

Density Functional Theory based on bare interaction

From ultra-cold atoms to nuclear matter

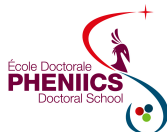
Antoine BOULET

1st year PhD student (2016–2019)

Supervisor: Denis LACROIX

Theory group, IPN Orsay

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Outline

- ▶ Introduction: DFT, EFT, interactions, etc
- ▶ Cold atoms and unitary: link with Neutron Matter
- ▶ Build a functional density based on the LEC (a_s, r_e, \dots)
- ▶ Some results in cold atoms (thermodynamic + linear response)
- ▶ From cold atoms to Neutron Matter case
- ▶ Conclusion and outlooks

Strongly correlated Fermions in infinite matter

Density Functional Theory (DFT) vs. Effective Field Theory (EFT)

DFT (Kohn-Sham, etc.)

$$\underbrace{|\psi_{1,\dots,N}\rangle}_{N\text{-body}} \mapsto \underbrace{\rho \mapsto E[\rho]}_{1\text{-body}}$$

Nuclear DFT (Hartree-Fock like)

$$E[\rho] = \langle \psi[\rho] | T + V_{\text{eff}} | \psi[\rho] \rangle$$

$$V_{\text{eff}} = t_0(1 + x_0 P_\sigma) + t_3(1 + x_3 P_\sigma) \rho^\beta$$

$\rho = \nu / (6\pi^2) k_F^3$ density

k_F Fermi momentum

ν degeneracy

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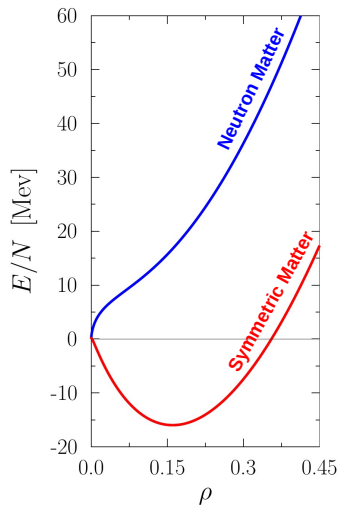
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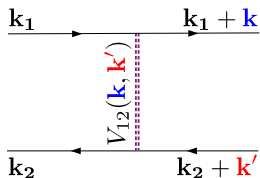
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EFT at low density (only s-scattering wave)

$$\langle \mathbf{k} | V_{12}^{(EFT)} | \mathbf{k}' \rangle = \frac{4\pi}{m} \left[a_s + \frac{r_e a_s^2}{4} (\mathbf{k}^2 + \mathbf{k}'^2) \right]$$

$$E(a_s k_F, r_e k_F) = E^{(1)} + E^{(2)} + \dots$$

a_s : s-wave scattering length

r_e : s-wave effective range

Neutron Matter:

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

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

How to relate low energy constants
(a_s, r_e, \dots) to density functionals?

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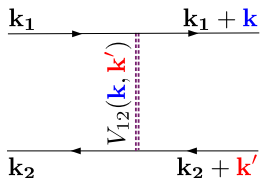
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New insight from ultra-cold atoms at unitary

Universality properties of strongly correlated fermions

$$\psi(r) \underset{r \rightarrow \infty}{\sim} \frac{e^{\delta(k)}}{kr} \sin(kr + \delta(k))$$

$$\lim_{k \rightarrow 0} k \cot \delta(k) = -\frac{1}{a_s} + r_e k^2$$

BEC regime ($a_s > 0$)

BCS regime ($a_s < 0$)

- ▶ When $a_s \rightarrow \pm\infty$ and $\rho \rightarrow 0$, the potential details has no influence: **Universality**

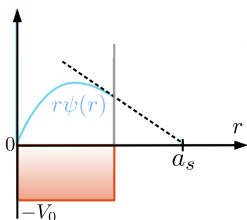
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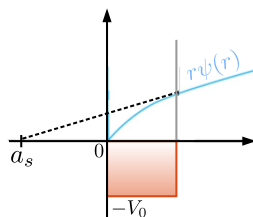
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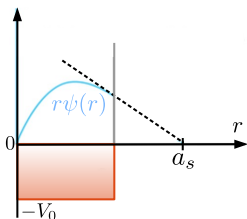
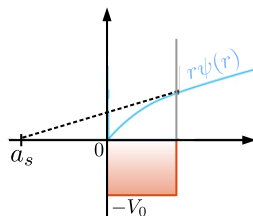
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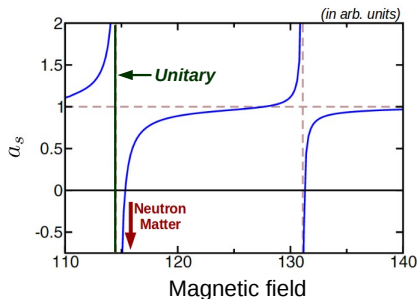
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Physical scales of interest

- ▶ At unitary: $a_s \rightarrow \pm\infty$ (in neutron matter, $a_s = -18.9$ fm).



[S. Kotochigova, Rep. Prog. Phys. **77** (9), 2015]

DFT at unitary ($r_e k_F$ expansion)

$$\frac{E[\rho]}{E_{FG}} = \xi_0 + (r_e k_F) \eta_e + (r_e k_F)^2 \delta_e$$

$\xi_0 \simeq 0.37$: Bertsch parameter

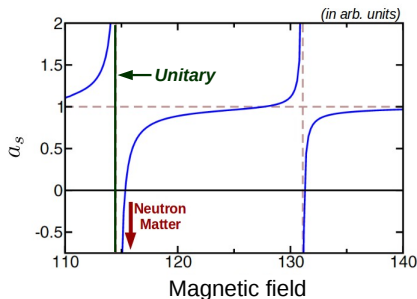
$$E_{FG} = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m}: \text{Free Gas energy}$$

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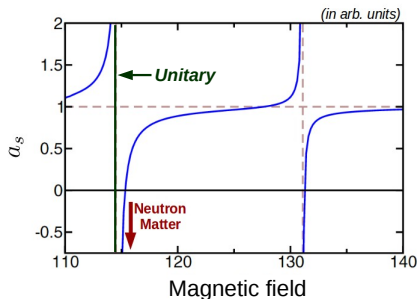
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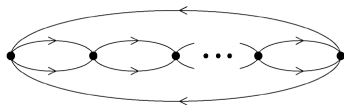
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New type of functional without free parameters

Resummation inspired by EFT

Particle-particle ladder diagrams contribution:



$$\frac{E_{pp}}{N} = \frac{4\pi\hbar^2 a_s}{m} \frac{3\pi^2}{k_F^3} \int \frac{d^3P}{(2\pi)^3} \frac{d^3k}{(2\pi)^3} \frac{\theta_k}{1 - (a_s k_F) f(k, P)}$$

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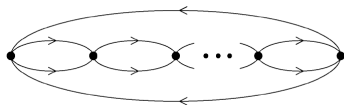
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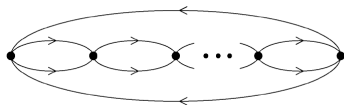
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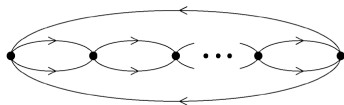
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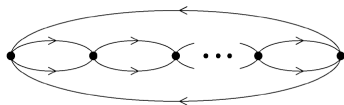
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Unitary limit

$$(a_s k_F \rightarrow -\infty, r_e k_F \ll 1)$$

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[D. Lacroix, PRA **94**, 043614 (2016)][D. Lacroix, **A.B. et al.**, PRC **95**, 054306 (2017)]

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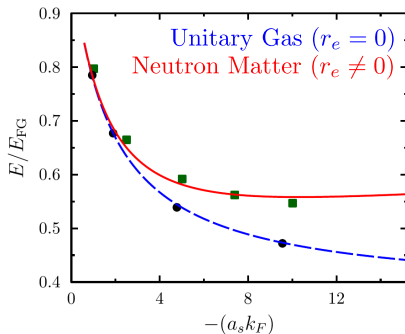
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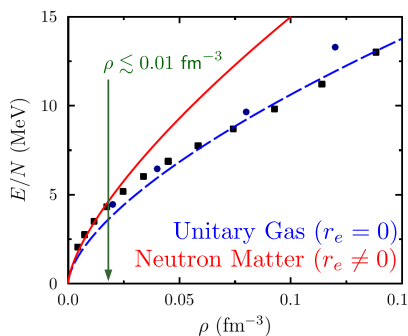
Comparison of energy with *ab initio* calculations

Low density



- [A. Gezerlis and J. Carlson, PRC **81**, 025803 (2010)]
- [J. Carlson, S. Gandolfi and A. Gezerlis, Prog. Theor. Exp. Phys. 01A209 (2012)]

Up to saturation density



- [A. Akmal, V. R. Pandharipande and D. G. Ravenhall, PRC **58**, 1804 (1998).]
- [B. Friedman and V. Pandharipande, Nucl. Phys. **A361**, 502 (1981)]

Some thermodynamical quantities

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

(FG : Free Gas)

$$P \equiv \rho^2 \frac{\partial E/N}{\partial \rho} \quad \frac{1}{\kappa} \equiv \rho \frac{\partial P}{\partial \rho}$$

$$\mu \equiv \frac{\partial \rho E/N}{\partial \rho} \quad \rho = \frac{k_F^3}{3\pi^2}$$

Pressure P

$$\frac{P}{P_{FG}} = \xi + \frac{k_F}{2} \frac{\partial \xi}{\partial k_F}$$

Chemical potential μ

$$\frac{\mu}{\mu_{FG}} = \xi + \frac{k_F}{5} \frac{\partial \xi}{\partial k_F}$$

Compressibility κ

$$\frac{\kappa_{FG}}{\kappa} = \xi + \frac{4k_F}{5} \frac{\partial \xi}{\partial k_F} + \frac{k_F^2}{10} \frac{\partial^2 \xi}{\partial k_F^2}$$

Sound velocity c_s

$$\left(\frac{c_s}{c}\right)^2 = (m\rho\kappa)^{-1}$$

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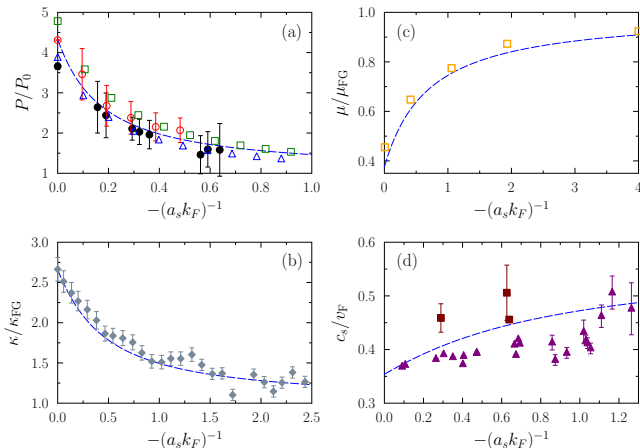
$$\frac{\kappa_{FG}}{\kappa} = \xi + \frac{4k_F}{5} \frac{\partial \xi}{\partial k_F} + \frac{k_F^2}{10} \frac{\partial^2 \xi}{\partial k_F^2}$$

Sound velocity c_s

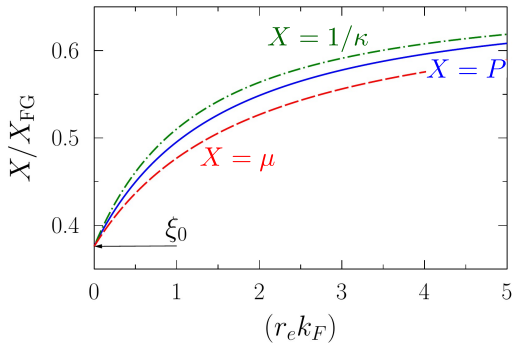
$$\left(\frac{c_s}{c}\right)^2 = (m\rho\kappa)^{-1}$$

Ultra-cold atoms results ($r_e = 0$) near unitary

Comparison between experimental and theoretical data



[A.B. and D. Lacroix, *in preparation*]

Effect of effective range at unitary ($a_s = -\infty$)[A.B. and D. Lacroix, *in preparation*]

Linear response theory in a nutshell

RPA formalism for infinite matter

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

Response function χ

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

$$\delta\rho = -\chi(q, \omega)\phi(q, \omega)$$

$$\chi = \chi_0 \left[1 - \frac{\delta^2 \mathcal{V}}{\delta \rho^2} \chi_0 \right]^{-1}$$

External field

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

Static response function

$$\chi(q) = \lim_{\omega \rightarrow 0} \chi(q, \omega)$$

Compressibility sum-rule

$$\lim_{q \rightarrow 0} \chi(q) = -\rho^2 \kappa$$

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Static response function

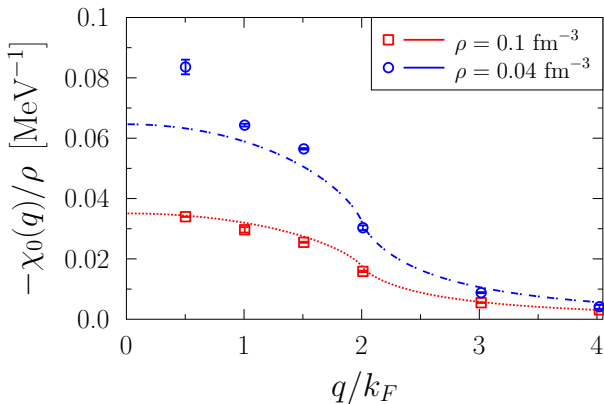
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Linear static response function for neutron matter ($r_e = 2.7$ fm)

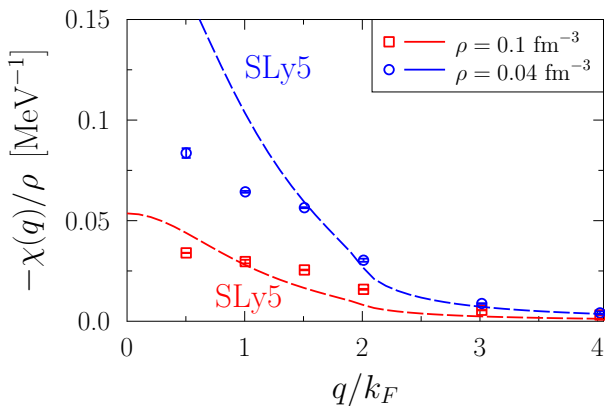
Comparison with recent QMC calculation



[M. Buraczynski and A. Gezerlis, PRL **116**, 152501 (2016)]
 [A.B. and D. Lacroix, *in preparation*]

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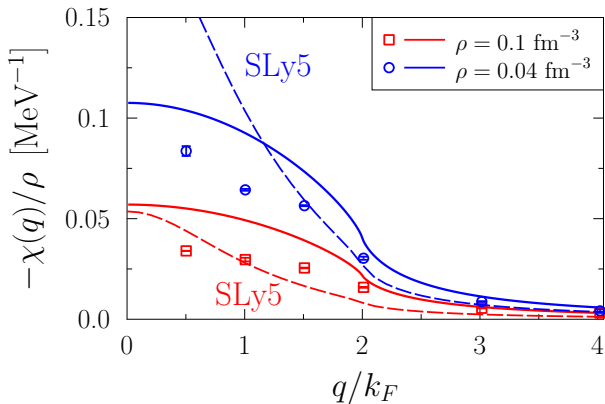
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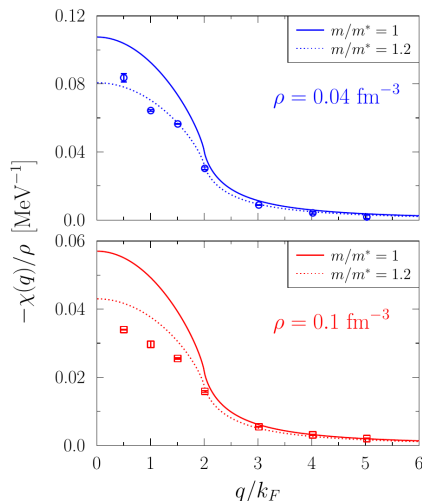
Comparison with recent QMC calculation



[M. Buraczynski and A. Gezerlis, PRL **116**, 152501 (2016)]
 [A.B. and D. Lacroix, *in preparation*]

Effective mass influence on the static response

Density independent effective mass case



Role of pairing and superfluidity on the dynamical response

Come back to unitary gas ($a_s \rightarrow -\infty$ and $r_e = 0$)

Dynamical external field

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

Response function

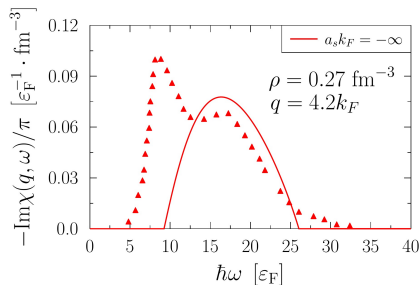
$$\chi(\mathbf{q}, \omega) = \frac{\chi_0(\mathbf{q}, \omega)}{1 - \frac{\delta^2 \mathcal{V}}{\delta \rho^2} \chi_0(\mathbf{q}, \omega)}$$

Role of pairing and superfluidity on the dynamical response

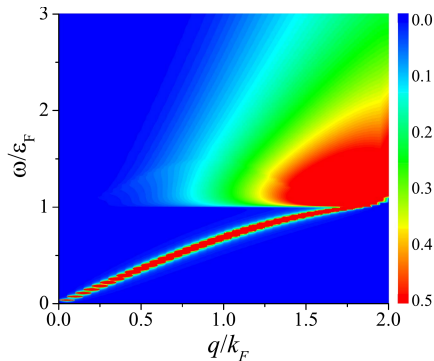
Come back to unitary gas ($a_s \rightarrow -\infty$ and $r_e = 0$)

Dynamical response

$$\hat{V}_{\text{ext}}(\mathbf{q}, \omega) \mapsto \chi(\mathbf{q}, \omega)$$



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



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

Summary

- ▶ A **functional without free parameters** was recently proposed and reproduce thermodynamical properties of cold atoms (without effective range)
- ▶ The functional reproduce the QMC results at low density ($\rho \lesssim 0.01 \text{ fm}^{-3}$) for Neutron Matter taking in account the effect of **effective range**
- ▶ The static response reproduce reasonably (better than phenomenological EDF) the recent QMC calculations
- ▶ **Short-term Outlook**
 - ▶ Include the **effective mass** effect
 - ▶ Include the **pairing** in the functional
 - ▶ Application to finite **Quantum Droplet** (statics and dynamics)
- ▶ **Long-term Outlook**
 - ▶ Extend the theory to **Symmetric Matter** and **finite nuclei**
 - ▶ Study more precisely the **BEC-BCS crossover**