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

From ultracold atoms to nuclear matter

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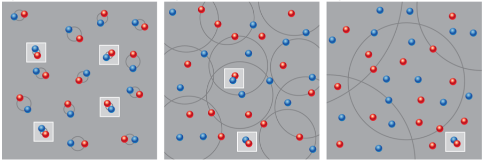
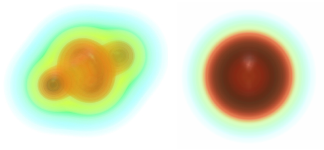
Collaborators: Jérémy BONNARD, Marcella GRASSO, Jerry YANG

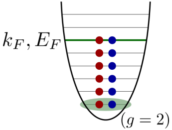
Content of the presentation



1. Motivations and context
   - DFT vs EFT
   - DFT at low density
   - DFT at unitarity

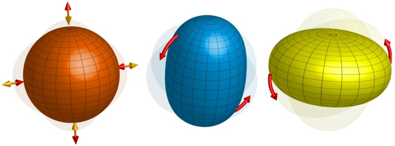


2. *Non-empirical* functional
   - Resummed formula for unitary gas
   - *Non-empirical* DFT for neutron matter



3. Self-energy resummation

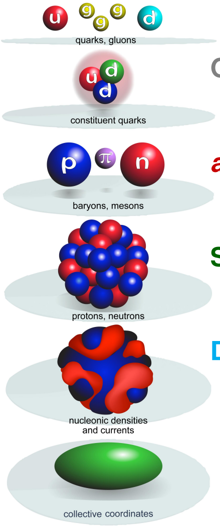
4. Summary and outlook



Nuclear theories landscape

Physics of Hadrons

Physics of Nuclei

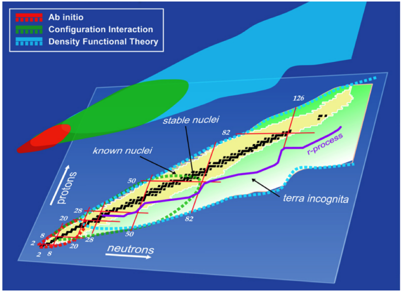


QCD

ab-initio

SM

DFT



Unified description of nuclear systems

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

Nuclear theories landscape

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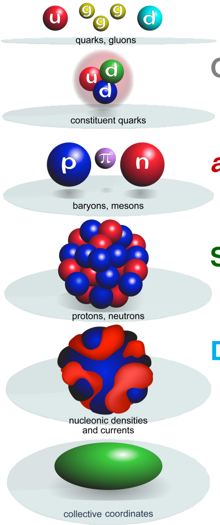

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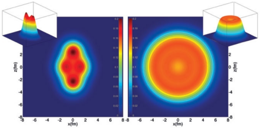

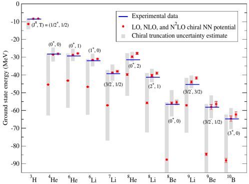

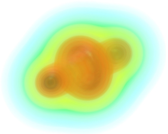

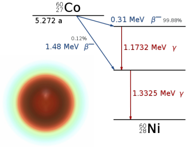

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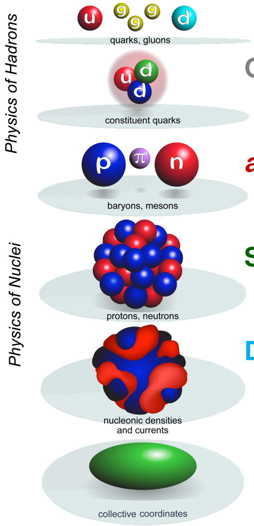

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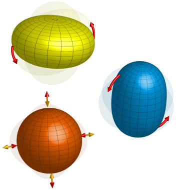

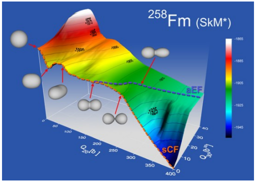

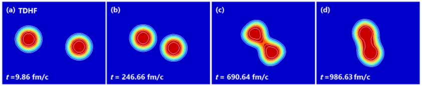

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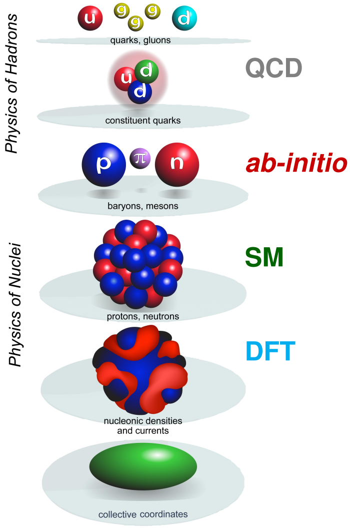

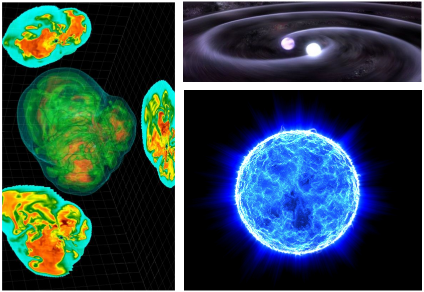

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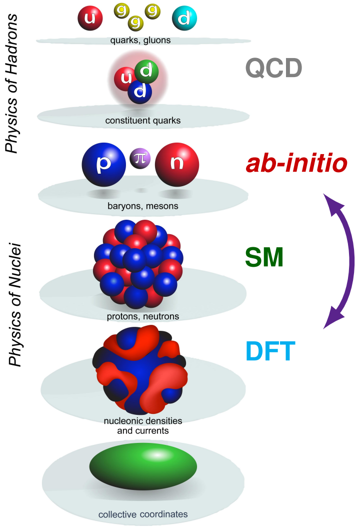

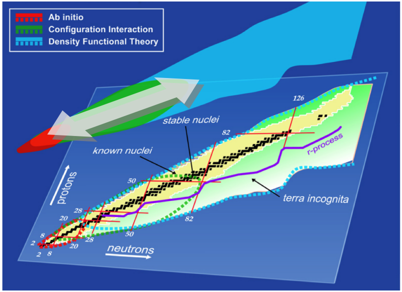

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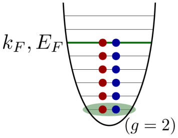
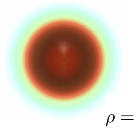
Strongly correlated Fermions in infinite matter

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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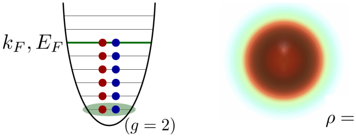

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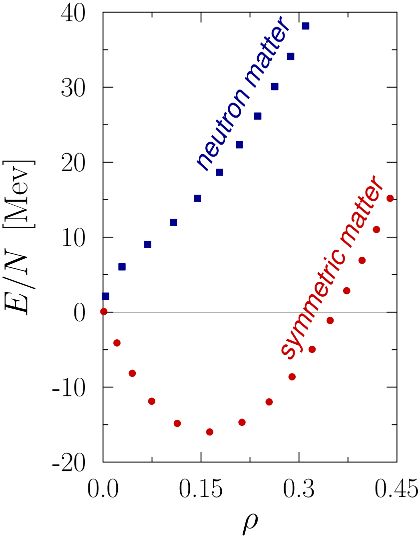

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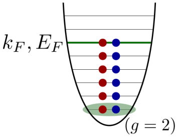

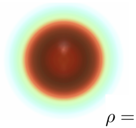

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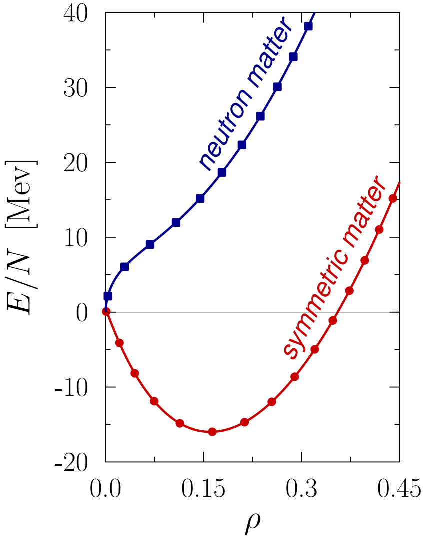
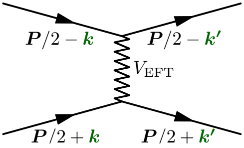
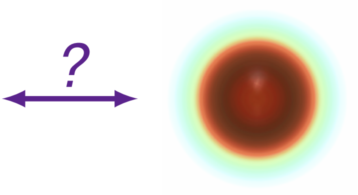


How to relate LECs to DFT?
and make it less empirical?





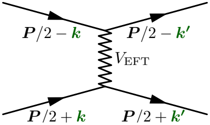
- **Low density expansion**
- **Unitary limit**

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*

$$|a_s k_F| \ll 1$$

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

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

(Free gas energy)

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

(Fermi momentum)

Strongly correlated Fermions in infinite matter

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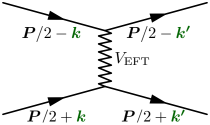
EFT at low density ($s-$scattering wave)

$$\langle \boldsymbol{k'} | V_{\mathrm{EFT}} | \boldsymbol{k} \rangle = \frac{4\pi \boldsymbol{a_s}}{m} \left[1 + \frac{\boldsymbol{r_e a_s}}{4} \left(\boldsymbol{k}^2 + \boldsymbol{k'}^2 \right) + \cdots \right]$$



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

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

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

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

$$\frac{E}{E_{FG}} = \frac{10}{9\pi}(\boldsymbol{a_s k_F}) + \frac{4}{21\pi^2}(11 - 2\ln 2)(\boldsymbol{a_s k_F})^2 + \cdots + \frac{1}{6\pi}(\boldsymbol{r_e k_F})(\boldsymbol{a_s k_F})^2 + \cdots$$

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New insight from unitary Fermi gas

Physical scales of interest

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

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

$\xi_0 \simeq 0.37$
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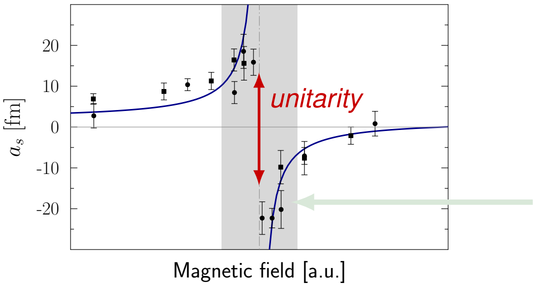

For Neutron Matter

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

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

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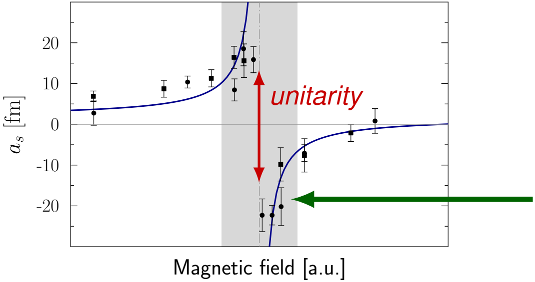

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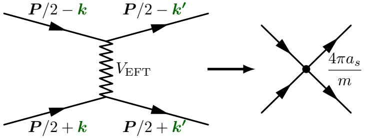
Resummed formula for unitary gas

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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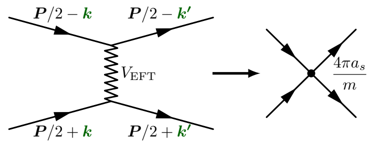

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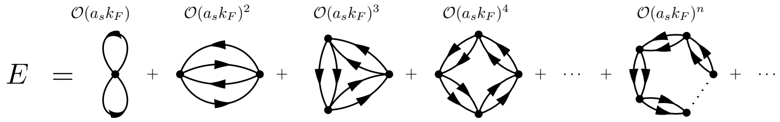

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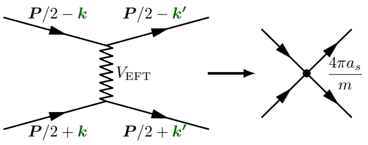

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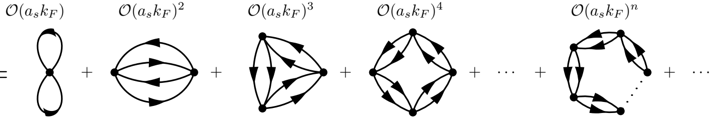

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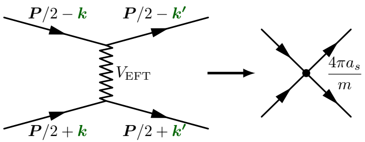

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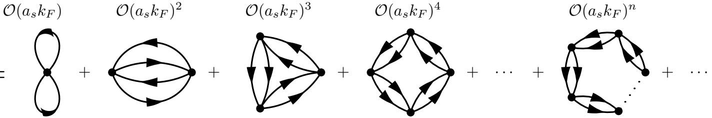

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Resummed formula for unitary gas

Pragmatic approach

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

Phase-space average

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

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

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

- Correct up to $\mathcal{O}(\boldsymbol{a_s k_F})^2$
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†Accepted value: $\xi_0 \simeq 0.37$

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$$E = \left(\frac{4\pi a_s}{m}\right) \iint \frac{d^3P}{(2\pi)^3} \frac{d^3k}{(2\pi)^3} \frac{\theta_{\boldsymbol{k}}^-}{1 - (\boldsymbol{a_s k_F}) \boldsymbol{F(P,k)}}$$
$$= \left[\frac{10}{9\pi}(\boldsymbol{a_s k_F}) + \frac{4}{21\pi}(11 - 2\ln 2)(\boldsymbol{a_s k_F})^2 + \cdots\right] E_{\mathrm{FG}}$$

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)]

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

  $\xi_0 = 0.37$ (exact)

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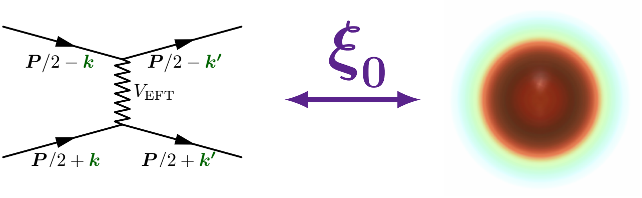
Non-empirical DFT based on LECs without free parameters: effective range generalization



Non-empirical DFT without free parameters

Effective range effect and neutron matter

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

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

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

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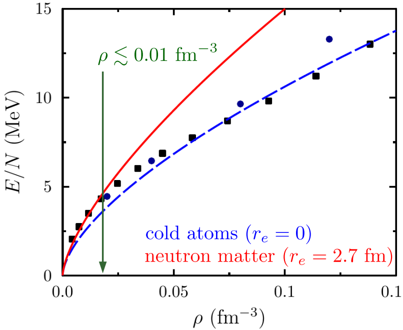

- [Gezerlis & Carlson, PRC (2010)]
- [Carlson *et al.*, PTEP (2012)]
- [Akmal & Pandharipande, PRC (1998)]
- [Friedman & Pandharipande, NPA (1981)]

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)]
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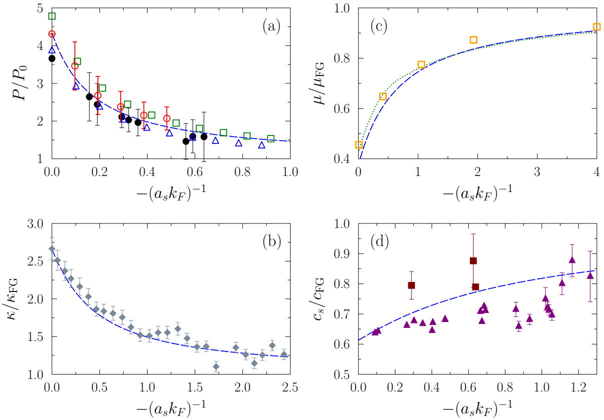

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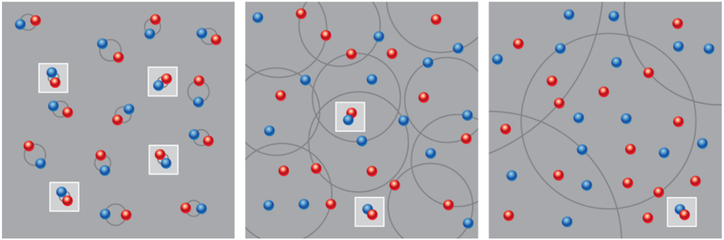
To a microscopic theory

exploration of resummation techniques



What about the quasi-particles properties?

Importance of the effective mass

Green functions and self-energy formalism

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

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Self-energy **resummation**

Relation with other theories

- Brueckner Hartree-Fock
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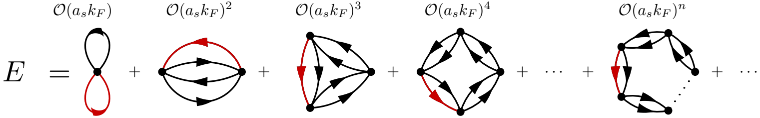

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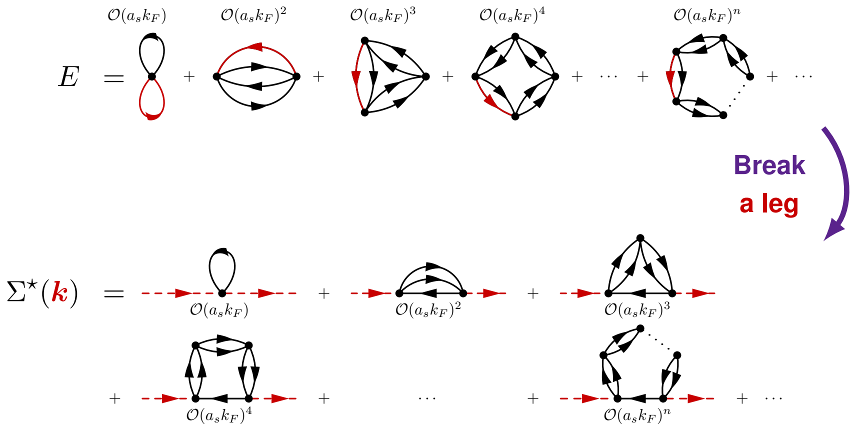

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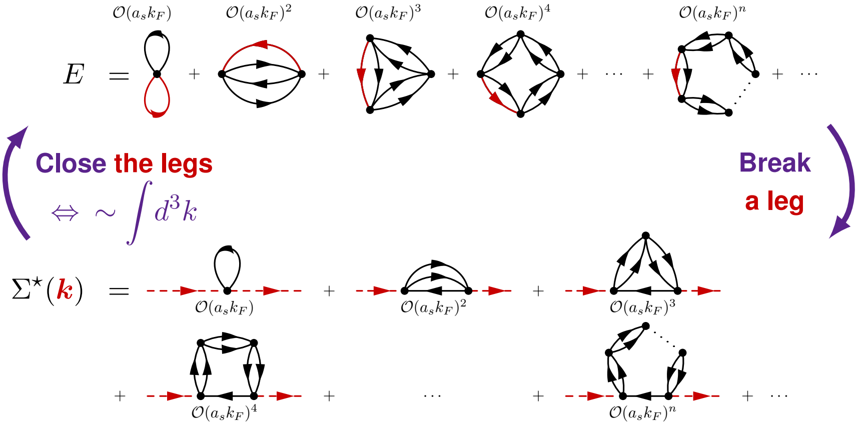

Summary and perspectives

- 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
- Applications: GS thermodynamics, static response and collective mode

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

***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 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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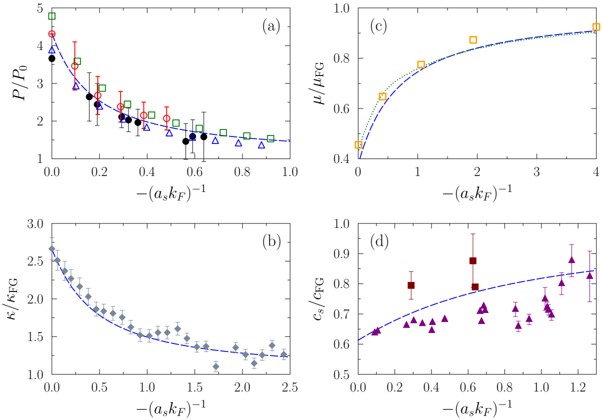

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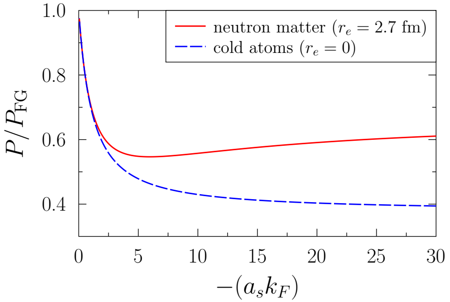
Neutron matter prediction



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

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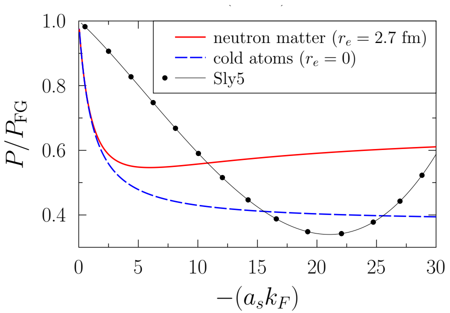

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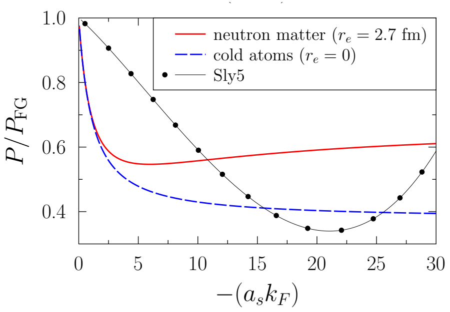

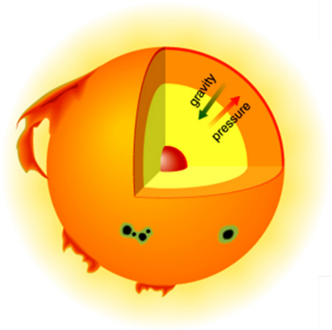

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System | **Weak external field**

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

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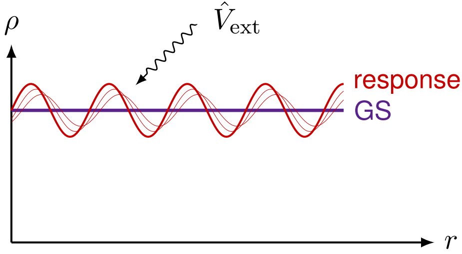

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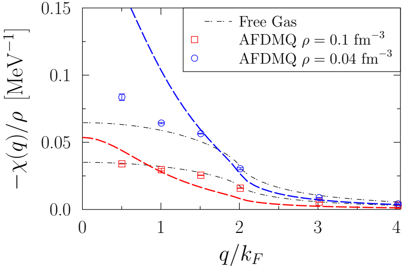

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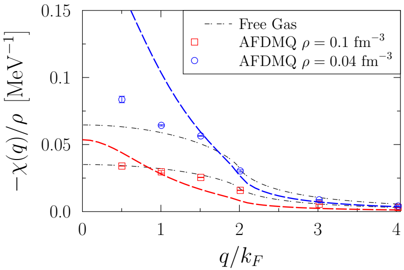

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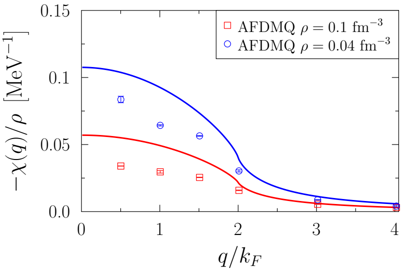

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  $\Gamma = \kappa P$ (adiabatic index of infinite system)

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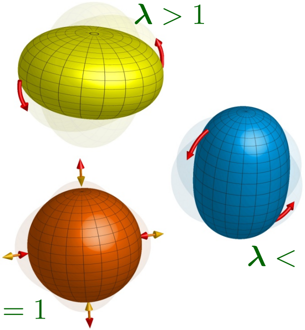

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$$\frac{\omega^p_{rad}}{\omega_0} = \sqrt{2\,\Gamma} \qquad \frac{\omega^p_{ax}}{\lambda\omega_0} = \sqrt{3 - \frac{1}{\Gamma}}$$

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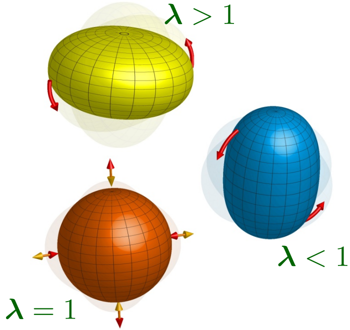

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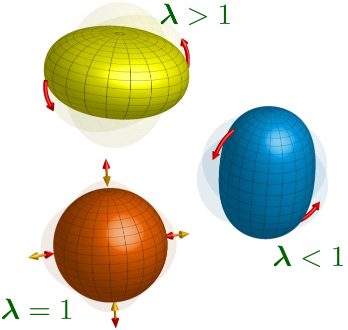

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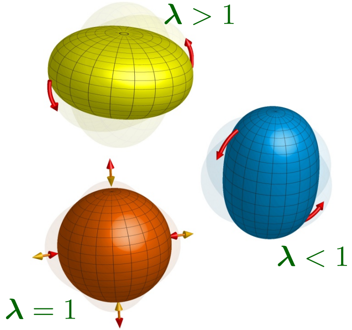

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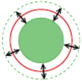

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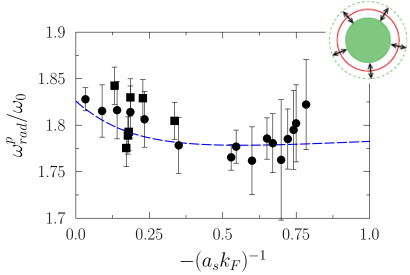

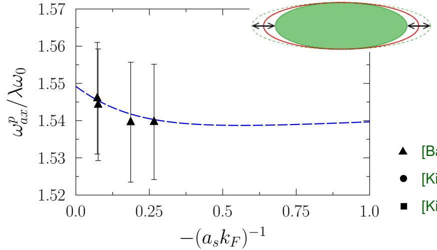

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- ● [Kinast, PRA **70** (2004)]
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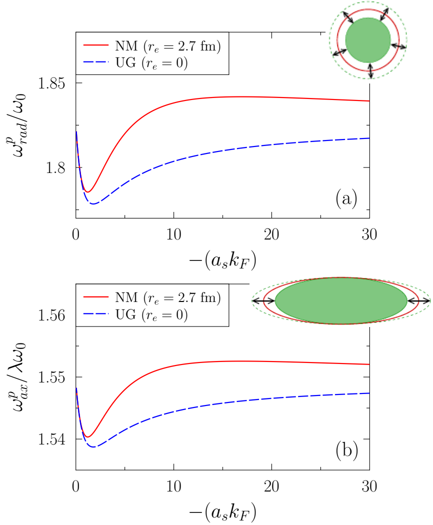

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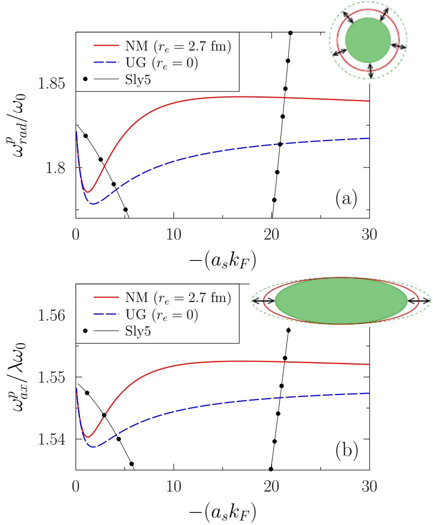
Tests and constrains DFT?

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



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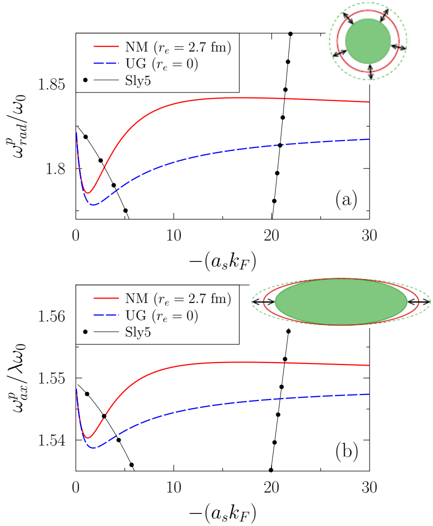
Collective mode in trapped neutron matter



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- $\mathrm{Re}\left[\Sigma^\star(\boldsymbol{k})\right] = \varepsilon(\boldsymbol{k}) \rightarrow \frac{\boldsymbol{k}^2}{2\boldsymbol{m}^\star} + U_0$ *(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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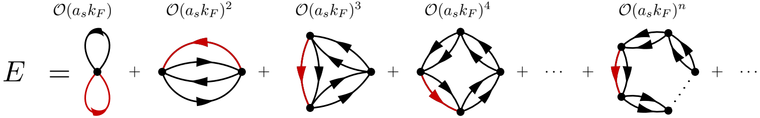
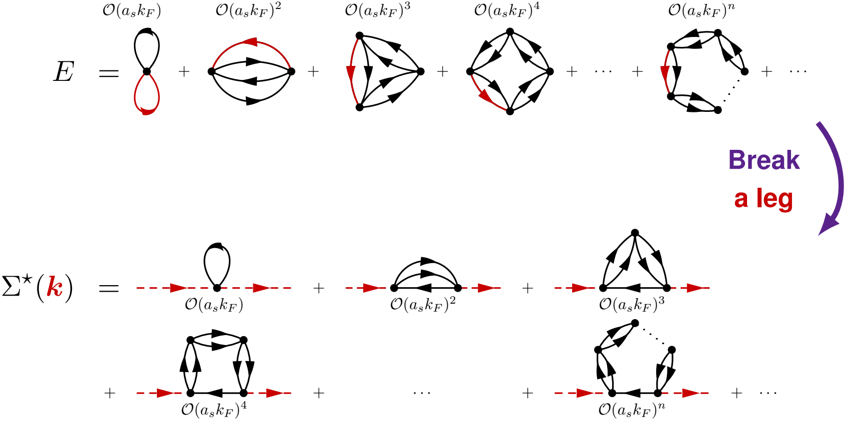
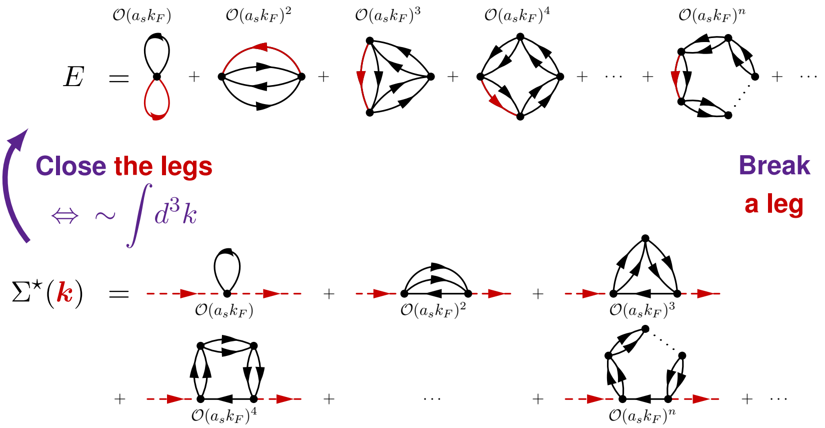
Self-energy resummation



What about the quasi-particles properties?

Self-energy resummation




$\mathcal{O}(a_s k_F)$
$\mathcal{O}(a_s k_F)^2$
$\mathcal{O}(a_s k_F)^3$
$\mathcal{O}(a_s k_F)^4$
$\mathcal{O}(a_s k_F)^n$
$E =$ + + + + ⋯ + + ⋯
Close the legs
$\Leftrightarrow \sim \int d^3k$
Break
a leg
$\Sigma^\star(\boldsymbol{k}) =$ + +
$\mathcal{O}(a_s k_F)$
$\mathcal{O}(a_s k_F)^2$
$\mathcal{O}(a_s k_F)^3$
+ + ⋯ + + ⋯
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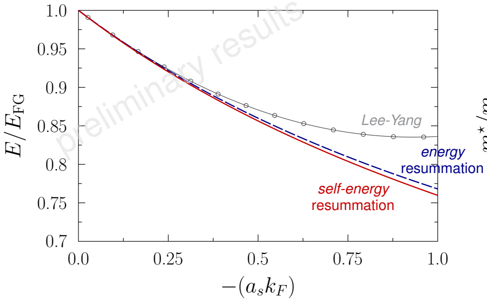

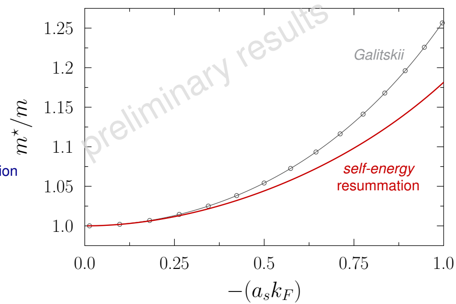

Lee-Yang formula

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

Galitskii formula

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

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