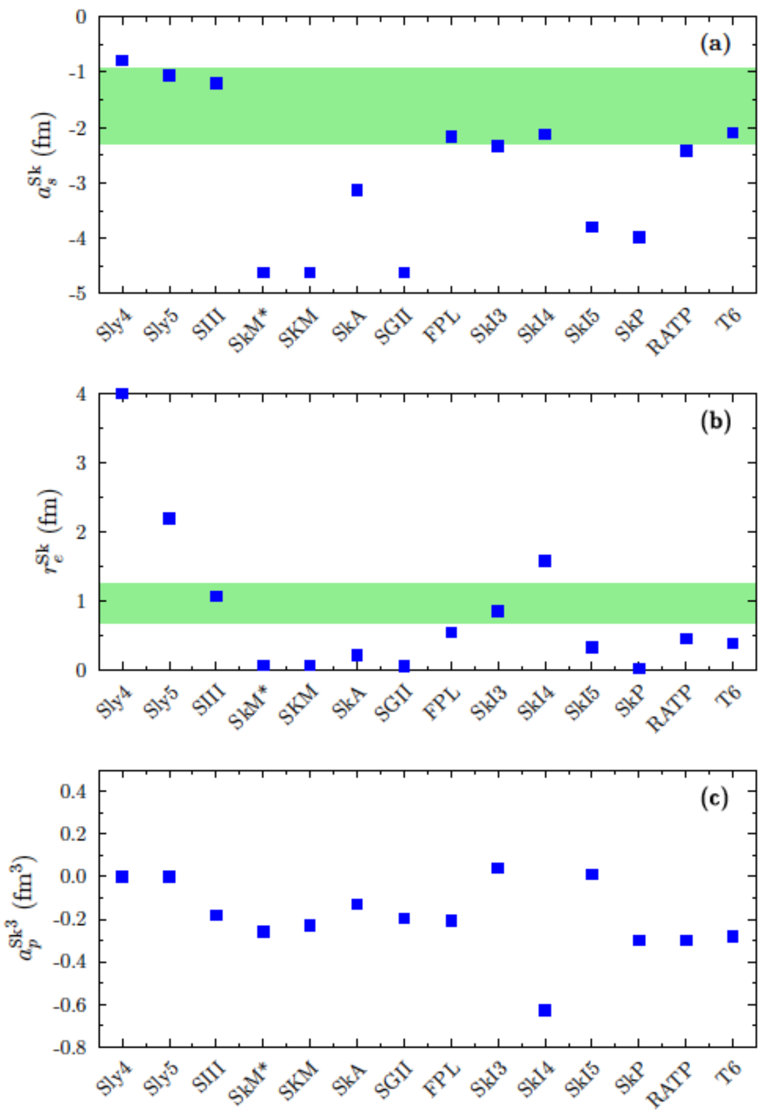
$$\tilde{r}_e(k_F) \simeq \frac{200}{27(\nu-1)}\frac{\eta_e}{(1-\xi_0)^2}\frac{r_e}{[1+\delta_e(r_e k_F)/\eta_e]}$$

Can we make contact with empirical functional ?

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

Bare values





Gives an empirical explanation of the Skyrme success

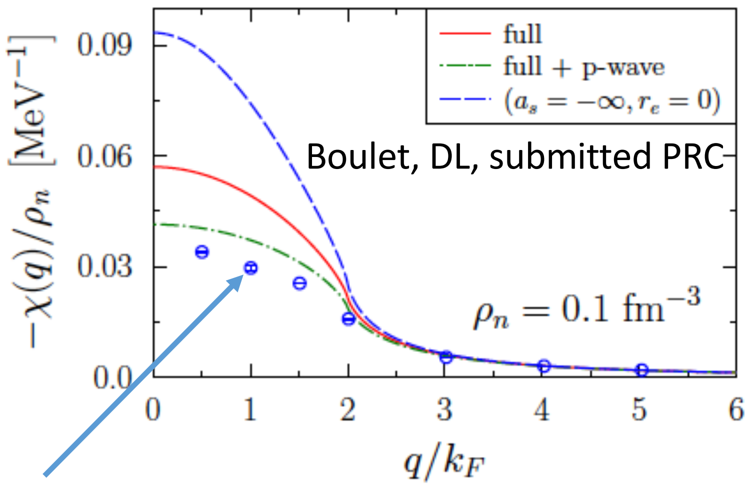
Conclusion and ongoing work

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 $\rho < 0.01 \text{ fm}^{-3}$
- 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 and dynamical response in neutron matter



Boulet, DL, submitted PRC

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