# Density Functional Theory based on bare interaction

## From ultra-cold atoms to nuclear matter

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$1^{st}$ year PhD student (2016–2019)
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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 ($a_s$, $r_e$, . . . )
- 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.)**

$$\underbrace{|\psi_{1,\ldots,N}\rangle}_{N-body} \longmapsto \underbrace{\rho \longmapsto E[\rho]}_{1-body}$$

**Nuclear DFT (Hartree-Fock like)**

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

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

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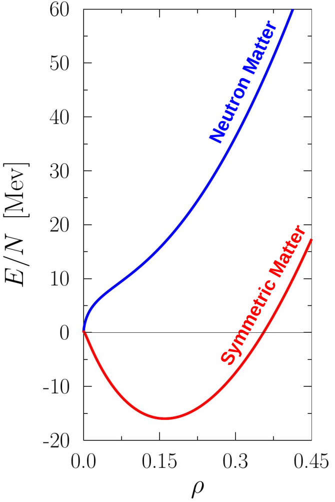

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**EFT at low density (only $s$-scattering wave)**

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

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

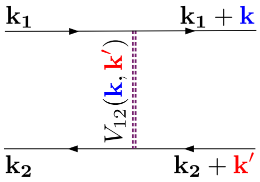
$a_s$: $s$-wave scattering length

$r_e$: $s$-wave effective range

Neutron Matter:

$a_s = -18.9$ fm

$r_e = 2.7$ fm

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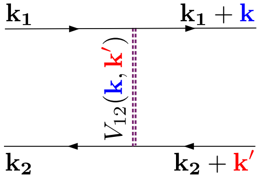


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## New insight from ultra-cold atoms at unitary

### Universality properties of strongly correlated fermions

$$\psi(r) \underset{r\to\infty}{\sim} \frac{e^{\delta(k)}}{kr} \sin\left(kr + \delta(k)\right) \qquad \lim_{k\to 0} k \cot\delta(k) = -\frac{1}{a_s} + r_e k^2$$

BEC regime ($a_s > 0$)

BCS regime ($a_s < 0$)

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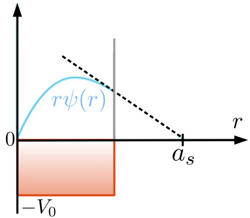


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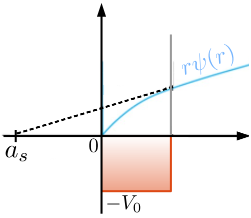


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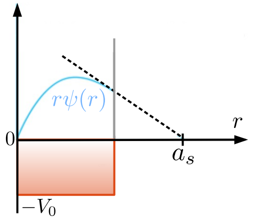


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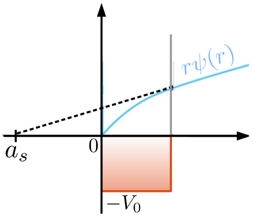


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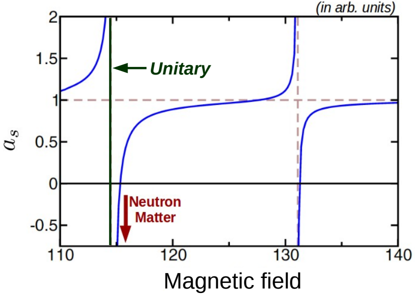


[S. Kotochigova, Rep. Prog. Phys. **77** (9), 2015]

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

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

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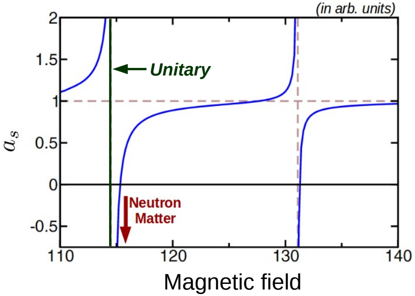


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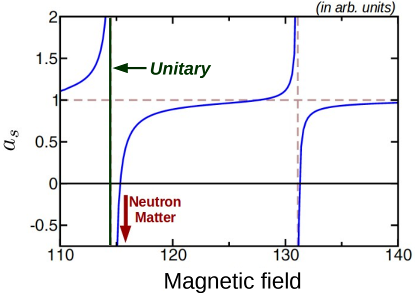


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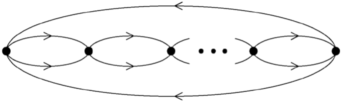
## New type of functional without free parameters

### Resummation inspired by EFT

# Particle-particle ladder diagrams contribution:



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\begin{aligned}
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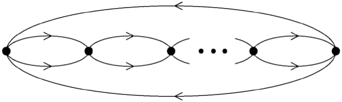

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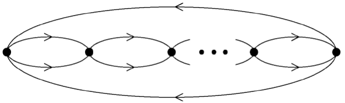

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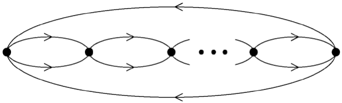

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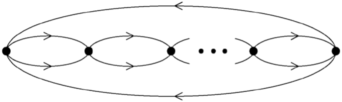

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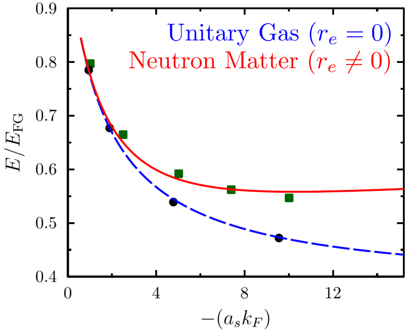
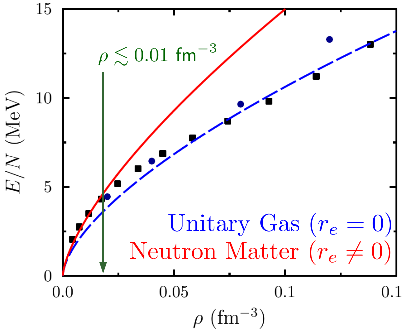
## Comparison of energy with *ab initio* calculations

### 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. A**361**, 502 (1981)]

## Some thermodynamical quantities

$$\frac{E}{E_{FG}} = \xi(a_s k_F, r_e k_F) \qquad \text{(FG : Free Gas)}$$

$$P \equiv \rho^2 \frac{\partial E/N}{\partial \rho} \qquad \frac{1}{\kappa} \equiv \rho \frac{\partial P}{\partial \rho} \qquad \mu \equiv \frac{\partial \rho E/N}{\partial \rho} \qquad \rho = \frac{k_F^3}{3\pi^2}$$

**Pressure $P$**

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

**Chemical potential $\mu$**

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

**Compressibility $\kappa$**

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

**Sound velocity $c_s$**

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

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$$P \equiv \rho^2 \frac{\partial E/N}{\partial \rho} \qquad \frac{1}{\kappa} \equiv \rho \frac{\partial P}{\partial \rho} \qquad \mu \equiv \frac{\partial \rho E/N}{\partial \rho} \qquad \rho = \frac{k_F^3}{3\pi^2}$$

### Pressure $P$

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

### Chemical potential $\mu$

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

### Compressibility $\kappa$

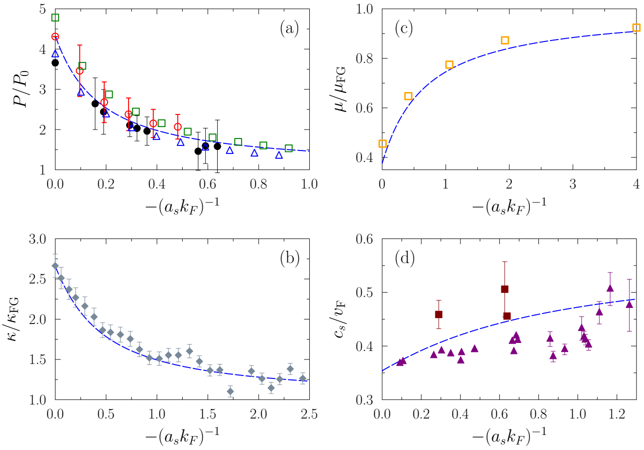
$$\frac{\kappa_{FG}}{\kappa} = \xi + \frac{4k_F}{5} \frac{\partial \xi}{\partial k_F} + \frac{k_F^2}{10} \frac{\partial^2 \xi}{\partial k_F^2}$$

### Sound velocity $c_s$

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

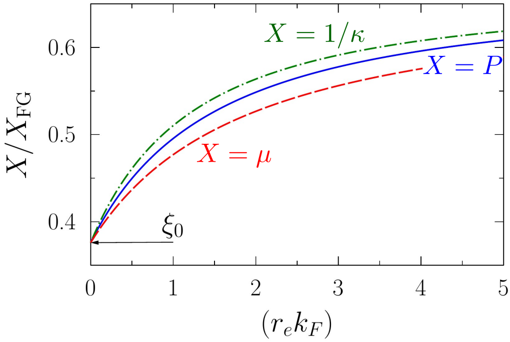
# Ultra-cold atoms results ($r_e = 0$) near unitary

## 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

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

### External field

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

### Response function $\chi$

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

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

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

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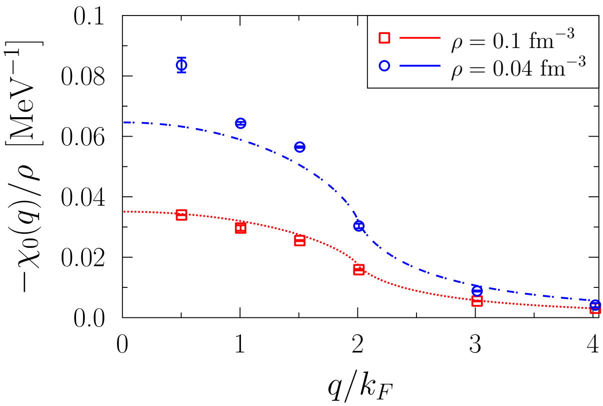
# Linear static response function for neutron matter ($r_e = 2.7$ fm)

## 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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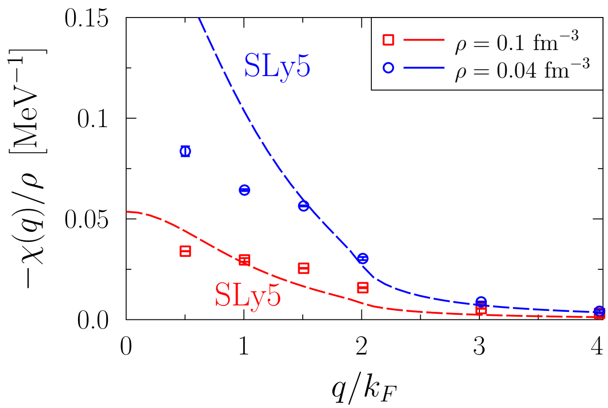


[M. Buraczynski and A. Gezerlis, PRL **116**, 152501 (2016)]
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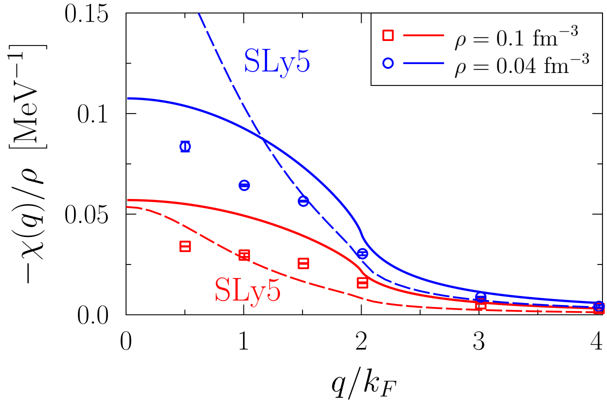
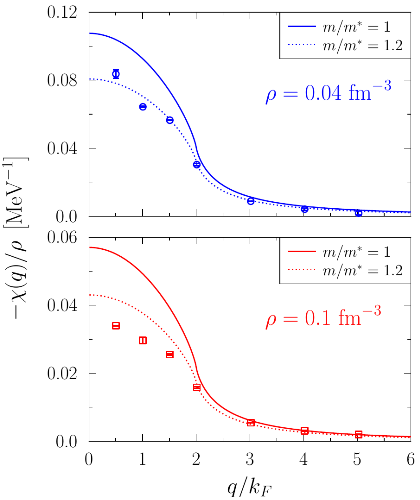



[M. Buraczynski and A. Gezerlis, PRL **116**, 152501 (2016)]
[**A.B.** and D. Lacroix, *in preparation*]

# 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 ($a_s \to -\infty$ and $r_e = 0$)

**Dynamical** external field

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

Response function

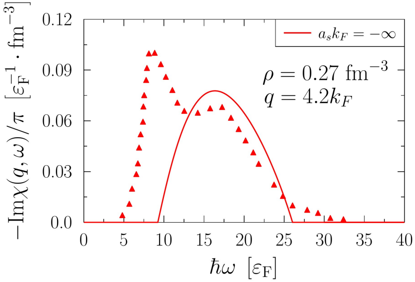
$$\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1 - \frac{\delta^2 \mathcal{V}}{\delta \rho^2}\chi_0(q,\omega)}$$

# Role of pairing and superfluidity on the dynamical response

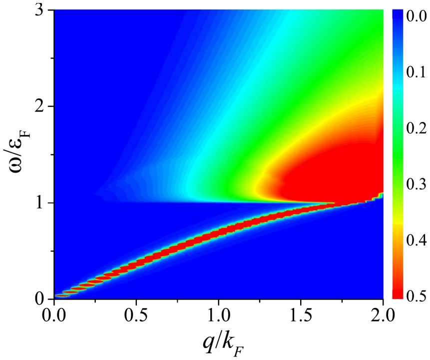
## Come back to unitary gas ($a_s \to -\infty$ and $r_e = 0$)

**Dynamical** response

$$\hat{V}_{\rm ext}(q,\omega) \longmapsto \chi(q,\omega)$$




[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 ($\rho \lesssim 0.01$ 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