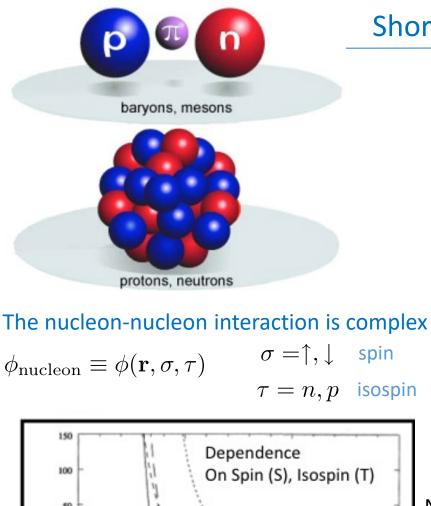
Density Functional approach to cold atoms and neutron matter

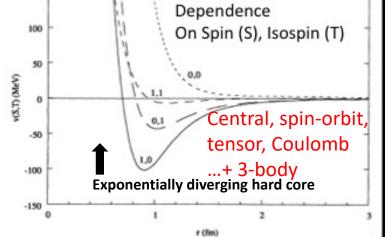


Outline:

- 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 (Ground state and excited states)

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





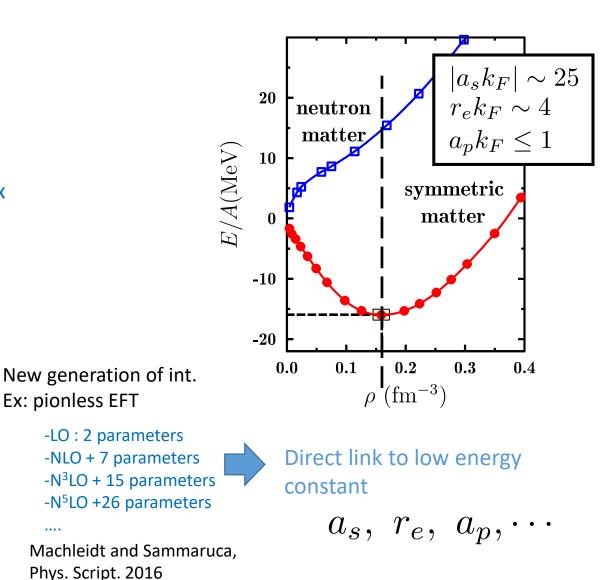
Wiringa, Rev. Mod. Phys. 1993

....

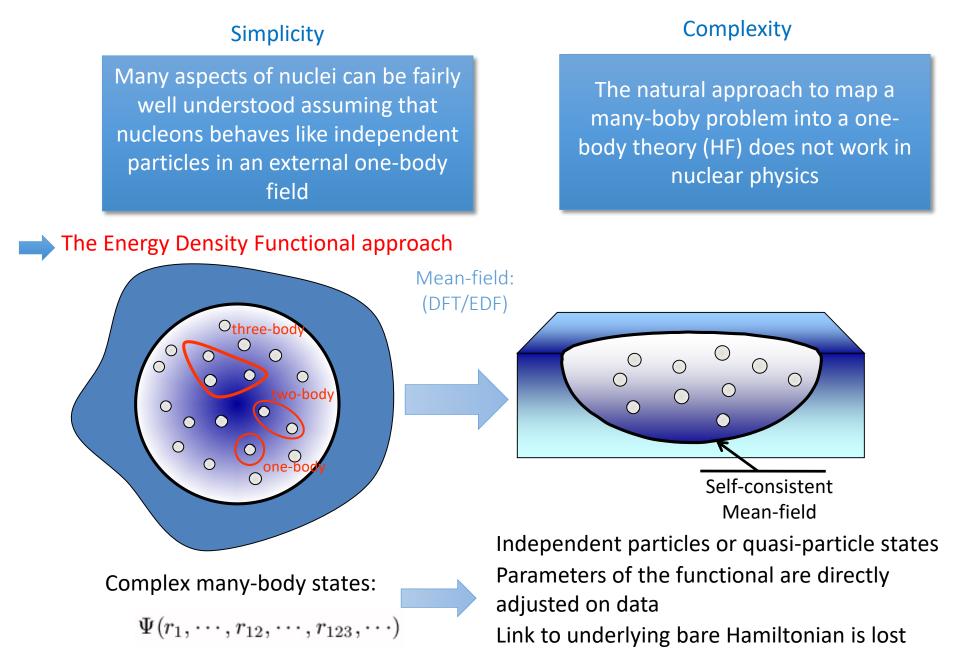
Short summary of the atomic nuclei properties

generalities

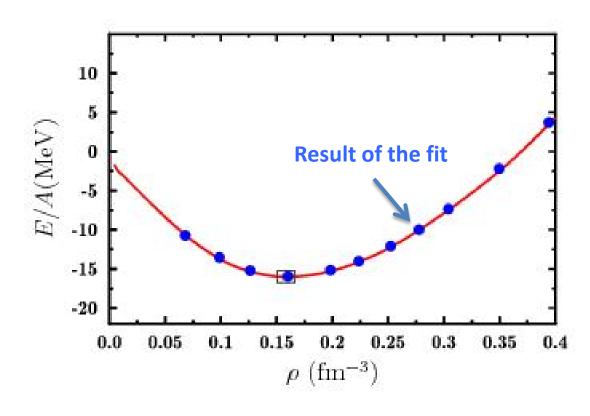
Some orders of magnitude and general aspects



Dilemma: failure of the Hartree-Fock theory /success of DFT/EDF



EDF from a simple perspective





Coefficients contains many-body physics

Contains resummation of many-body effects to all orders

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)

Basic aspects of Functional approach to nuclear systems

Nuclear takes different names:

Skyrme/Gogny Hartree-Fock, Nuclear Density Functional Theory (nuclear DFT) Energy Density Functional (EDF) Relativistic Mean-Field ...

What type of Density Functional Theory we use ?

In its simplest form in DFT, the exact ground state of an N-body problem can be replaced by the minimization of an energy functional of the local one-body density $\rho(r)$. At the minimum, the energy and the density corresponds to the exact energy

Hohenberg, Kohn, Phys. Rev. (1965)

Extensions:

Introduction of auxiliary state $\Psi = \mathcal{A}(\varphi_1(r_1), \cdots \varphi_N(r_N))$ Kohn, Sham. Phys. Rev. (1965) $o(r) = \sum |\varphi_1(r_1)|^2$

, Sham, Phys. Rev. (1965)
$$ho(r) = \sum_i |arphi_i(r)|^2$$

 $\{\varphi_i\} \to \rho(r) \to \mathcal{E} \to U_{KS}(r) \to \{\varphi_i\}...$ $h[\rho]|\varphi_i\rangle = \varepsilon_i |\varphi_i\rangle \text{ with } h[\rho] = \frac{\partial \mathcal{E}}{\partial \rho}$

GGA, Meta GGA, ...

A primer to DFT, Lectures notes in Physics 620 (2003)

DFT with pairing

Oliveira et al, PRL (1988) Time-dependent DFT

Runge, Gross PRL (1984)

$$\mathcal{E} = \mathcal{E}[\rho(r), \nabla \rho, \Delta \rho, \tau, \ldots]$$

$$\mathcal{E} = \mathcal{E}[\rho, \kappa...]$$
 (and much more ...)

 $\langle \Psi | \hat{H} | \Psi \rangle \Longrightarrow \mathcal{E}[\rho(r)]$

Nuclear Energy Density Functional based on effective interaction Illustration with the Skyrme Functional

Vautherin, Brink, PRC (1972)

$$\begin{aligned} v(\mathbf{r}_{1} - \mathbf{r}_{2}) &= t_{0} \left(1 + x_{0} \hat{P}_{\sigma} \right) \delta(\mathbf{r}) \\ &+ \frac{1}{2} t_{1} \left(1 + x_{1} \hat{P}_{\sigma} \right) \left[\mathbf{P}^{\prime 2} \, \delta(\mathbf{r}) + \delta(\mathbf{r}) \, \mathbf{P}^{2} \right] \\ &+ t_{2} \, \left(1 + x_{2} \hat{P}_{\sigma} \right) \mathbf{P}^{\prime} \cdot \delta(\mathbf{r}) \, \mathbf{P} \\ &+ i W_{0} \sigma. \left[\mathbf{P}^{\prime} \times \delta(\mathbf{r}) \, \mathbf{P} \right] \\ &+ \frac{1}{6} t_{3} \left(1 + x_{3} \hat{P}_{\sigma} \right) \rho^{\alpha}(\mathbf{R}) \, \delta(\mathbf{r}) \end{aligned}$$

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

$$\begin{split} \mathcal{H} &= \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_3 + \mathcal{H}_{\rm eff} \\ &+ \mathcal{H}_{\rm fin} + \mathcal{H}_{\rm so} + \mathcal{H}_{\rm sg} + \mathcal{H}_{\rm Coul} \end{split}$$

$$\begin{aligned} \mathcal{H}_{0} &= \frac{1}{4} t_{0} \left[(2+x_{0})\rho^{2} - (2x_{0}+1)(\rho_{p}^{2}+\rho_{n}^{2}) \right] \\ \mathcal{H}_{3} &= \frac{1}{24} t_{3} \rho^{\alpha} \left[(2+x_{3})\rho^{2} - (2x_{3}+1)(\rho_{p}^{2}+\rho_{n}^{2}) \right] \\ \mathcal{H}_{\text{eff}} &= \frac{1}{8} \left[t_{1}(2+x_{1}) + t_{2}(2+x_{2}) \right] \tau \rho \\ &+ \frac{1}{8} \left[t_{2}(2x_{2}+1) - t_{1}(2x_{2}+1) \right] (\tau_{p}\rho_{p} + \tau_{n}\rho_{n}) \\ \mathcal{H}_{\text{fin}} &= \frac{1}{32} \left[3t_{1}(2+x_{1}) - t_{2}(2+x_{2}) \right] (\nabla \rho)^{2} \\ &- \frac{1}{32} \left[3t_{1}(2x_{1}+1) + t_{2}(2x_{2}+1) \right] \left[(\nabla \rho_{p})^{2} + (\nabla \rho_{n})^{2} \right] \end{aligned}$$

$$\mathcal{H}_{so} = \frac{1}{2} W_0 \big[\mathbf{J} \cdot \nabla \rho + \mathbf{J}_p \cdot \nabla \rho_p + \mathbf{J}_n \cdot \nabla \rho_n \big]$$

$$\mathcal{H}_{sg} = -\frac{1}{16} (t_1 x_1 + t_2 x_2) \mathbf{J}^2 + \frac{1}{16} (t_1 - t_2) \big[\mathbf{J}_p^2 + \mathbf{J}_n^2 \big]$$

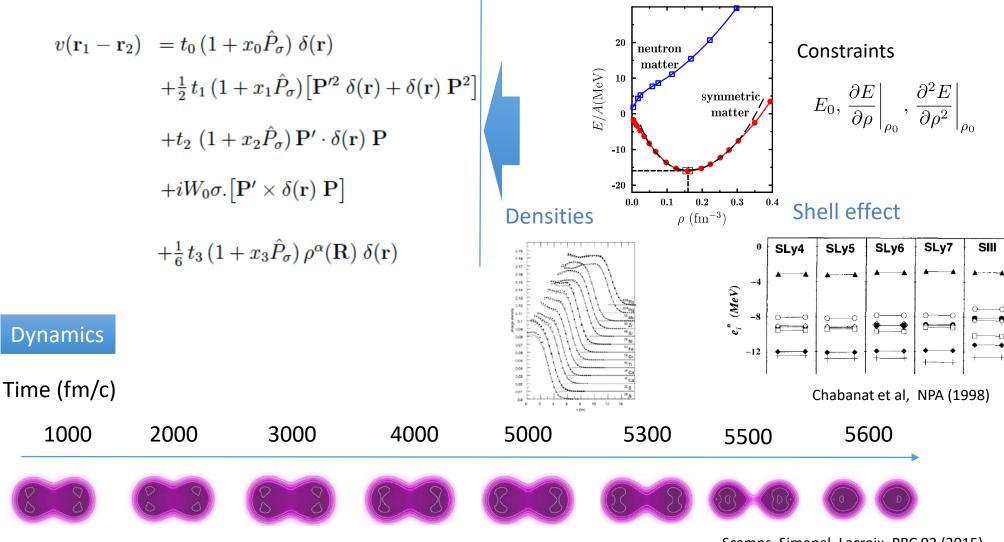
Functional of $\rho, \rho_n, \rho_p, \tau, \tau_n, \tau_p, \mathbf{J}, \dots$ Around 10-14 parameters to be adjusted

Nuclear Energy Density Functional based on effective interaction

Constraining the functional

Infinite nuclear matter and Nuclear Masses

See for instance, Meyer EJC1997



Vautherin, Brink, PRC (1972)

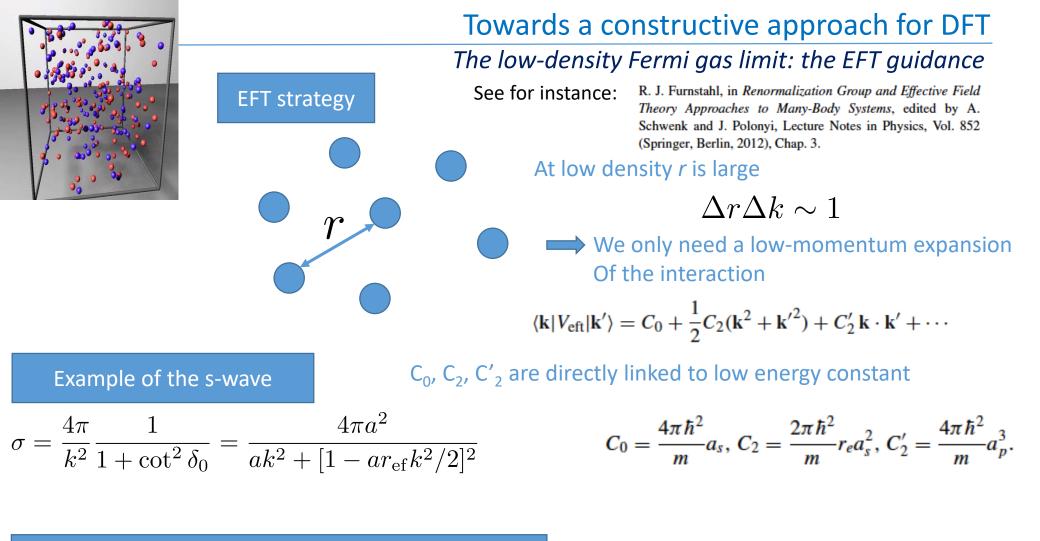
Scamps, Simenel, Lacroix, PRC 92 (2015) Tanimura, Lacroix, Scamps, PRC 92 (2015) Since we directly fit on experiments Complex correlation much beyond Hartree-Fock are included



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



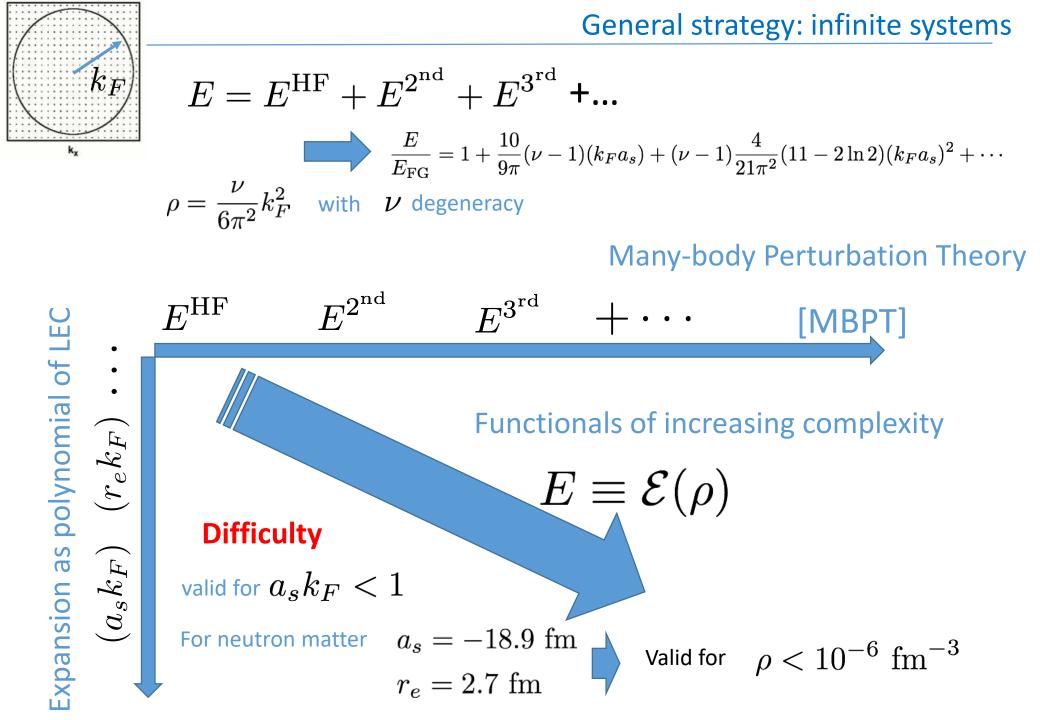
Can we link the energy density functional to the low energy constants of the bare interaction? and render it less empirical?



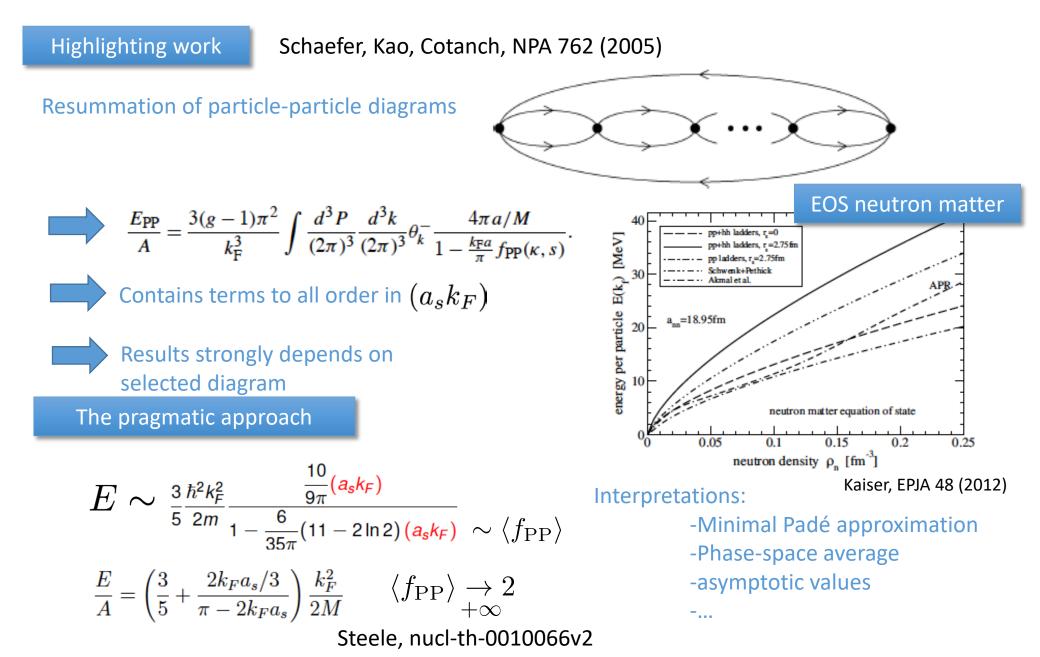
Constructive many-body perturbative approach

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

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



The "magic" technique: resummation



Resummed formula for Unitary gas

Great interest of resummed expression: 3000 It has a finite limit for Unitary gas 2000 scattering length (a) 1000 For unitary gas: -low density system -1000 $a_s \rightarrow +\infty$ -2000 -3000 $\frac{\frac{3}{5}\frac{\hbar^{2}k_{F}^{2}}{2m}}{1-\frac{6}{35\pi}(11-2\ln 2)(a_{s}k_{F})} =$ $\rightarrow 0.32 \frac{3}{5} \frac{\hbar^2 k_F^2}{2m}$ $=\langle f \rangle$ $\frac{E}{A} = \left(\frac{3}{5} + \frac{2k_F a_s/3}{\pi - 2k_F a_s}\right) \frac{k_F^2}{2M} \longrightarrow 0.4 \frac{3}{5} \frac{\hbar^2 k_F^2}{2m}$

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

220

B (gauss)

225

230

215

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

 $\mathcal{E}[\rho] = \xi \times \mathcal{E}_{FG}[\rho]$ $\xi = 0.37$ 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

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

 $|a_{\circ}k_{F}| \ll 1$

 $|a_s k_F| \gg 1$

$$\frac{E}{E_{\rm FG}} = 1 + \frac{10}{9\pi}(\nu - 1)(k_Fa_s) + \frac{(\nu - 1)\frac{4}{21\pi^2}(11 - 2\ln 2)(k_Fa_s)^2 + \cdots}{Adjusting \text{ only on low density}}$$

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

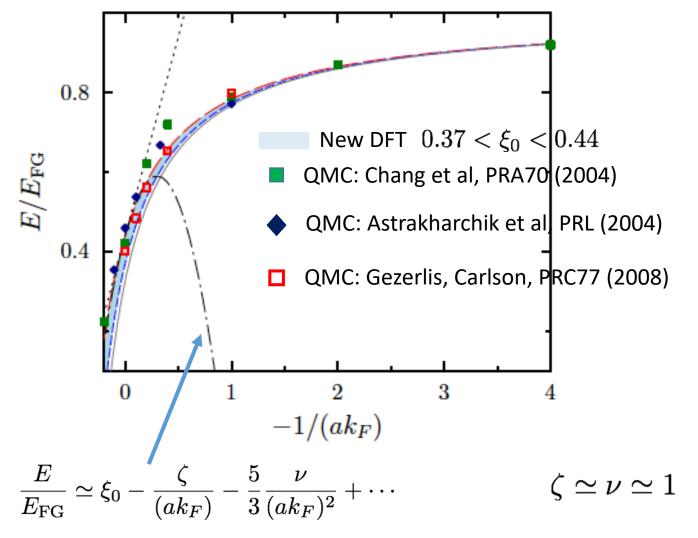
$$A_0A_1 = (\nu - 1)\frac{4}{21\pi^2}(11 - 2\ln 2)$$

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



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

Example of applications

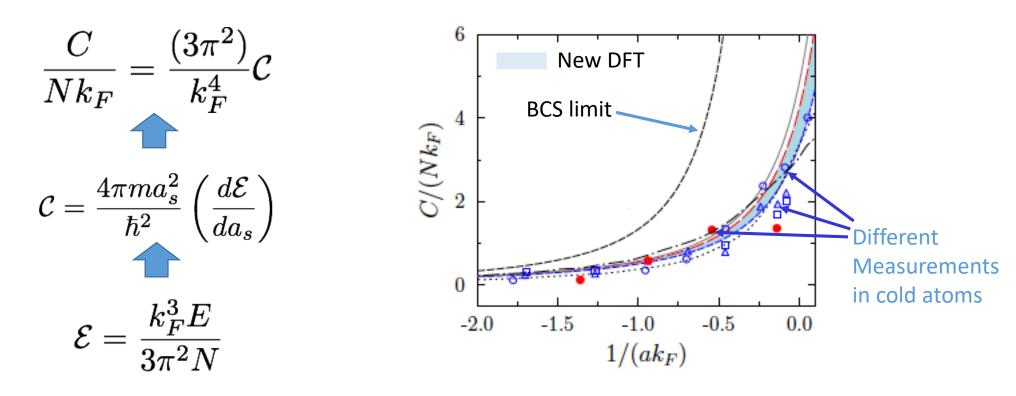
Lacroix, PRA 94 (2016)

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

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

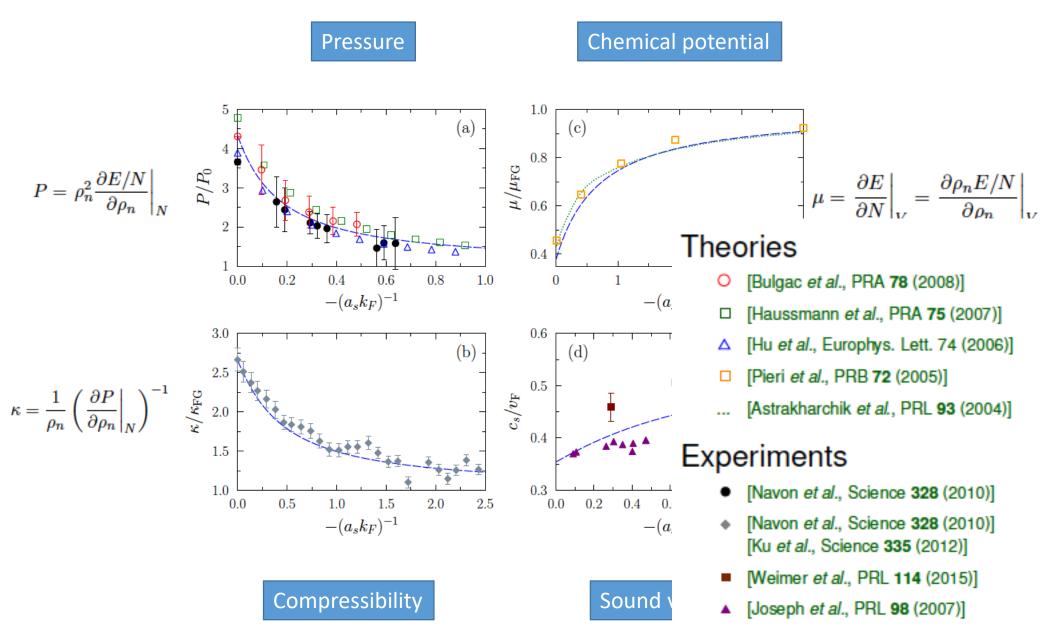
Estimate of the density dependence of the Tan contact parameter

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

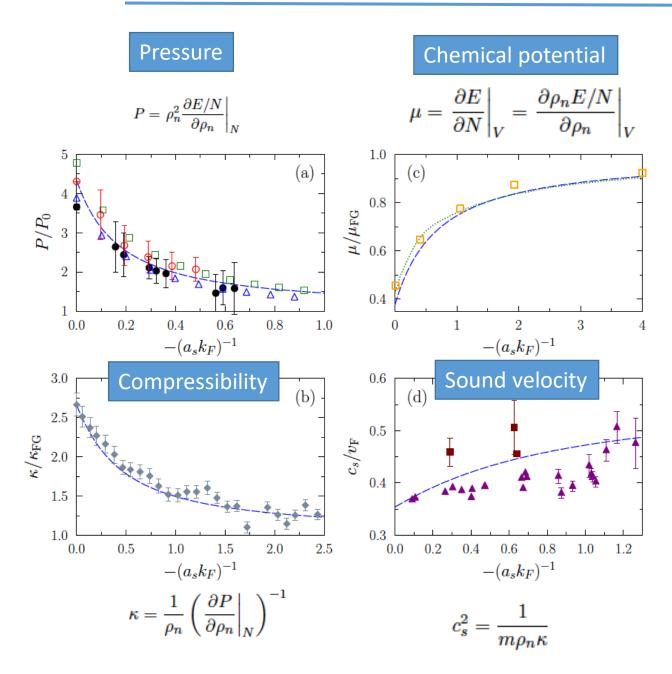


Example of applications: thermodynamical quantities around unitarity

Boulet, DL, Phys. Rev. C 97 (2018)



Example of applications: thermodynamical quantities around unitarity



Boulet, DL, Phys. Rev. C 97 (2018)

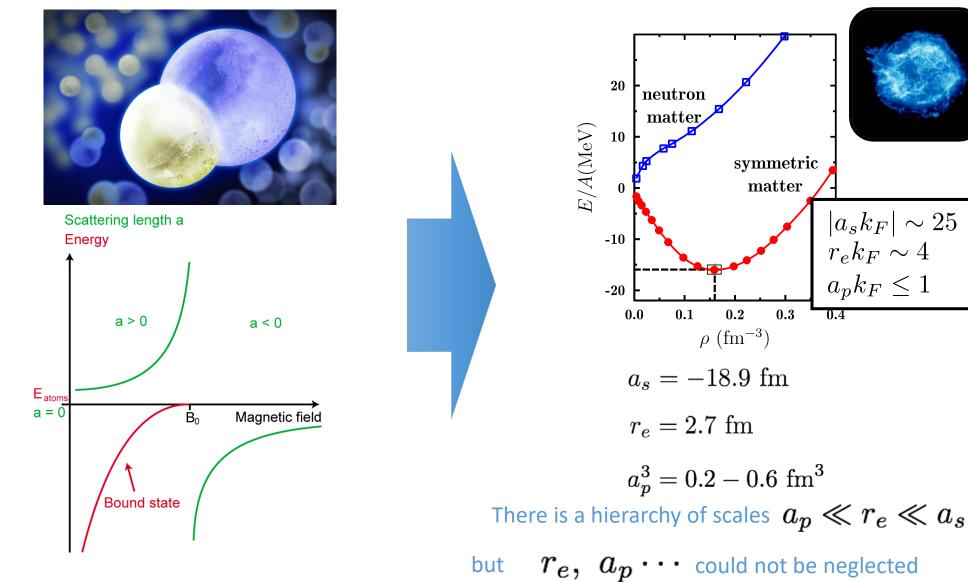
Theories

- [Bulgac et al., PRA 78 (2008)]
- [Haussmann et al., PRA 75 (2007)]
- △ [Hu et al., Europhys. Lett. 74 (2006)]
- [Pieri et al., PRB 72 (2005)]
- ... [Astrakharchik et al., PRL 93 (2004)]

Experiments

- [Navon et al., Science 328 (2010)]
- [Navon et al., Science 328 (2010)]
 [Ku et al., Science 335 (2012)]
- [Weimer et al., PRL 114 (2015)]
- ▲ [Joseph et al., PRL 98 (2007)]

From cold atom to neutron matter



Most often, only a_s matter

and $\,\,k_F\,\,$ is not small

From cold atom to neutron matter: inclusion of effective range

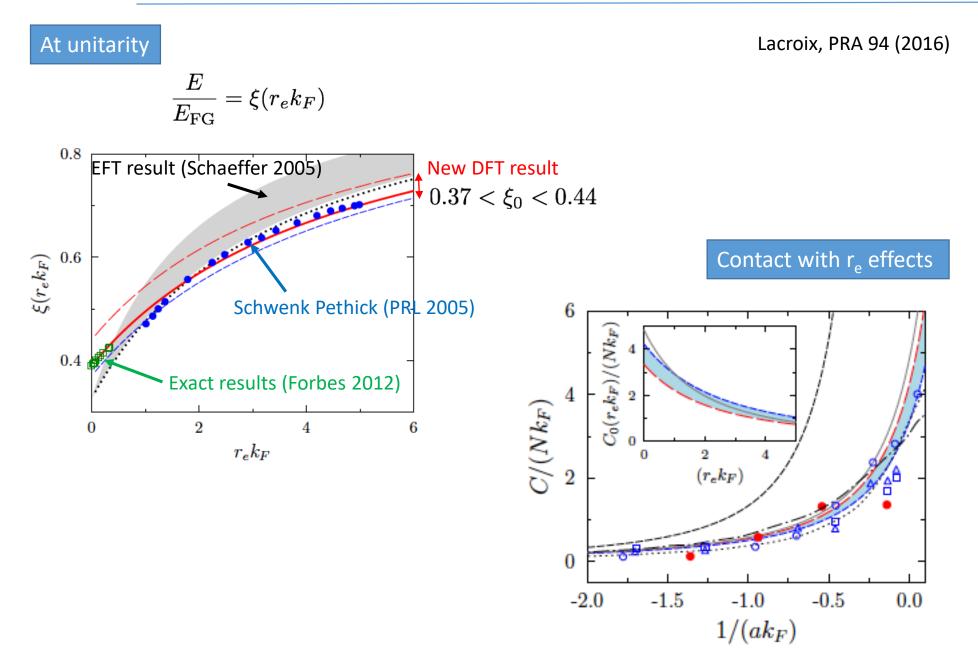
Lacroix, PRA 94 (2016)

$$\frac{E}{E_{\rm FG}} = 1 - \frac{U_0}{1 - (a_s k_F)^{-1} U_1} + \frac{R_0 (r_e k_F)}{[1 - R_1 (a_s k_F)^{-1}][1 - R_1 (a_s k_F)^{-1} + R_2 (r_e k_F)]} \qquad \text{Effective range part} (form obtained by resumming effective range effects in HF theory)}$$

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

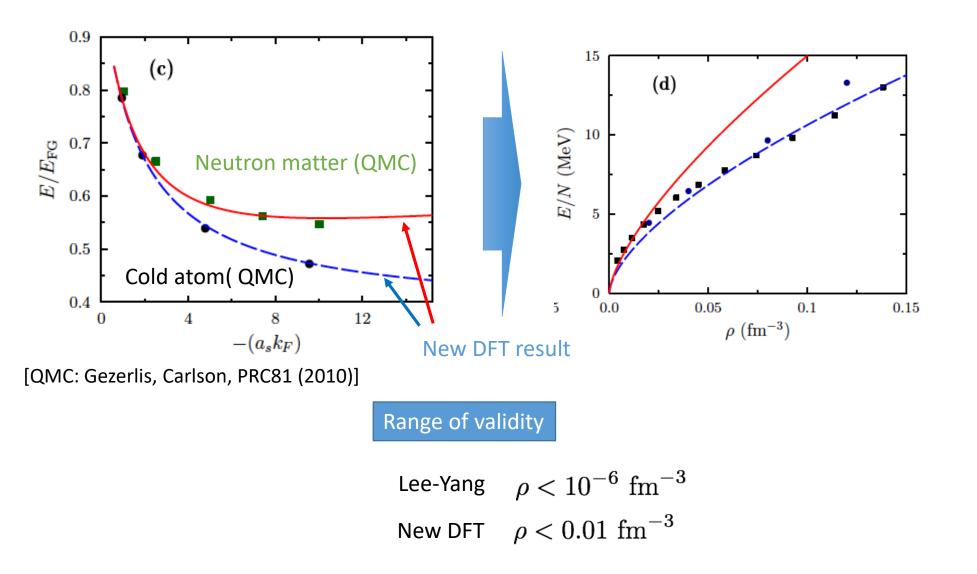
$$\frac{E}{E_{\rm FG}} 1 + \frac{10}{9\pi} (\nu - 1)(k_F a_s) + (\nu - 1) \frac{1}{6\pi} (k_F r_e)(k_F a_s)^2 + \cdots \qquad \xi(+\infty, r_e k_F) \equiv \xi_0 + (r_e k_F) \eta_e + (r_e k_F)^2 \delta_e$$
Forbes, Gandolfi, Gezerlis, PRA86 (2012)
$$U_0 = (1 - \xi_0) = 0.62400, \qquad \xi_0 = 0.376, \\U_1 = \frac{9\pi}{10} (1 - \xi_0) = 1.76432, \qquad \eta_e = 0.127 \\R_0 = \eta_e = 0.12700, \qquad \delta_e = -0.055 \\R_1 = \sqrt{\frac{6\pi\eta_E}{(\nu - 1)}} = 1.54722, \\R_2 = -\delta_e/\eta_e = 0.43307.$$

Inclusion of effective range effects in cold atoms

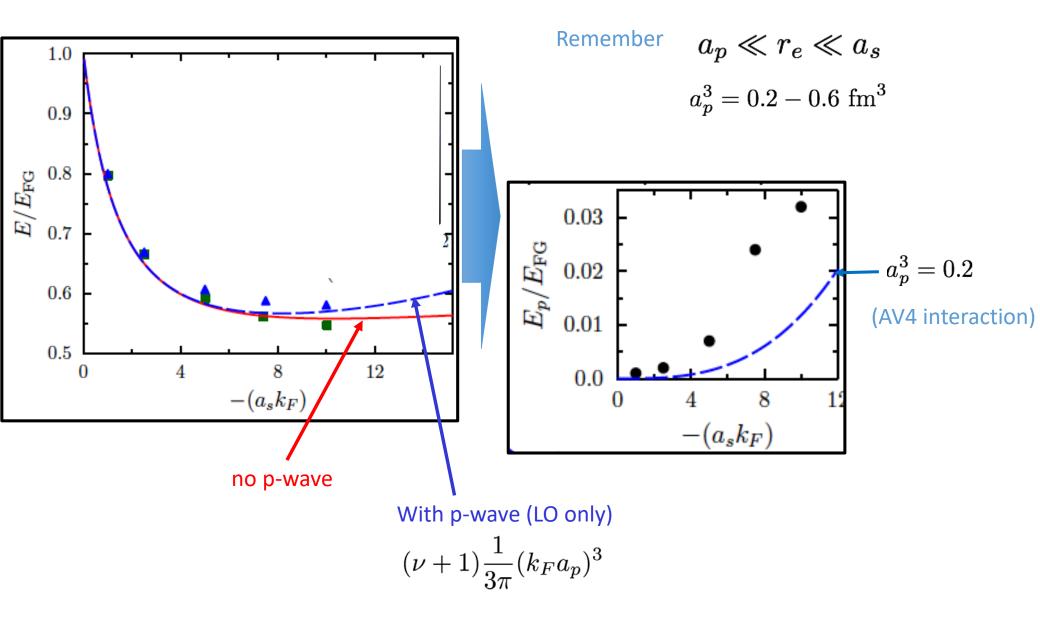


EDF with no-free parameters: Predictive power for neutron matter

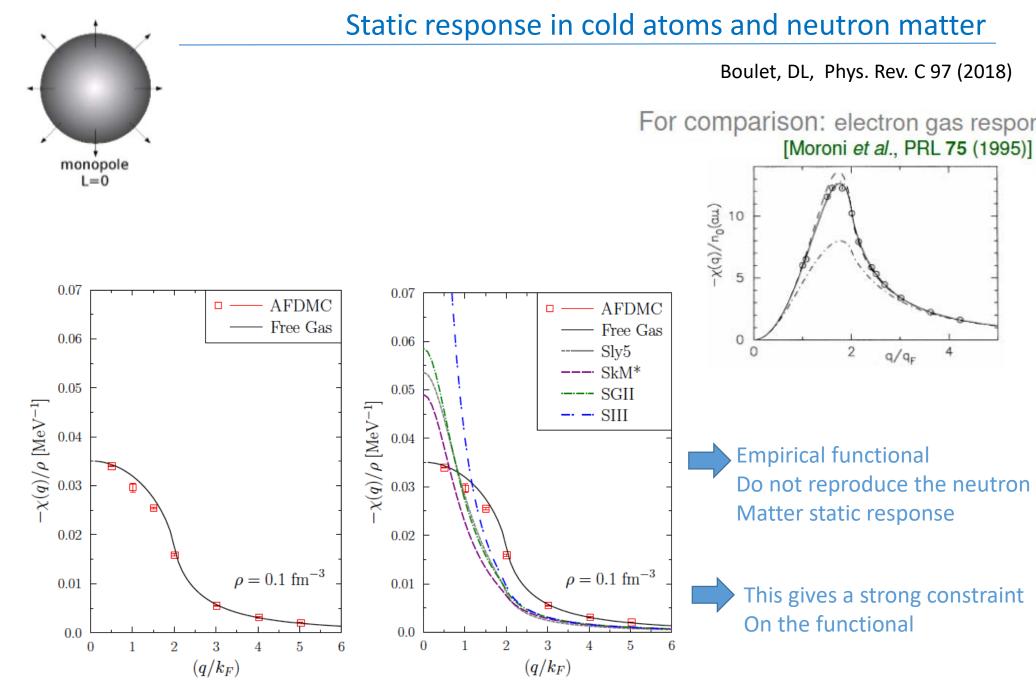
Lacroix, Boulet, Grasso, Yang, PRC 95 (2017)



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



From static to dynamic



[Buraczynski and Gezerlis, PRL 116 (2016)]

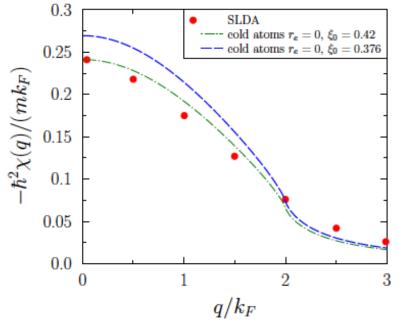
Static response in cold atoms and neutron matter

Boulet, DL, Phys. Rev. C 97 (2018)

External field

$$\hat{V}_{\text{ext}} = \sum_{j} \phi(\boldsymbol{q}, \omega) e^{i \mathbf{q} \cdot \mathbf{r}_{j} - i \omega t}$$

Comparison with Superfluid LDA (Bulgac et al) in cold atoms



SLDA: [Forbes and Sharma, PRA 90 (2014)]

Assuming
$$m^* = m$$

Response function χ

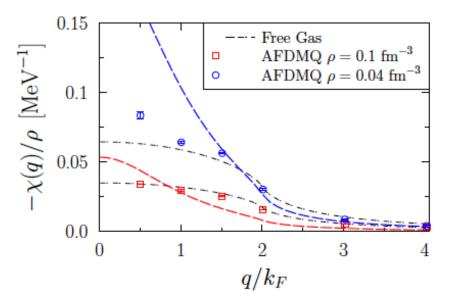
$$\rho(\mathbf{r}) \equiv \rho \to \rho + \delta \rho$$

$$\delta \rho = -\chi(\boldsymbol{q}, \omega) \phi(\boldsymbol{q}, \omega)$$
$$\chi = \chi_0 \left[1 - \frac{\delta^2 \mathcal{V}}{\delta \rho^2} \chi_0 \right]^{-1}$$

$$E = \int d\mathbf{r} \left(\underbrace{\mathcal{K}[\rho(\mathbf{r})]}_{kinetic} + \underbrace{\mathcal{V}[\rho(\mathbf{r})]}_{interaction} \right)$$

Boulet, DL, Phys. Rev. C 97 (2018)

Empirical functional (Sly5)

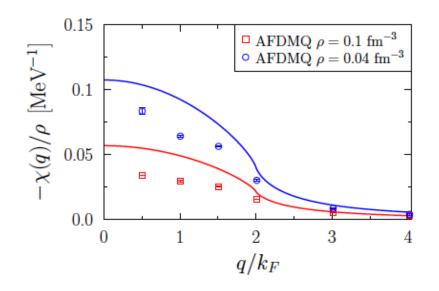


[Buraczynski and Gezerlis, PRL 116 (2016)]

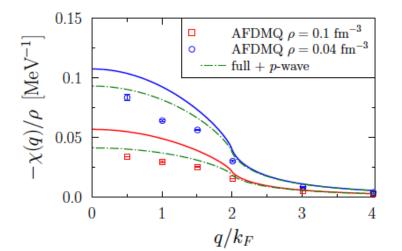
Adding *p*-wave (leading order term only)

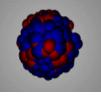
$$\frac{E_p}{E_{\rm FG}} = \frac{1}{\pi} (a_p k_F)^3$$

Non-empirical functional



Non-empirical functional + *p*-wave

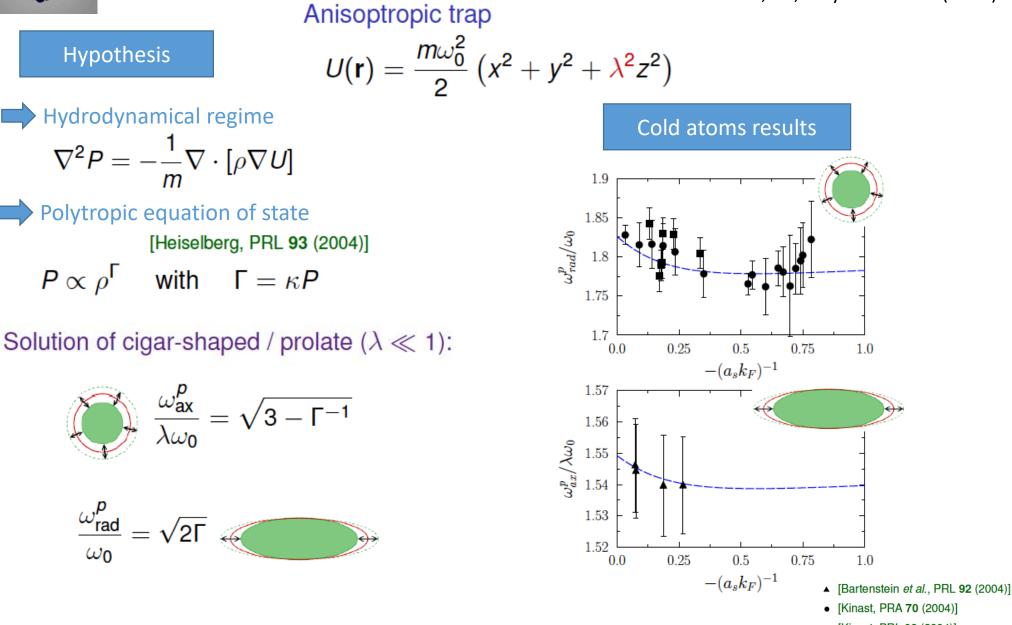




ωn

Dynamical response in cold atoms and neutron matter

Boulet, DL, Phys. Rev. C 97 (2018)



[Kinast, PRL 92 (2004)]



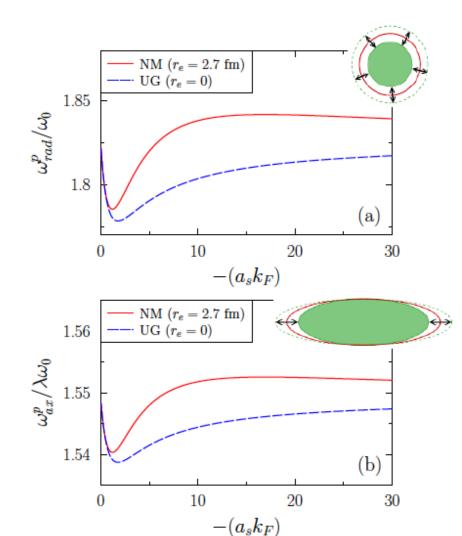
Dynamical response in cold atoms and neutron matter

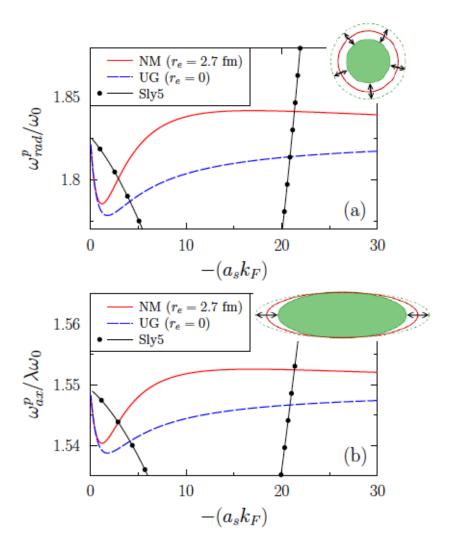
Neutron matter

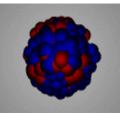
Boulet, DL, Phys. Rev. C 97 (2018)

$$U(\mathbf{r}) = \frac{m\omega_0^2}{2} \left(x^2 + y^2 + \lambda^2 z^2 \right)$$

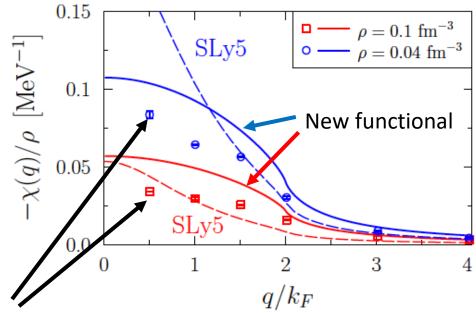
Anisoptropic trap



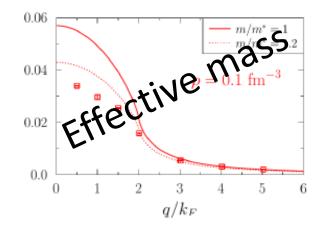




Static response of neutron matter



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

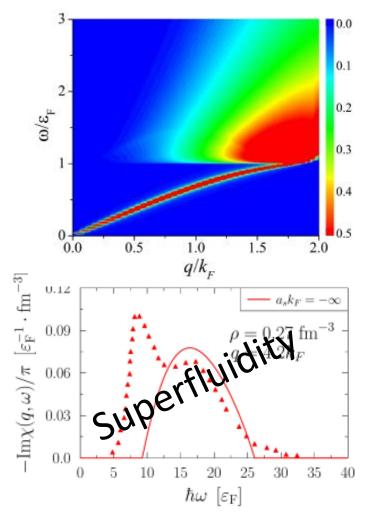


Superfluidity and effective mass

Boulet, DL, Phys. Rev. C 97 (2018)

Dynamical response (atomic gases)

[S. Hoinka et al., PRL 109, 050403 (2012)]



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

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 $ho < 0.01 \ {\rm fm}^{-3}$

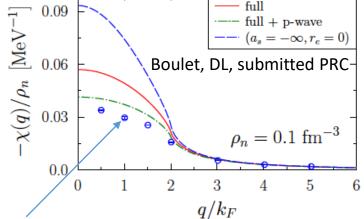
The new DFT reproduces ab-initio results in cold atoms and neutron matter

Transition from s-wave driven (low density) to unitary gas driven (Bertsch parameter) regime

Link between non-empirical and empirical DFT

Applications and on-going work

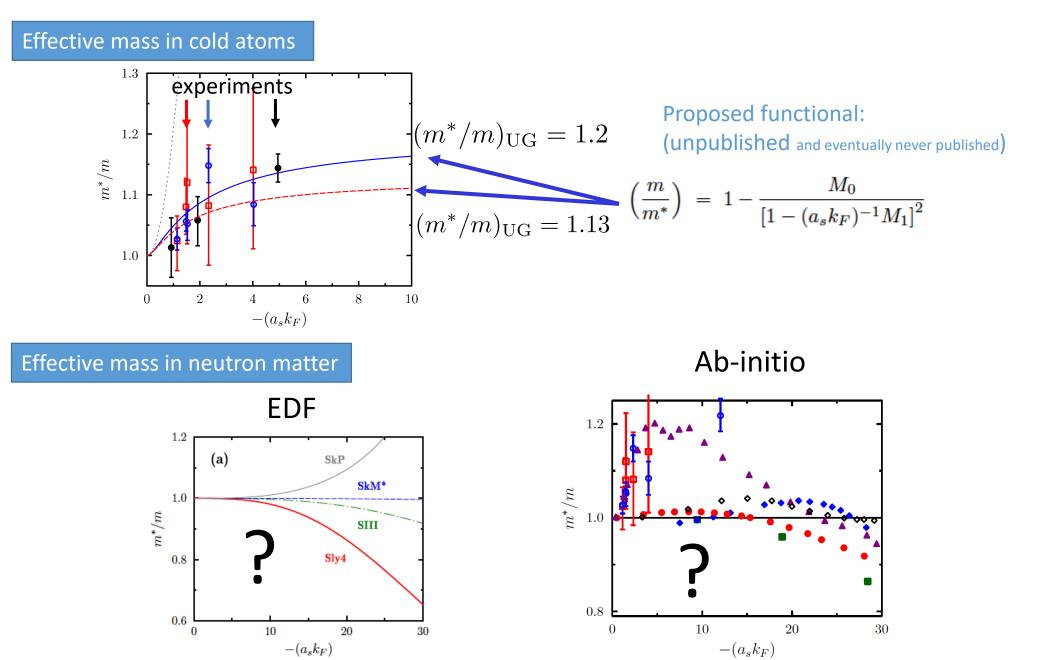




AFDMC: Buraczynski, Gezerlis, PRL 116 (2016)]

Some Opportunities: cross-fertilization between atomic and nuclear physics

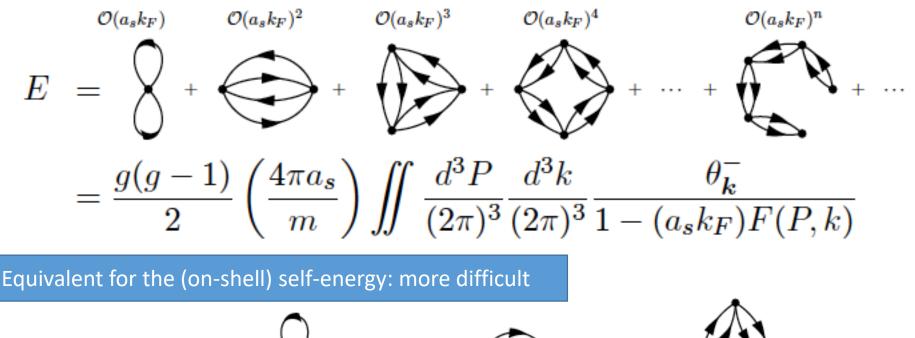
Some Fermi liquid properties are scarcely known: effective mass, ...

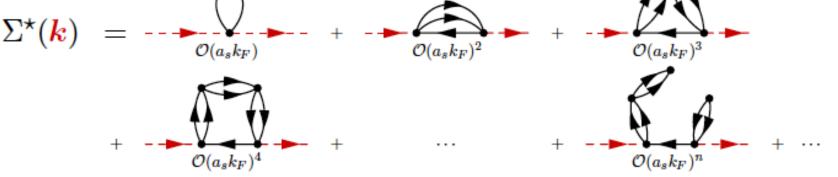


Some follow up: Fermi liquid or non-Fermi liquid

theory of strongly interacting systems

Resummation technique for the energy





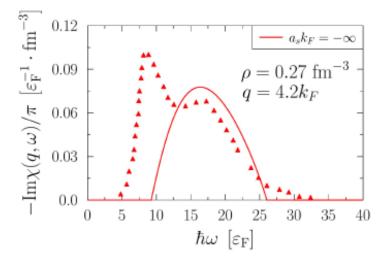
(courtesy A. Boulet)

Odd-even effects in nuclei

Dynamical response in neutron matter and cold atoms, vortices, ...

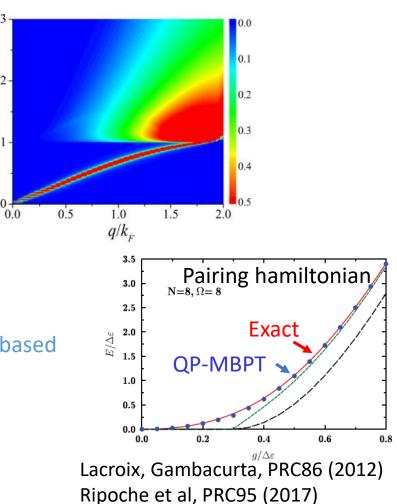
2

 ω/ϵ_F

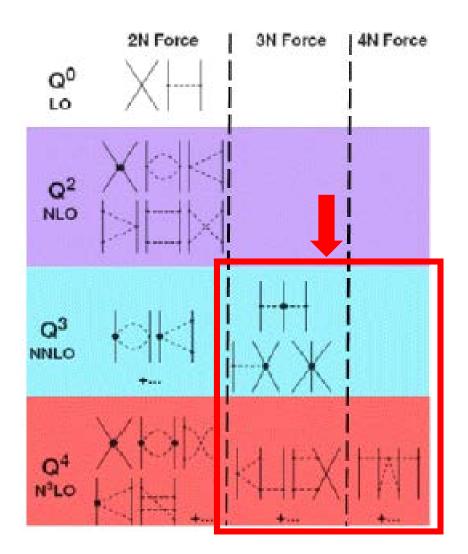


[P. Zou et al., New J. Phys. 18, 113044 (2016)]

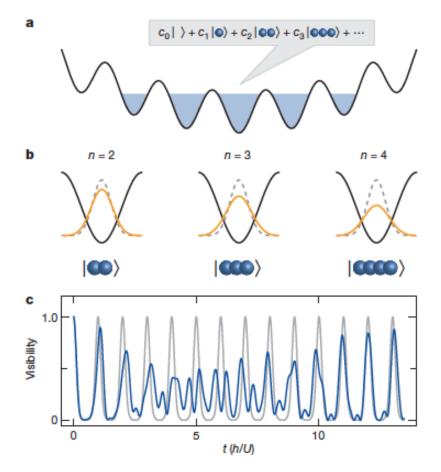
Towards a *resummation technique with pairing* based on MBPT of quasi-particles? Green-Gorkov, ...



Nucleon-nucleon interaction from chiral EFT

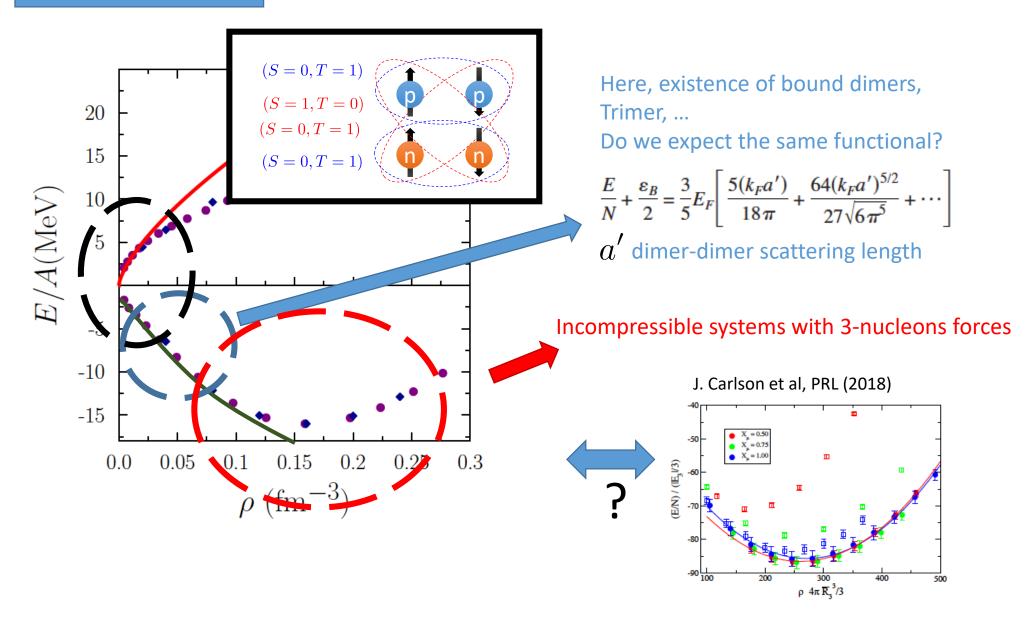


Systems with tunable multi-body interaction Can now be formed on a lattice

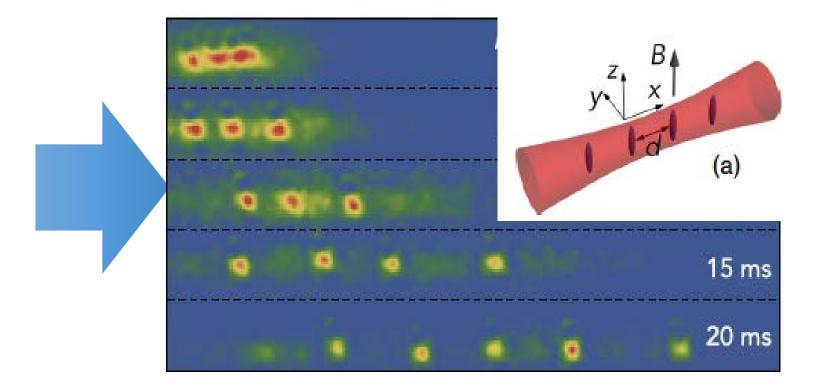


S. Will et al, Nature (2010)

Some common interest



Quantum droplet physics



Ferrier-Barbut, PRL 116, (2016)

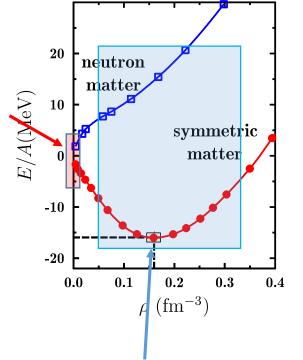
Additional discussion

Difficulty in nuclear systems

Yang, Grasso, Lacroix PRC94 (2016)

Skyrme functional

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



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

Additional remarks on traditional Skyrme

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

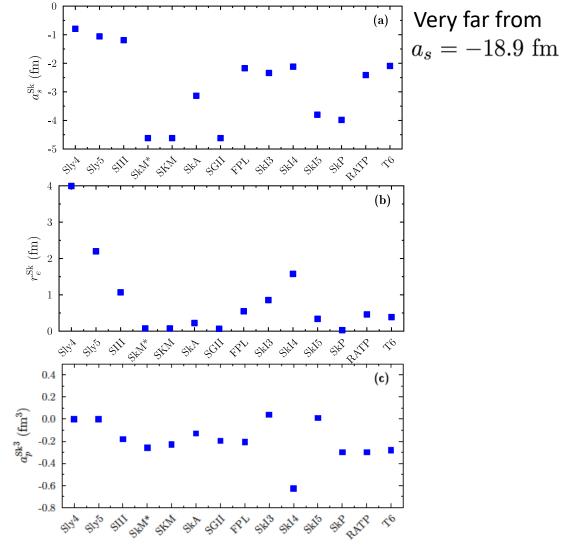
Due to the analogy, one can define equivalent low energy constant

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

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

$$C'_2 = t_2(1 + x_2) = \frac{4\pi\hbar^2}{m}a_p^3.$$

See discussion in Furnstahl, EFT for DFT (2007)



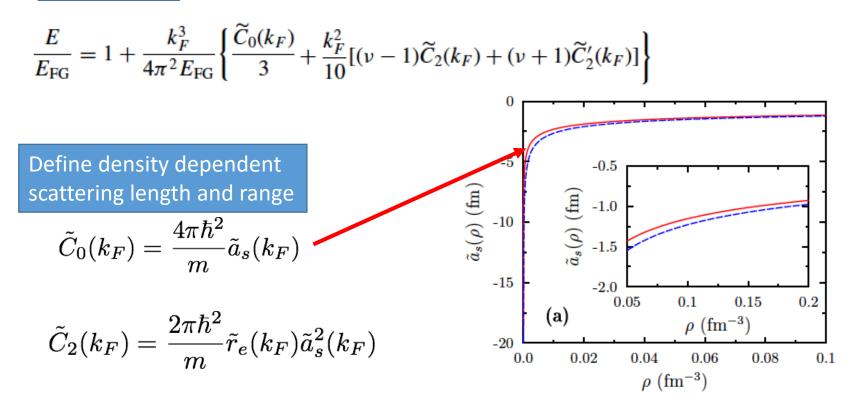
Can we make contact with Skyrme like empirical functional ?

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

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

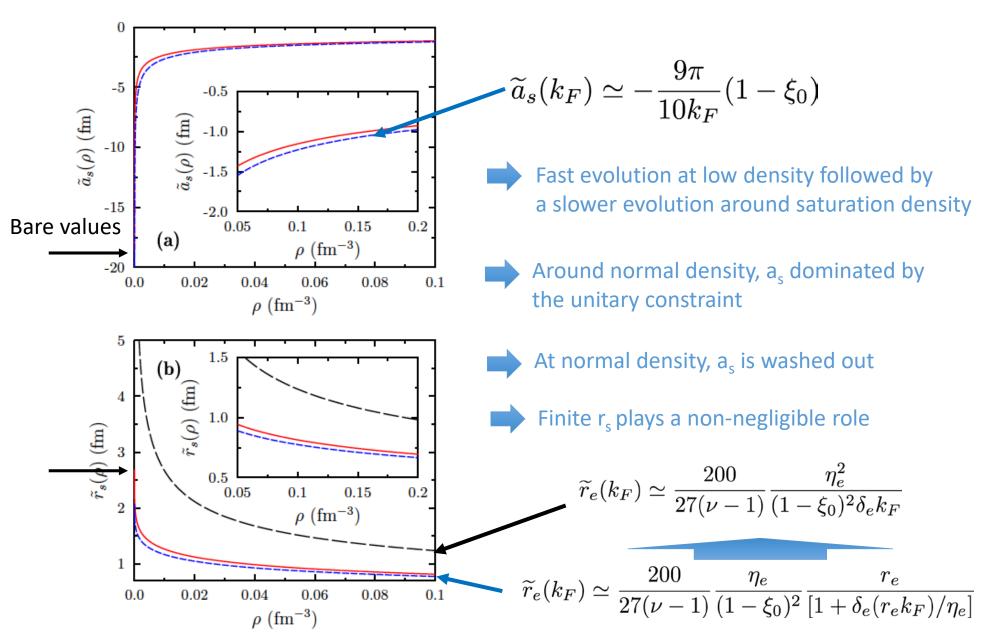


Starting point

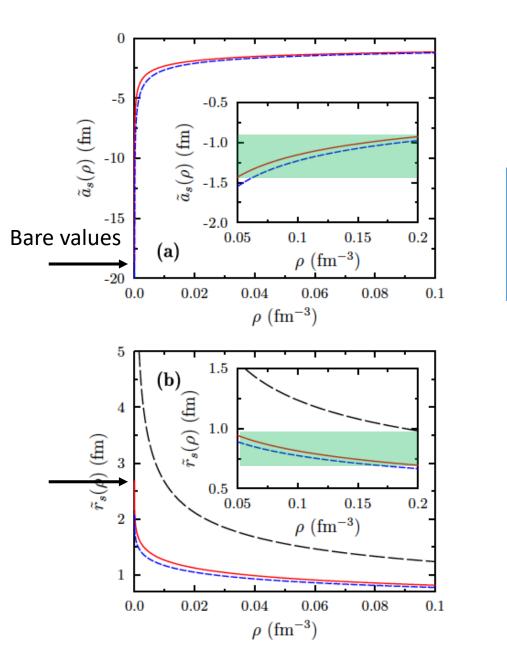


Can we make contact with empirical functional ?

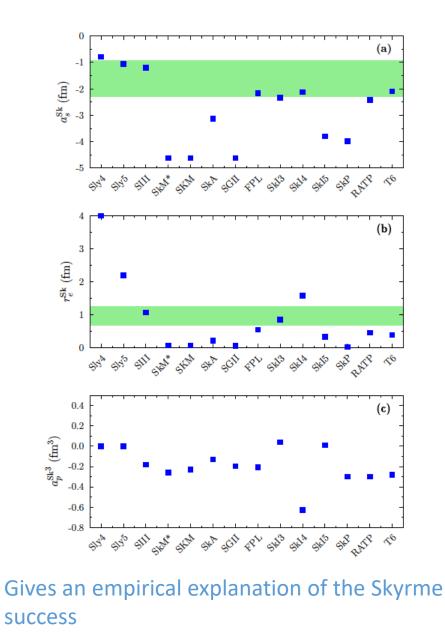
Lacroix, Boulet, Grasso, Yang, PRC 95 (2017)



Can we make contact with empirical functional ?



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



Backup

Resummation of effective range effect in the HF theory

Assume a gaussian interaction
$$v(\mathbf{r}_1, \mathbf{r}_2) = \left\{ v_0 + v_\sigma P_\sigma \right\} \frac{e^{-(r^2/\mu^2)}}{(\mu\sqrt{\pi})^3}$$

 $\frac{E_G^{(1)}}{N} = \frac{\rho}{2} \left[A - BF\left(\mu k_F\right) \right]$

HF energy

with

$$F(x) = \frac{12}{x^6}(1 - e^{-x^2}) + \frac{6}{x^4}(e^{-x^2} - 3) + \frac{6\sqrt{\pi}}{x^3}\operatorname{Erf}(x)$$

Low density expansion is recovered if:

$$A = -\frac{2\hbar^2 \pi}{\nu m \mu^2} [(\nu - 1)r_e a_s^2 - 2(\nu + 1)a_p^3]$$

$$B = +\frac{2\hbar^2 \pi}{\nu m \mu^2} [(\nu - 1)r_e a_s^2 + 2(\nu + 1)a_p^3]$$

$$\mu^2 = -(r_e a_s)$$

