# Bridging nuclear *ab-initio* methods and Energy Density Functional Theories

## From ultracold atoms to nuclear matter

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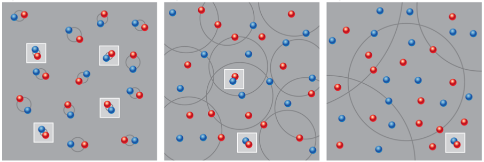
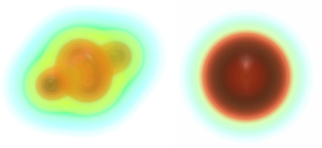
*Collaborators:* Jérémy BONNARD, Marcella GRASSO, Jerry YANG

# Content of the presentation

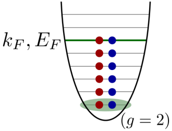
1. Motivations and context
   - DFT vs EFT
   - Cold Fermi Gas



2. *Non-empirical* functional
   - Resummed formula for unitary gas
   - *Non-empirical* DFT for neutron matter

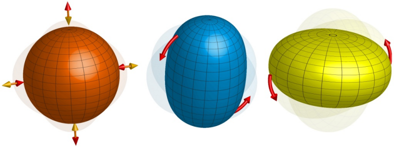


3. Recent applications
   - Ground State thermodynamical properties
   - Static linear response
   - Dynamical response (hydrodynamical regime)

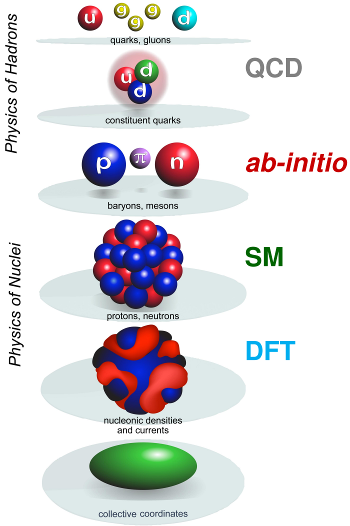


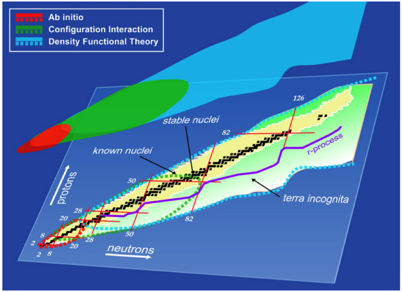

4. Self-energy resummation

5. Summary and outlook



# Nuclear theories landscape



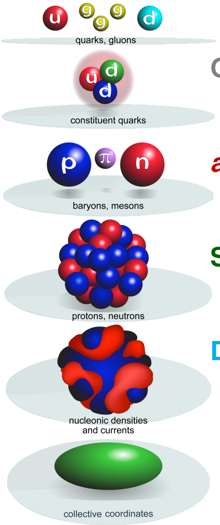

**Unified description of nuclear systems**

- GS structure of the atomic nuclei
- Small and large amplitude dynamics
- Thermodynamics (finite/infinite systems)

## Nuclear theories landscape

*Physics of Hadrons*

*Physics of Nuclei*

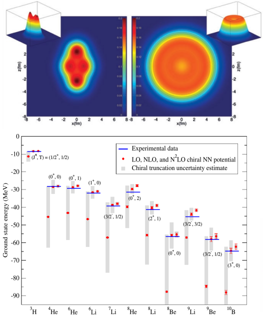


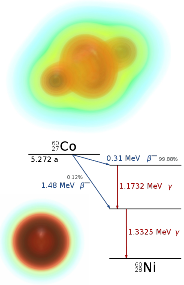

**QCD**

***ab-initio***

**SM**

**DFT**

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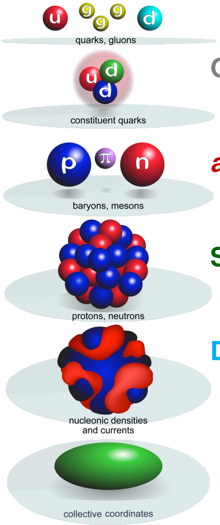


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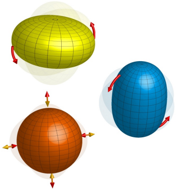

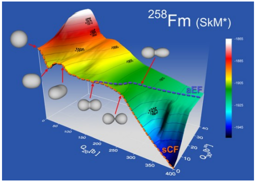


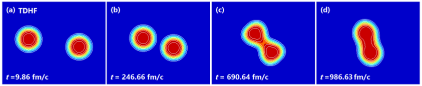


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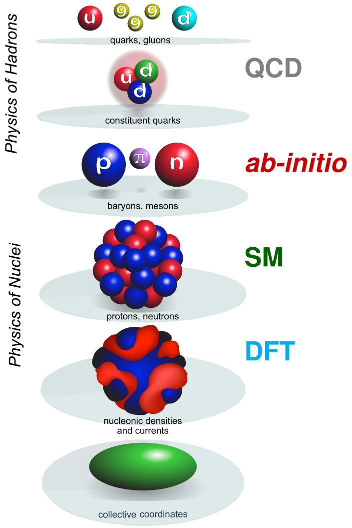


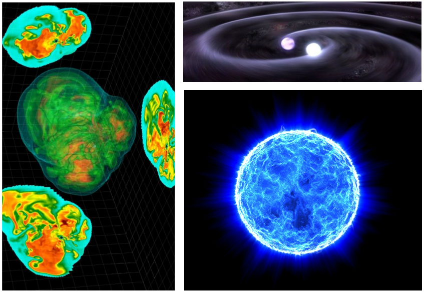

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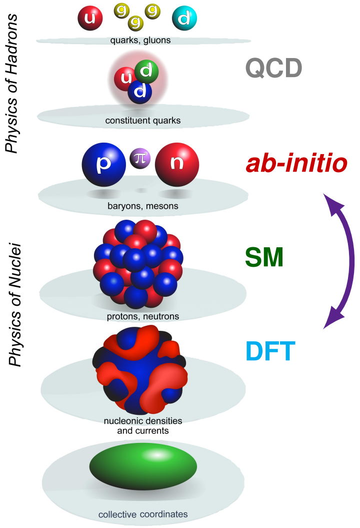


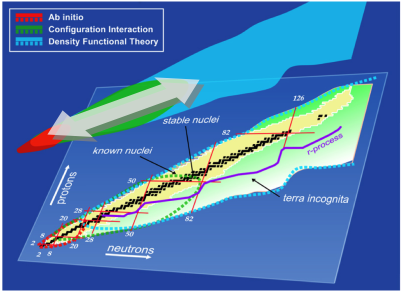


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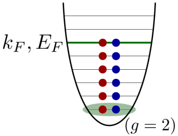
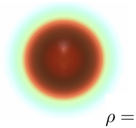
## Strongly correlated Fermions in infinite matter

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

### DFT / (N)EDF

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



$$\rho = \frac{g k_F^3}{6\pi^2}$$

### Nuclear DFT (Hartree-Fock like)

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

$$= \langle T \rangle + c_1 \rho^{\beta_1} + c_2 \rho^{\beta_2} + \cdots$$

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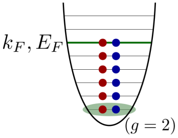


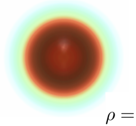

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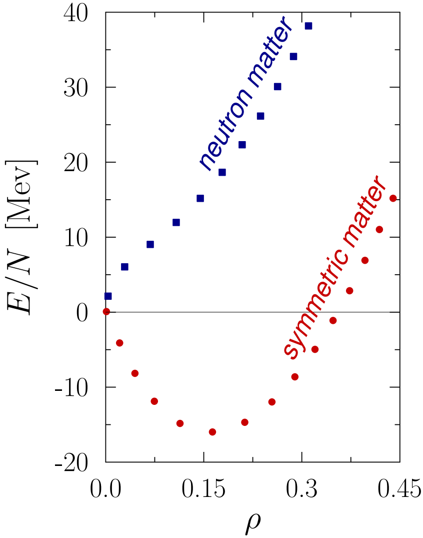

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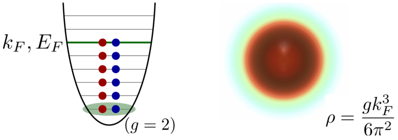


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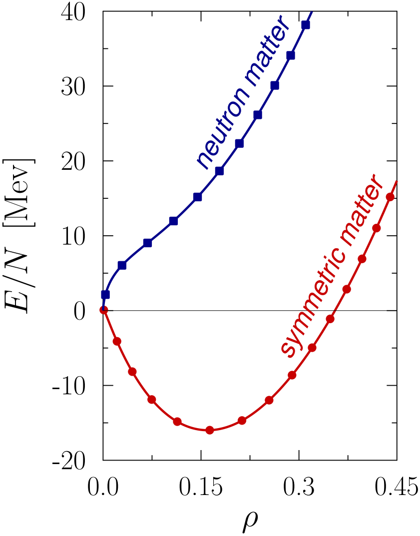
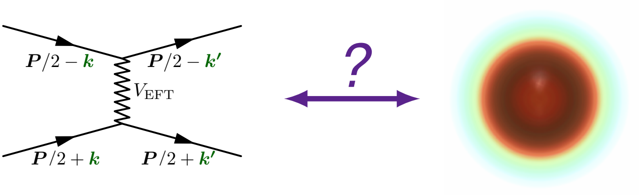


# *How to relate LECs to DFT? and make it less empirical?*



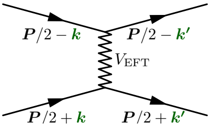

- **Low density expansion**
- **Unitary limit**

# Strongly correlated Fermions in infinite matter

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

### EFT at low density ($s-$scattering wave)

$$\langle \boldsymbol{k}' | V_{\text{EFT}} | \boldsymbol{k} \rangle = \frac{4\pi \boldsymbol{a_s}}{m}$$




$\boldsymbol{a_s}$: $s$-wave scattering length

### Many-Body Perturbation Theory: *Lee-Yang formula*

$$|a_s k_F| \ll 1$$

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

$$E_{FG} = \frac{3}{5}\frac{k_F^2}{2m}$$

(Free gas energy)

$$k_F = \left(3\pi^2 \rho\right)^{1/3}$$

(Fermi momentum)

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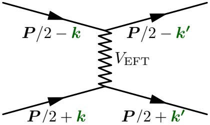


$\boldsymbol{a_s}$: $s$-wave scattering length

$\boldsymbol{r_e}$: $s$-wave effective range

**Many-Body Perturbation Theory: *Lee-Yang formula***

$$|a_s k_F| \ll 1 \quad \text{and} \quad |r_e k_F| \ll 1$$

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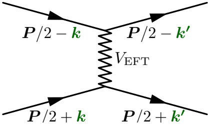


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**MBPT** →

$$E = \begin{array}{l} \quad E^{(1)}_{\boldsymbol{a_s}} + E^{(2)}_{\boldsymbol{a_s}} + \cdots \\ + \; E^{(1)}_{\boldsymbol{a_s},\boldsymbol{r_e}} + E^{(2)}_{\boldsymbol{a_s},\boldsymbol{r_e}} + \cdots \\ + \; \vdots \end{array}$$

↓ **LECs**

**Increasing complexity**

### For neutron matter

$a_s = -18.9$ fm | $r_e = 2.7$ fm

- *Validity* ($|a_s k_F| < 1$): $\rho < 10^{-6}\ \text{fm}^{-3}$

# New insight from unitary Fermi gas

## Physical scales of interest

**DFT at unitarity ($a_s \to \pm\infty$)**

$$\frac{E[\rho]}{E_{FG}} = \xi_0$$

$\xi_0 \simeq 0.37$
(Bertsch parameter)

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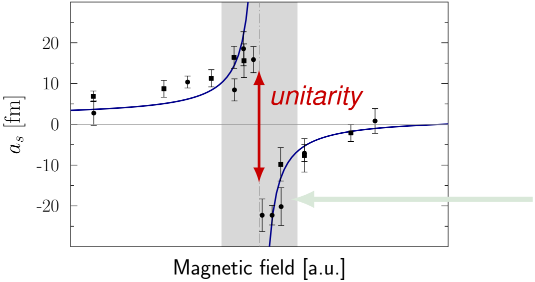


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[Regal & Jin, PRL **90** (2003)]

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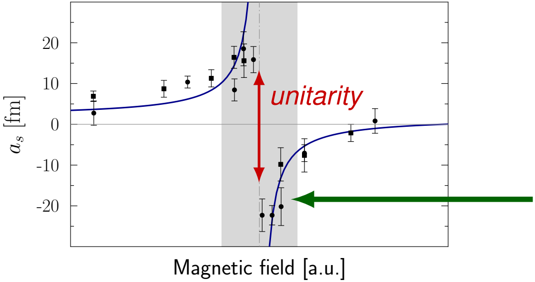


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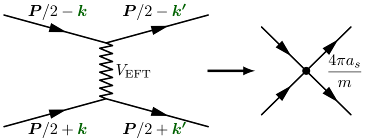
## Resummed formula for unitary gas
### Ladder particle-particle diagrams resummation

**Contact interaction (EFT)**




[Steele, arXiv:nucl-th/0010066 (2000)]

- Contains terms to **all order** in $(a_s k_F)$
- **Finite limit** for Unitary gas $(a_s \to \pm\infty)$
- Results strongly depends on selected diagram

$E =$




$$= \left(\frac{4\pi a_s}{m}\right) \iint \frac{d^3P}{(2\pi)^3} \frac{d^3k}{(2\pi)^3} \frac{\theta^-_{\boldsymbol{k}}}{1-(a_s k_F)F(P,k)}$$

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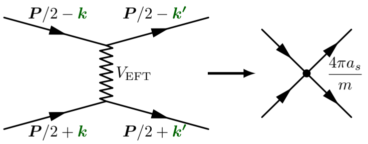


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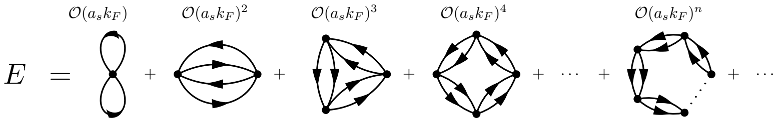


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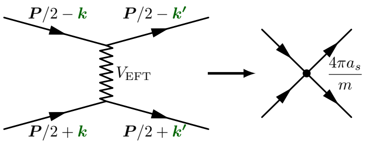


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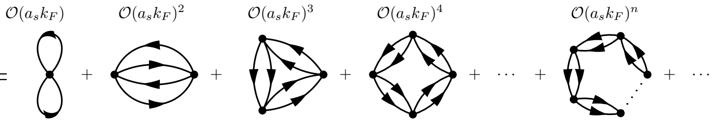


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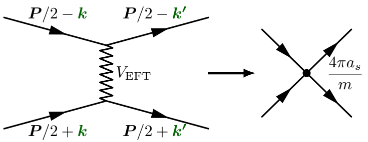


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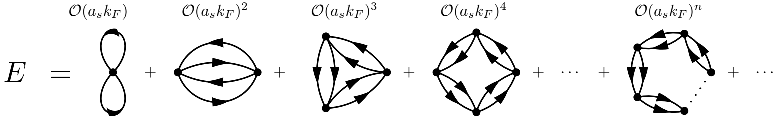


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**Phase-space average**

$$F(P,k) \longmapsto \frac{6}{35\pi}(11 - 2\ln 2)$$

$$\frac{E}{E_{\mathrm{FG}}} = \frac{\frac{10}{9\pi}(a_s k_F)}{1 - \frac{6}{35\pi}(11 - 2\ln 2)(a_s k_F)}$$

[Schäfer *et al.*, NPA **762** (2005)]

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$$\frac{E}{E_{\mathrm{FG}}} = \frac{\frac{10}{9\pi}(\boldsymbol{a_s k_F})}{1 - \frac{6}{35\pi}(11 - 2\ln 2)(\boldsymbol{a_s k_F})}$$

[Schäfer *et al.*, NPA **762** (2005)]

- Correct up to $\mathcal{O}(\boldsymbol{a_s k_F})^2$
- Bertsch parameter† $(a_s k_F \to \infty)$:

  $\boldsymbol{\xi_0} = 0.32$

†Accepted value: $\xi_0 \simeq 0.37$

# Resummed formula for unitary gas

## Pragmatic approach

$$E = \left(\frac{4\pi a_s}{m}\right) \iint \frac{d^3P}{(2\pi)^3} \frac{d^3k}{(2\pi)^3} \frac{\theta_{\boldsymbol{k}}^-}{1 - (\boldsymbol{a_s k_F}) \boldsymbol{F(P,k)}}$$

$$= \left[\frac{10}{9\pi}(\boldsymbol{a_s k_F}) + \frac{4}{21\pi}(11 - 2\ln 2)(\boldsymbol{a_s k_F})^2 + \cdots\right] E_{\mathrm{FG}}$$

**Unitary limit ($E \to \xi_0 E_{\mathrm{FG}}$)**

$$\boldsymbol{F(P,k)} \longmapsto \frac{10}{9\pi}(1-\xi_0)^{-1}$$

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[Lacroix, PRA **94** (2016)]

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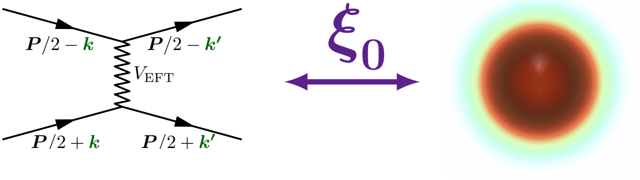
# *Non-empirical DFT based on LECs without free parameters: effective range generalization*



# *Non-empirical* DFT without free parameters

## Effective range effect and neutron matter

[Lacroix, PRA **94** (2016)]
[Lacroix, AB, Grasso and Yang, PRC **95** (2017)]

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

$$= \underbrace{1 - \frac{\boldsymbol{U_0}}{1-(a_s k_F)^{-1}\boldsymbol{U_1}}}_{\text{zero-range part}} + \underbrace{\frac{(r_e k_F)\boldsymbol{R_0}}{[1-\boldsymbol{R_1}(a_s k_F)^{-1}][1-\boldsymbol{R_1}(a_s k_F)^{-1}+\boldsymbol{R_2}(r_e k_F)]}}_{\text{effective range part}}$$

$(\boldsymbol{U_0}, \boldsymbol{U_1}, \boldsymbol{R_0}, \boldsymbol{R_1}, \boldsymbol{R_2})$ adjusted without free parameter to reproduce:

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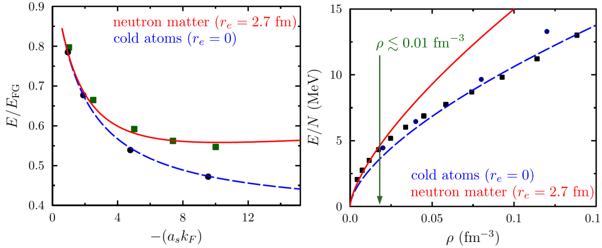



- ● [Gezerlis & Carlson, PRC (2010)]
- ■ [Carlson *et al.*, PTEP (2012)]
- ● [Akmal & Pandharipande, PRC (1998)]
- ■ [Friedman & Pandharipande, NPA (1981)]

*Ground State*
*thermodynamical properties*

## Some GS thermodynamical quantities

### Infinite systems

**_Non-empirical_ DFT: $E = \xi(a_s k_F, r_e k_F) E_{FG}$**

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

**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 $c_s$**

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

# Cold atoms results ($r_e = 0$) near unitary

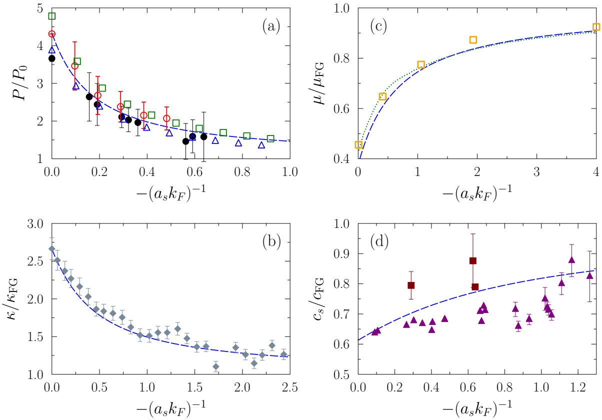
## Survey of experimental and theoretical data

### 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

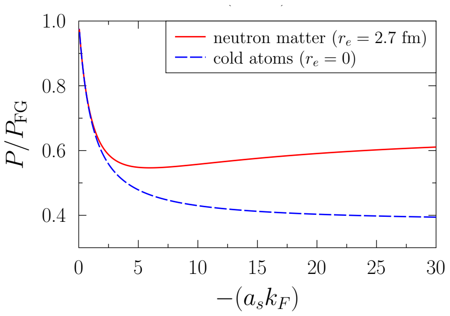
- ● [Navon *et al.*, Science **328** (2010)]
- ◆ [Navon *et al.*, Science **328** (2010)] [Ku *et al.*, Science **335** (2012)]
- ■ [Weimer *et al.*, PRL **114** (2015)]
- ▲ [Joseph *et al.*, PRL **98** (2007)]




In general the non-empirical DFT **works very well in cold atoms** at unitarity and away from unitarity.

## Effective range effect
### Application to neutron matter

#### Neutron matter prediction




- **Strong effective range dependence**

[AB & Lacroix, PRC **97** (2018)]

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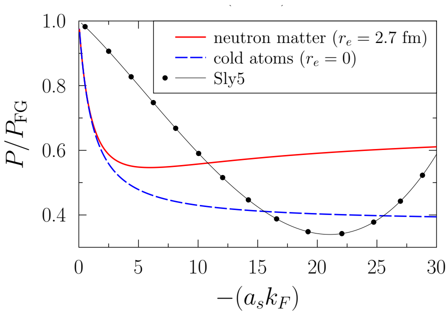


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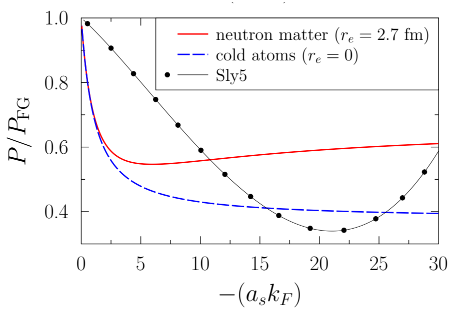


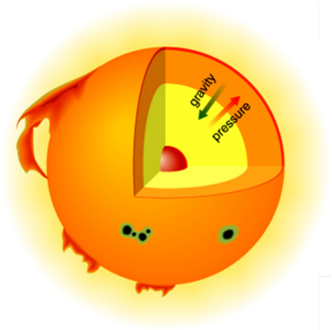


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*Static linear response*

# Linear response theory

## RPA formalism for infinite matter

**System** | **Weak external field**

$$E = \int d^3r \Big( \underbrace{\mathcal{K}[\rho(\boldsymbol{r})]}_{\text{kinetic}} + \underbrace{\mathcal{V}[\rho(\boldsymbol{r})]}_{\text{interaction}} \Big) \leftsquigarrow \hat{V}_{\text{ext}} = \sum_j \phi(q,\omega) e^{i\boldsymbol{q}\cdot\boldsymbol{r}_j - i\omega t}$$

**Response function $\chi$**

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

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

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

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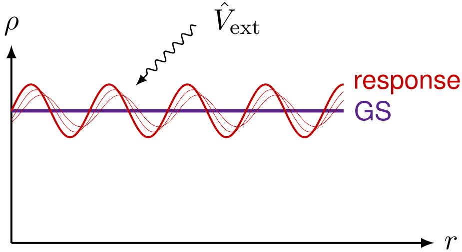
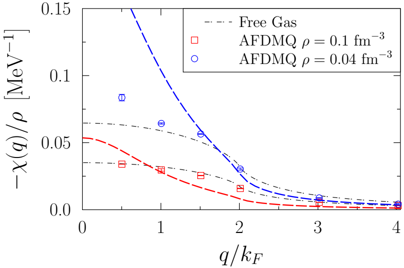


## Linear static response function for neutron matter
### Comparison with recent QMC calculation

### *Empirical* DFT (Sly5)




AFDMC match Free Fermi Gas response (unlike *empirical* DFT)

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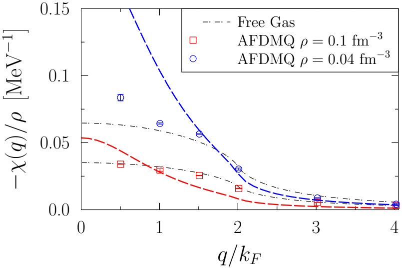


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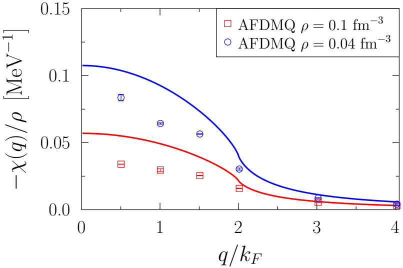


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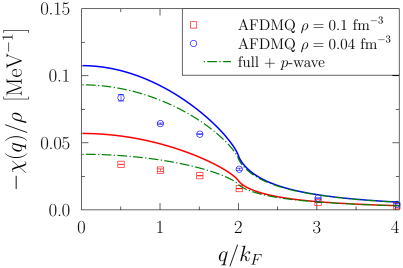
***Non-empirical* DFT + $p$ – wave**

Adding LO $p$ – wave

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

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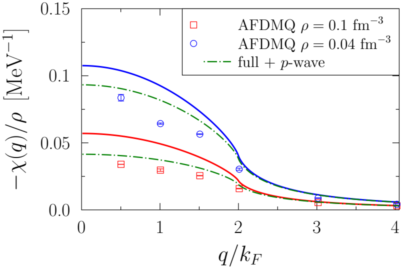


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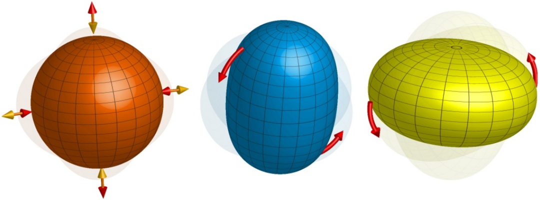
# *Dynamical response: hydrodynamical regime*



## Collective modes in trapped Fermi systems

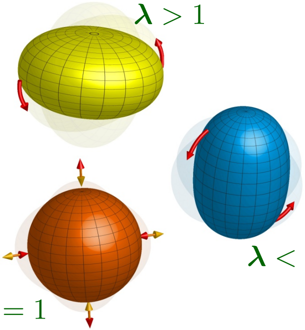
- **Anisoptropic trap**

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

- **Polytropic EoS** $P \propto \rho^{\Gamma}$

  $\Gamma = \kappa P$ (adiabatic index of infinite system)

- **Linearized hydrodynamic**




Solution of cigar-shaped / prolate ($\boldsymbol{\lambda} \ll 1$):

$$\frac{\omega^p_{rad}}{\omega_0} = \sqrt{2\,\Gamma} \qquad \frac{\omega^p_{ax}}{\boldsymbol{\lambda}\omega_0} = \sqrt{3 - \frac{1}{\Gamma}}$$

[Heiselberg, PRL **93** (2004)]

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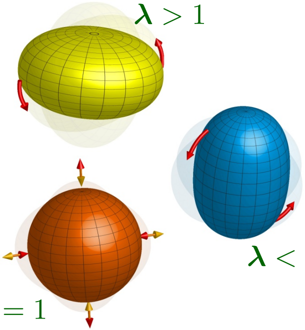


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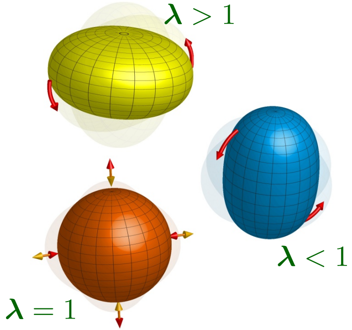


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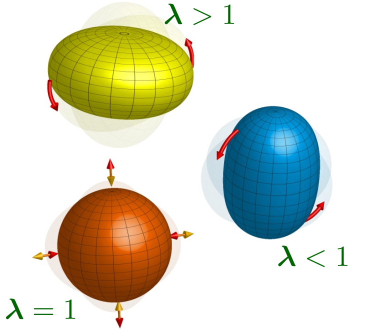


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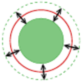

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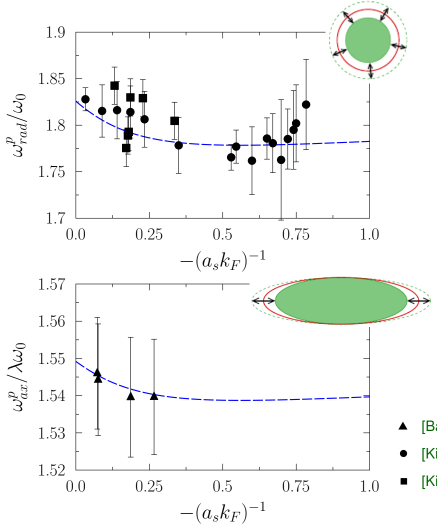


### Prolate collective modes

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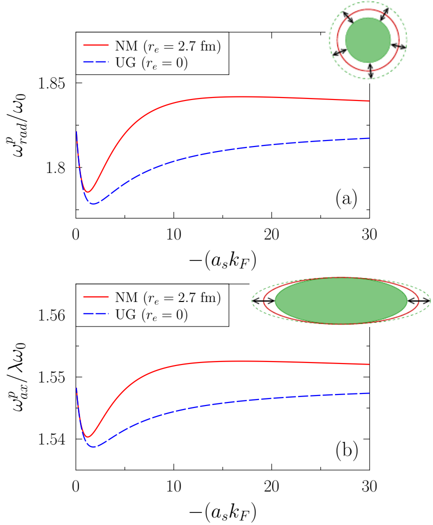
- ▲ [Bartenstein *et al.*, PRL **92** (2004)]
- ● [Kinast, PRA **70** (2004)]
- ■ [Kinast, PRL **92** (2004)]

[AB & Lacroix, PRC **97** (2018)]

## Collective mode in trapped neutron matter

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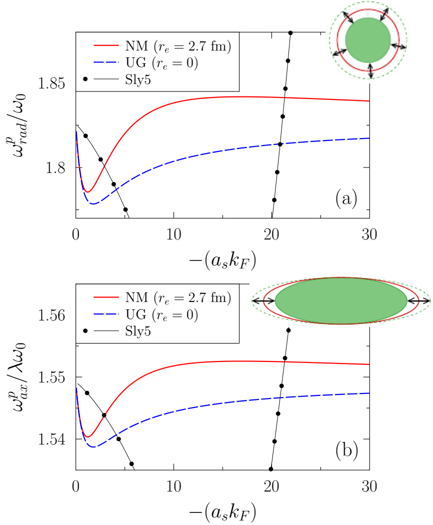


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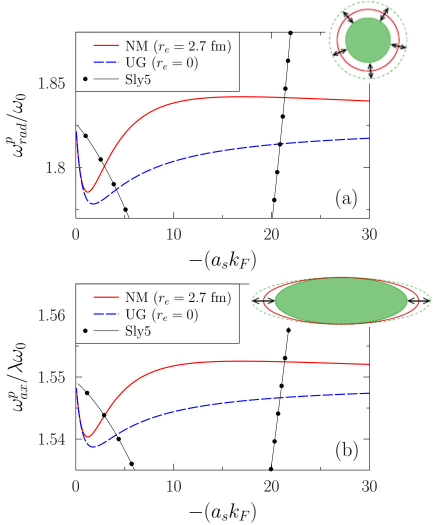


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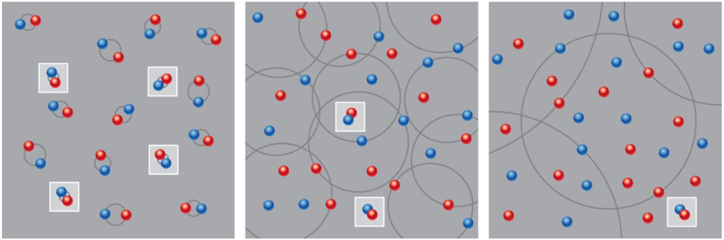
# *To a microscopic theory*

*exploration of resummation techniques*



## What about the quasi-particles properties?

### Importance of the effective mass

**Green functions and self-energy formalism**

$$E = \int \frac{d^3k}{(2\pi)^3} G(\boldsymbol{k}) \Sigma^\star(\boldsymbol{k})$$

- $\mathrm{Re}\left[\Sigma^\star(\boldsymbol{k})\right] = \varepsilon(\boldsymbol{k}) \rightarrow \frac{\boldsymbol{k}^2}{2\boldsymbol{m}^\star} + U_0$ *(sp energy of qp)*
- $\mathrm{Im}\left[\Sigma^\star(\boldsymbol{k})\right] = \gamma(\boldsymbol{k})$ *(life time of qp)*

*Self-energy* **resummation**

**Relation with other theories**

- Brueckner Hartree-Fock
- Landau Fermi liquid theory

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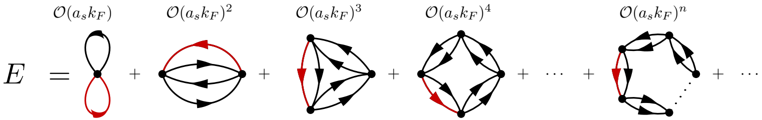
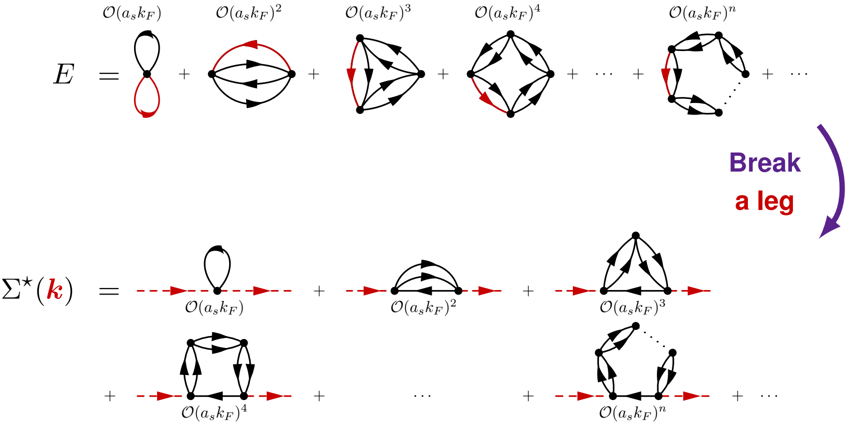


# What about the quasi-particles properties?

## Self-energy resummation



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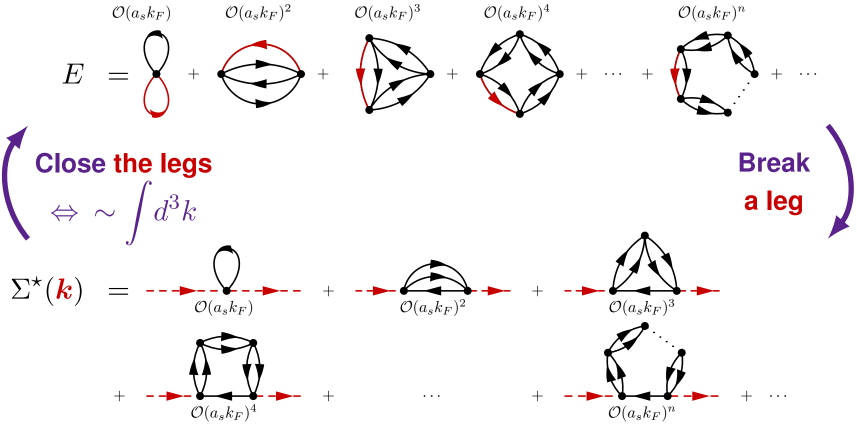

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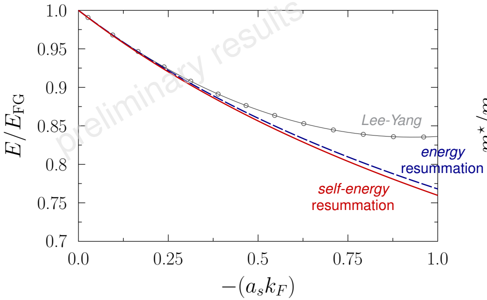


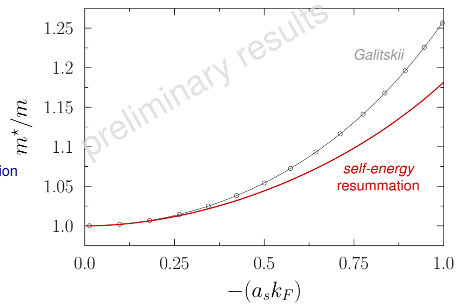


### *Lee-Yang formula*

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

### *Galitskii formula*

$$\frac{m^\star}{m} = 1 + \frac{4}{15\pi^2}(7\ln 2 - 1)(a_s k_F)^2$$

## Summary and perspectives

- A functional without free parameters was recently proposed and reproduce very well the properties of cold atoms
- The functional reproduce the *ab-initio* results at low density for neutron matter taking in account the effective range effect
- The static response reproduces reasonably AFDMC calculation for neutron matter
- The collective mode should be efficient to test and constrain the functional theories

## Summary and perspectives

- **Short-term project**
  - Validity of ressumation to justify the functional
  - Include the effective mass effect
  - Include the pairing in the functional (study more precisely the BEC-BCS crossover)
- **Long-term project**
  - Include the 3-body interaction
  - Extend the theory to symmetric matter, finite nuclei and finite quantum droplet (statics and dynamics)
  - Include other partial waves

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