Approximate self-energy for Fermi systems with large s-wave scattering length:

A step towards density functional theory

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Collaborator: Denis Lacroix (IPN Orsay)

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15th July 2019

Selected applications and/or extensions (see Denis' talk)

Constraint on unitarity limits
$a_s \to \pm\infty$ (ultracold atoms + NM)

- thermodynamics of Fermi gas

$$\frac{E}{E_{FG}} = 1 + \frac{(a_s k_F) A_0}{1 - (a_s k_F) A_1}$$

Range of validity:

- MBPT: $\rho \sim 10^{-6}$ fm^{-3}
- This work: $\rho \sim 10^{-2}$ fm^{-3}

Including quasi-particle properties

[AB, Lacroix, J. Phys. G]

- effective mass of Fermi gas

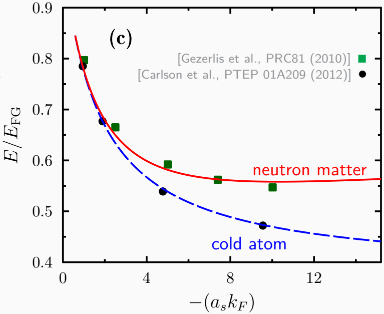
Generalization including effective range effect

- EOS of dilute neutron matter

[Lacroix, AB, et al., PRC 95 (2017)]

- static and dynamical linear response + collective modes

[AB, Lacroix, PRC97 (2018)]



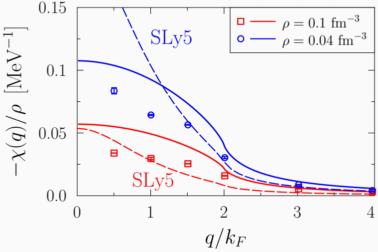
Motivation to include quasi-particle properties

External field V_{ext} applied on the system $E = \int d^3r[\mathcal{K}(r) + \mathcal{V}(r)]$
induce a change in density $\rho \to \rho + \delta\rho$ (here: $m^\star = m$)

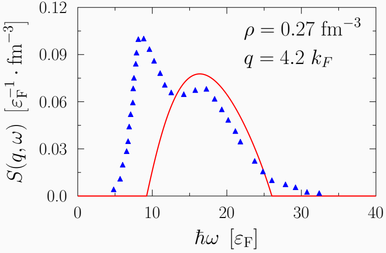
$$\text{with} \quad \delta\rho = \chi(q,\omega) \times V_{ext} = \frac{\chi_0(q,\omega) \times V_{ext}}{1 - \chi_0(q,\omega)\frac{\delta^2\mathcal{V}}{\delta\rho^2}}$$

(χ_0 : Lindhard functions)

Static response ($\omega = 0$)



Dynamical response $\propto Im[\chi(q,\omega)]$



✗ effective mass $m^\star$

✗ pairing gap Δ

[AB, Lacroix, PRC97 (2018)]

Extend to self-energy → quasi-particle properties (focus on $m^\star$)

Strategy

1. Non-empirical functionals based on resummation technique
    - Resummation of Ladder diagrams for the energy
    - Phase-Space average approximation
2. Non-perturbative approach:
   resummation of the quasi-particle properties

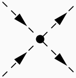
   Goal: obtain explicit and simple form for the self-energy

    - extend the Phase-Space average to the self-energy
    - coherently according to the approximate energy (HvH theorem)

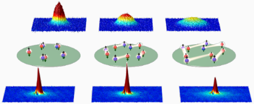
Basics of diagrammatic framework at zero temperature

$E = \frac{3}{5}\frac{k_F^2}{2m} + E^{(1)} + E^{(2)} + \cdots$ [Hammer and Furnstahl, NPA678 (2000)]

$G(\omega, \boldsymbol{k}) =$  : Green's functions

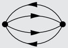
$\langle \boldsymbol{k} | V_{EFT} | \boldsymbol{k'} \rangle =$  $= C_0 = \dfrac{4\pi a_s}{m}$

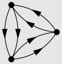
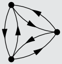
(Directly connected to ultracold atoms physics)

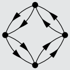
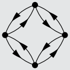
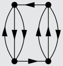
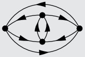
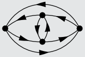


Contributing energy diagrams

$E_{(1)} =$  $\rightarrow (a_s k_F) \rightarrow$ *Hartree – Fock*

$E_{(2)} =$  $\rightarrow (a_s k_F)^2 \rightarrow$ *Lee – Yang*

$E_{(3)} =$  $+$ 

$E_{(4)} =$  $+$  $+$  $+$  $+$ 

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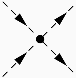
$\langle \boldsymbol{k} | V_{EFT} | \boldsymbol{k'} \rangle =$  $= C_0 = \dfrac{4\pi a_s}{m}$

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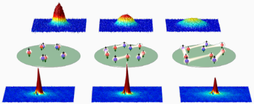
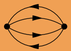
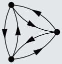
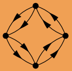
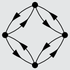
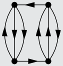
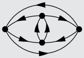
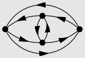


Contributing energy diagrams [Ladder approximation]

$E_{(1)} =$  $\rightarrow (a_s k_F) \rightarrow$ *Hartree – Fock*

$E_{(2)} =$  $\rightarrow (a_s k_F)^2 \rightarrow$ *Lee – Yang*

$E_{(3)} =$  $+$ 

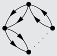
$E_{(4)} =$  $+$  $+$  $+$  $+$ 

[Kaiser, NPA860 (2011)]

Ladder approximation for the energy

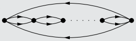
Energy resummation

$$E_{int} = \sum_{n=1}^{\infty}$$



$$= \frac{80}{\pi k_F^5} E_{FG} \int_0^{k_F} s^2 ds \int_0^{\sqrt{k_F^2 - s^2}} t dt \ \mathrm{atan} \frac{(a_s k_F) \pi I(s,t)}{\pi - (a_s k_F) R(s,t)}$$

$$E_{int}^{pp} = \sum_{n=1}^{\infty}$$



$$= \frac{80}{\pi k_F^5} E_{FG} \int_0^{k_F} s^2 ds \int_0^{\sqrt{k_F^2 - s^2}} t dt \frac{(a_s k_F) \pi I(s,t)}{\pi - (a_s k_F) F(s,t)}$$

[Kaiser, NPA860 (2011)] (no pairing, no self-consistency)

$$F(s,t) = 1 + \frac{s}{k_F} - \frac{t}{k_F} \ln \left| \frac{k_F + s + t}{k_F + s - t} \right| + \frac{k_F^2 - s^2 - t^2}{2 s k_F} \ln \left| \frac{(k_F + s)^2 - t^2}{k_F - s^2 - t^2} \right|$$

$$R(s,t) = F(s,t) + F(-s,t)$$

$$I(s,t) = \begin{cases} t/k_F & \text{for } 0 \le t < k_F - s \\ (k_F^2 - s^2 - t^2)/2 s k_F & \text{for } k_F - s \le t < \sqrt{k_F^2 - s^2} \end{cases}$$

Ladder approximation for the energy

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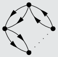
$$= \frac{80}{\pi k_F^5} E_{FG} \int_0^{k_F} s^2 ds \int_0^{\sqrt{k_F^2 - s^2}} t dt \, \mathrm{atan} \frac{(a_s k_F) \pi I(s,t)}{\pi - (a_s k_F) R(s,t)}$$

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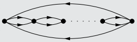
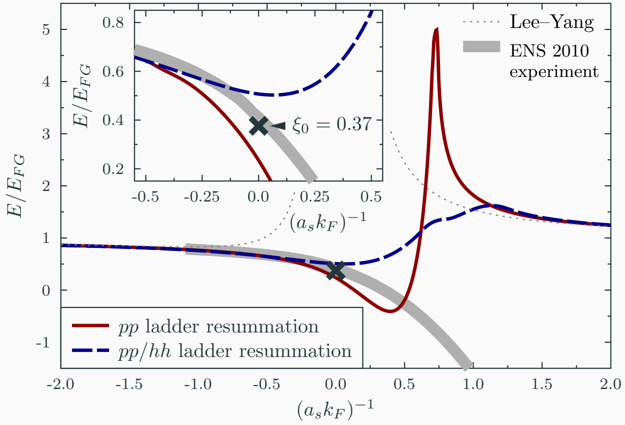

$$= \frac{80}{\pi k_F^5} E_{FG} \int_0^{k_F} s^2 ds \int_0^{\sqrt{k_F^2 - s^2}} t dt \frac{(a_s k_F) \pi I(s,t)}{\pi - (a_s k_F) F(s,t)}$$

[Kaiser, NPA860 (2011)] (no pairing, no self-consistency)

- ✓ Contains terms to all order in $(a_s k_F)$ in a compact form
- ✓ Expansion in $(a_s k_F) \to$ Lee–Yang formula
- ✓ Finite limit at unitarity $(a_s \to \infty)$
- ✗ Implicit function of $\rho = k_F^3 / 3\pi^2$ (goal: explicit function)

Ladder approximation for the energy



- ✓ correct limit at $a_s k_F \ll 1$ (Lee-Yang expansion)
- ✓ finite limit at unitarity
- ✗ strong dependence of retained diagrams
- ✗ complicated function of $(a_s k_F)$

Phase-space average Approximation (PSA)

$$\frac{E_{pp}}{E_{FG}} = 1 + \frac{80}{\pi k_F^5} \underbrace{\int s^2 ds \int t dt}_{phase\ space} \frac{(a_s k_F)\pi I(s,t)}{1 - (a_s k_F/\pi) F(s,t)} \xrightarrow[a_s k_F \to \infty]{} 0.24$$

PSA of *pp* ladder resummation = GPS functional

$$\frac{E}{E_{FG}} = 1 + \frac{10}{9\pi} \frac{(a_s k_F)}{1 - (a_s k_F/\pi)\langle F \rangle} \xrightarrow[a_s k_F \to \infty]{} 0.32$$

[Heiselberg, PRA63 (2001)] [Schäfer et al., NPA762 (2005)] [Haussmann et al., PRA75 (2007)]

- ✓ Lee–Yang formula $\langle F \rangle = \frac{6}{35}(11 - 2\ln 2)$
- ∼ More predictive near unitarity: $\xi_0 = 0.37$ (accepted value)

Phase-space average Approximation (PSA)

$$\frac{E}{E_{FG}} = 1 + \frac{80}{\pi k_F^5} \int s^2 ds \int t dt \, \text{atan} \frac{(a_s k_F) I(s,t)}{1 - (a_s k_F/\pi) R(s,t)} \underset{a_s k_F \to \infty}{=} 0.51$$

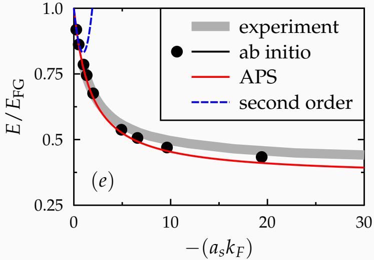
PSA of full ladder resummation = APS functional

$$\frac{E}{E_{FG}} = 1 + \frac{16}{3\pi} \text{atan} \frac{5/24 (a_s k_F)}{1 - (a_s k_F/\pi) \langle R \rangle} \underset{a_s k_F \to \infty}{=} \mathbf{0.36}$$

- ✓ Unitary limit well reproduced (accepted value: $\xi_0 = 0.37$)
- ✓ Exact Lee–Yang expansion
- ✓ **No adjustment !**

[AB, Lacroix, J. Phys. G]

EOS in cold atoms systems



Quasi-particle properties:
Self-Energy Resummation

Ladder Resummation +

Phase-Space average Approximation

Link with Landau theory of Fermi liquid

$$E_{int} = \sum_{kk'} V_{eff}(k,k') n_k n_{k'}$$

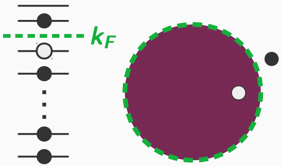
Low-lying excited states $\quad n_k \to n_k + \delta n_k$

$$\delta E = \sum_k \Sigma^\star(k) \delta n_k \longmapsto$$

$$\Sigma^\star(k) = U(k) + iW(k) = \frac{\delta E}{\delta n_k}$$

Close to Fermi surface $\quad v_{k_F} \equiv \partial_k \epsilon_k \big|_{k=k_F} \equiv \frac{k_F}{m^\star}$

$$\epsilon_k = \epsilon_{k_F} + (k - k_F)\frac{k_F}{m^\star} + \cdots$$



[Landau (1957)]

$$\left[\begin{array}{ccc} \epsilon_k & = & \frac{k^2}{2m} + U(k) \\ \frac{1}{2\gamma_k} & = & -W(k) \end{array}\right]$$

Link with Landau theory of Fermi liquid

$$E_{int} = \sum_{kk'} V_{eff}(k,k') n_k n_{k'}$$

Low-lying excited states $\quad n_k \to n_k + \delta n_k$

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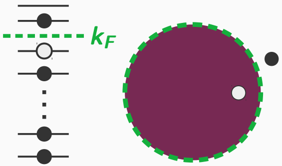
$$\epsilon_k = \epsilon_{k_F} + (k - k_F)\frac{k_F}{m^\star} + \cdots$$



[Landau (1957)]

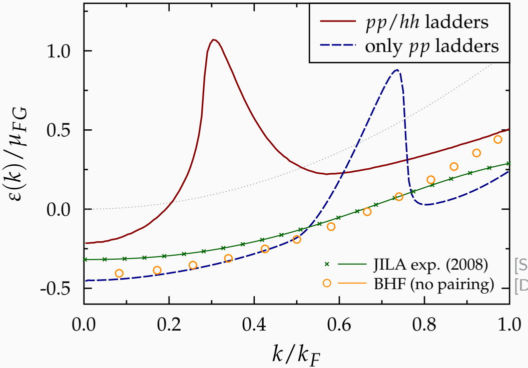
$$\left[\begin{array}{lll} \epsilon_k & = & \frac{k^2}{2m} + U(k) \\ \frac{1}{2\gamma_k} & = & -W(k) \end{array}\right]$$

Hugenholtz – van Hove theorem (HvH theorem)

$$\mu = E(N+1) - E(N) = \frac{\partial E}{\partial N} = \epsilon_{k_F}$$

[Hugenholtz, Van Hove, Physica XXIV (1958)]

Ladder approximation: single-particle energy [Kaiser, EPJA49 (2013)]



[Stewart, Gaebler, Jin, Nature 454 (2008)]
[Doggen et al., Nature (2015)]

✓ valid at low density → Galitskii formula [Galitskii, JETP34 (1958)]:

$$\frac{\varepsilon(k)}{\mu_{FG}} = \frac{4}{3\pi}(a_s k_F) + \phi_2(k)(a_s k_F)^2 + \cdots$$

✓ finite limit at unitarity ($a_s k_F \to \infty$)

✗ non-predictive for $a_s k_F \gg 1$: pathologies

✗ strong dependence of retained diagrams

Phase-Space Average approximation of the resummed self-energy

Focus on the single particle potential $U(k)$ inside the Fermi surface $(k \leq k_F)$

Strategy of the Self-energy resummation

$$E = E_{FG} + \int_{st} \mathcal{E}(s,t)$$

$$\epsilon(k) = \frac{k^2}{2m} + \int_{st} \mathcal{U}(s,t,k)$$

Strategy of the Self-energy resummation

$$E = E_{FG} + \int_{st} \mathcal{E}(s,t)$$

$$\mu = \left.\frac{\partial E}{\partial N}\right|_{V} = \epsilon(k_F)$$

$k = k_F$

HvH theorem

$$\epsilon(k) = \frac{k^2}{2m} + \int_{st} \mathcal{U}(s,t,k)$$

Strategy of the Self-energy resummation

$$E = E_{FG} + \int_{st} \mathcal{E}(s,t)$$

PS approx.

Lee-Yang

$$E_{PS}$$

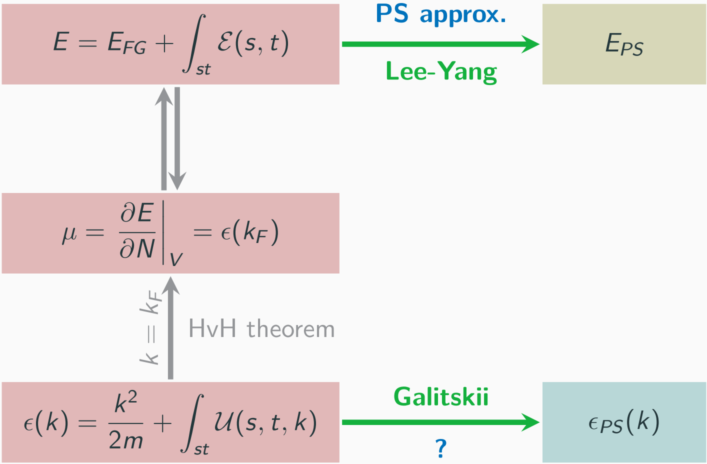
$$\mu = \left.\frac{\partial E}{\partial N}\right|_V = \epsilon(k_F)$$

$k = k_F$

HvH theorem

$$\epsilon(k) = \frac{k^2}{2m} + \int_{st} \mathcal{U}(s,t,k)$$

Strategy of the Self-energy resummation



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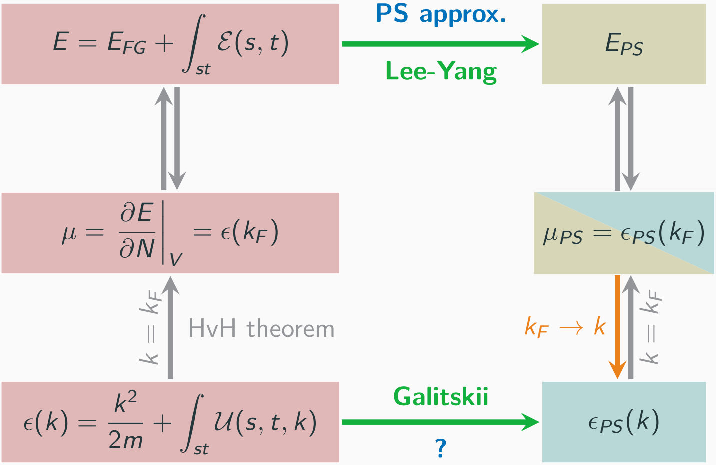

Phase-space average approximation: GPS case

$$\frac{E}{E_{FG}} = 1 + \frac{10}{9\pi} \frac{(a_s k_F)}{1 - (a_s k_F/\pi) \frac{9\pi^2}{14} \phi_2(k_F)}$$

Phase-space average approximation: GPS case

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$$\mu = \left.\frac{\partial E}{\partial N}\right|_V$$

$$\frac{\mu}{\mu_{FG}} = 1 + \frac{4}{3} \frac{(a_s k_F)}{\pi - (a_s k_F)\frac{9\pi^2}{14}\phi_2(k_F)} + \frac{2}{9} \frac{(a_s k_F)^2 \frac{9\pi^2}{14}\phi_2(k_F)}{\left[\pi - (a_s k_F)\frac{9\pi^2}{14}\phi_2(k_F)\right]^2}$$

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$$\phi_2(k_F) \rightarrow \phi_2(k)$$

$$\frac{\epsilon(k)}{\mu_{FG}} = 1 + \frac{4}{3}\frac{(a_s k_F)}{\pi - (a_s k_F)\frac{9\pi^2}{14}\phi_2(k)} + \frac{2}{9}\frac{(a_s k_F)^2 \frac{9\pi^2}{14}\phi_2(k)}{\left[\pi - (a_s k_F)\frac{9\pi^2}{14}\phi_2(k)\right]^2}$$

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$$\mu = \left.\frac{\partial E}{\partial N}\right|_V$$

✓ Lee-Yang Formula

$$\frac{\mu}{\mu_{FG}} = 1 + \frac{4}{3}\frac{(a_s k_F)}{\pi - (a_s k_F)\frac{9\pi^2}{14}\phi_2(k_F)} + \frac{2}{9}\frac{(a_s k_F)^2\frac{9\pi^2}{14}\phi_2(k_F)}{\left[\pi - (a_s k_F)\frac{9\pi^2}{14}\phi_2(k_F)\right]^2}$$

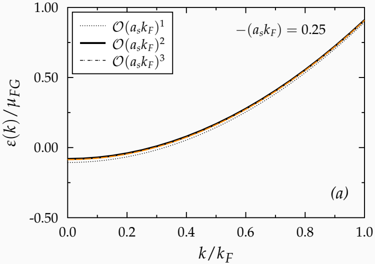
$$\phi_2(k_F) \to \phi_2(k)$$

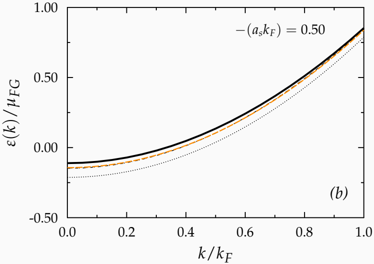
✓ HvH theorem $\mu = \epsilon(k_F)$

$$\frac{\epsilon(k)}{\mu_{FG}} = 1 + \frac{4}{3}\frac{(a_s k_F)}{\pi - (a_s k_F)\frac{9\pi^2}{14}\phi_2(k)} + \frac{2}{9}\frac{(a_s k_F)^2\frac{9\pi^2}{14}\phi_2(k)}{\left[\pi - (a_s k_F)\frac{9\pi^2}{14}\phi_2(k)\right]^2}$$

✓ Galitskii Formula

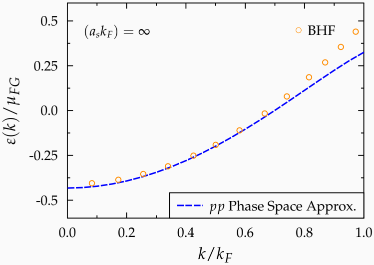
Single particle energy





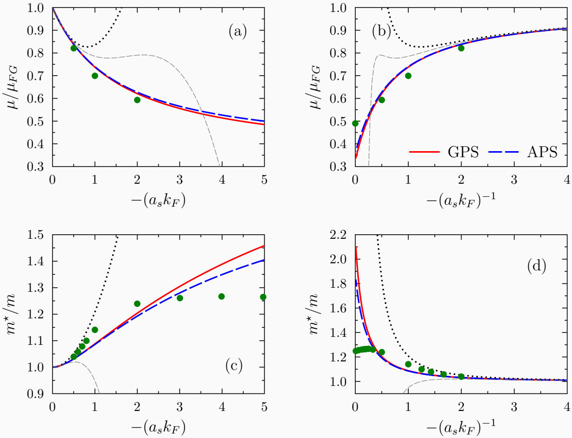
MBPT: [Platter *et al.*, NPA714 (2003)]
[AB, Lacroix, J. Phys. G]

- ✓ exact expansion up to $(a_s k_F)^2$
  $\rightarrow$ Galitskii formula
- ✓ pathologies removed for
  $a_s k_F \gg 1$ (more predictive)
- ✓ simpler function of the density



BHF: [Doggen et al., Nature (2015)]

Chemical potential and effective mass



$\mu = \epsilon(k_F)$

$$\frac{m}{m^\star} = \frac{m}{k_F}\frac{\partial \epsilon_k}{\partial k}\bigg|_{k_F}$$

MBPT:
[Platter *et al.*, NPA714 (2003)]

BHF (●):
[Doggen et al., Nature (2015)]

- ✓ Expansion valid up to $(a_s k_F)^2 \rightarrow$ Galitskii formula
- ✓ Simple and explicit dependence in density
- ✓ Finite limit at Unitarity

[AB, Lacroix, J. Phys. G]

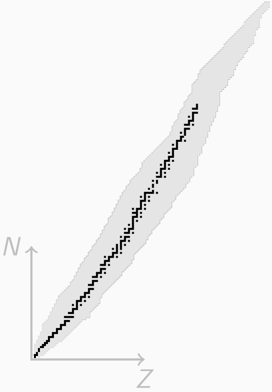
Summary and outlook

- Ladder (*pp* or *pp*/*hh*) resummation from E to $\Sigma^{\star}(k)$
  - ✗ quite complex density dependence
  - ✗ strong dependence on the selected diagrams
- **Phase-space approximation of the energy**
  - ✓ **simple and explicit density dependence**
  - ✓ **predictive from low density to unitarity without adjustment**
- **Phase-space approximation of the self-energy**
  - ✓ **simple and explicit density dependence**
  - ✓ **predictive at low and intermediate density**
  - ✗ Unitary limit far from expected results: need to be adjusted
  - ✗ Pairing effect: from normal to superfluid

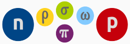
Perspectives towards non-empirical EDF

- Cross-fertilization: EDF vs. *ab initio* → experiment
- Complicated but generalizable
  (higher order in the interaction, pairing, bound states,...)
- *Make explicit the link with density functional theory*
  → *apply to finite systems*

Context and motivation



Context and motivation



$V_2, V_3, \ldots$

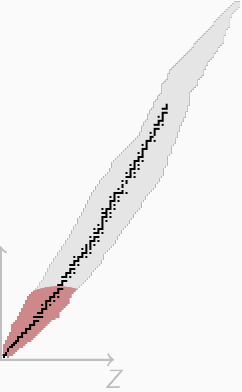
$\rightarrow$ LECs

Ab-initio

BHF,SCGF,QMC,...

static (also a bit of dynamic)
properties of some nuclei
and infinite nuclear matter

Results



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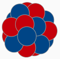

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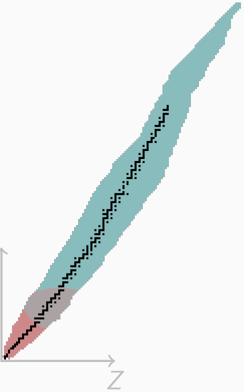
Results

structure of atomic nuclei
small/large amplitude dynamics
thermodynamics

Density Functional Theory (DFT)



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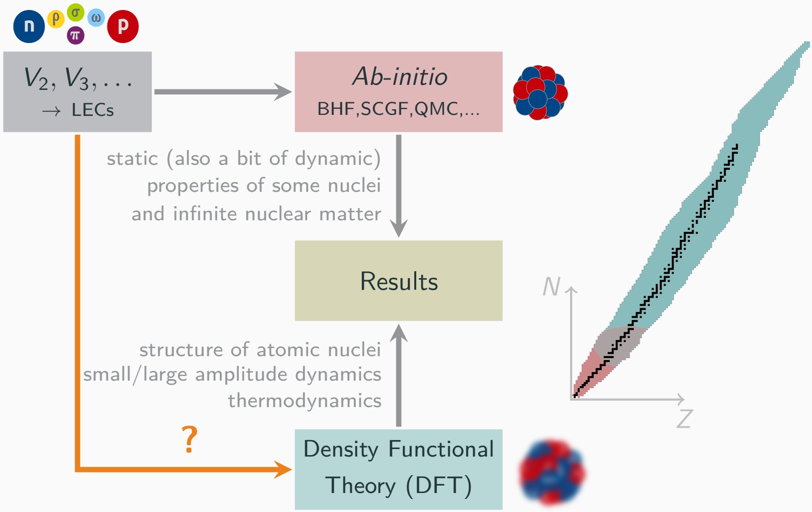

How to relate the bare interaction to DFT and make it less empirical?

In this work $\rightarrow$ a focus on infinite matter

Low density Fermi gas limit as a guidance

$$\langle \boldsymbol{k} | V_{EFT} | \boldsymbol{k'} \rangle = \underbrace{C_0 + \frac{C_2}{2}\left[\boldsymbol{k}^2 + \boldsymbol{k'}^2\right]}_{s-wave} + \cdots$$

[Steele and Furnstahl, NPA762 (2000)]
[Beane et al., nucl-th/0008064 (2000)]
[Hammer and Furnstahl, NPA678 (2000)]

$$C_0 = \frac{4\pi}{m} a_s \quad C_2 = \frac{2\pi}{m} a_s^2 r_s$$

Neutron Matter

$a_s = -18.9$ fm $\quad r_s = 2.7$ fm

$$E\left(\rho = \frac{k_F^3}{3\pi^2}\right) = \frac{3}{5}\frac{k_F^2}{2m} + E^{(1)} + E^{(2)} + \cdots = \frac{3}{5}\frac{k_F^2}{2m}\left[1 + \frac{10}{9\pi}(a_s k_F) + \cdots\right]$$

Difficulties of the perturbative approach

- Perturbative approach valid if $|a_s k_F| \ll 1$
- Non perturbative approaches
  - Standard MB techniques: BHF, SCGF, QMC, AFDMC, ...
    - ✗ non-analytical in $a_s k_F$
  - Resummation technique
    - ✓ analytical in $a_s k_F$ (compatible with a DFT point of view)

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Connect EFT to EDF? (neuron matter case in s-wave channel)

Pionless EFT

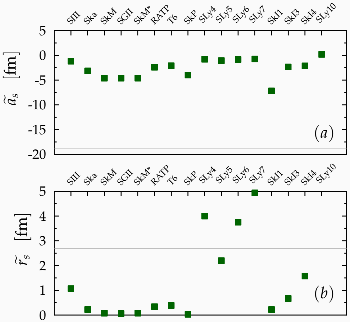
$$\langle \boldsymbol{k'} | V_{nn}^{EFT} | \boldsymbol{k} \rangle = C_0 + \frac{C_2}{2}\left[\boldsymbol{k'}^2 + \boldsymbol{k}^2\right] + \cdots$$

$$C_0 = \frac{4\pi a_s}{m} \quad \& \quad \frac{C_2}{C_0} = \frac{a_s r_s}{2}$$

Skyrme effective interaction

$$\langle \boldsymbol{k'} | V_{nn}^{Sk} | \boldsymbol{k} \rangle = t_0(1 - x_0) + \frac{1}{2} t_1(1 - x_1)\left[\boldsymbol{k'}^2 + \boldsymbol{k}^2\right] + \cdots$$

$$t_0(1 - x_0) = \frac{4\pi \widetilde{a}_s}{m} \quad \& \quad \frac{t_1(1 - x_1)}{t_0(1 - x_0)} = \frac{\widetilde{a}_s \widetilde{r}_s}{2}$$



- Similar expression
- Skyrme parameters $\neq$ physical LECs

Strong renormalization of the LECs from vacuum to saturation

How to relate the bare interaction to DFT and make it less empirical?

$\downarrow$

Can we understand the value of parameters entering in the empirical EDFs?

One of the explored solution $\rightarrow$ resummation techniques

Can we understand the empirical Skyrme parameters?

Starting point:

$$\frac{E}{E_{FG}} = 1 + \frac{16}{3\pi}\,\text{atan}\,\frac{5/24(a_s k_F)}{1-(a_s k_F/\pi)\langle R\rangle}$$

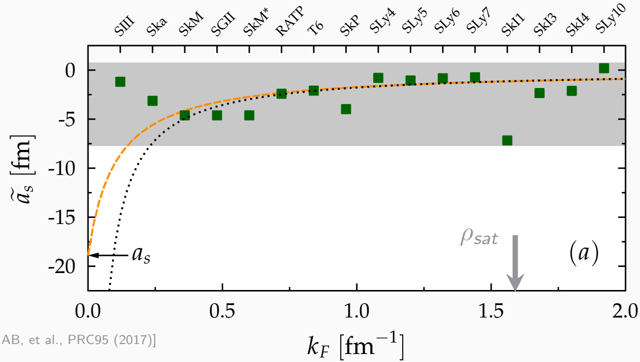
Rewritten as:

$$\frac{E}{E_{FG}} = 1 + \frac{10}{9\pi}\left[\widetilde{a}_s(k_F)k_F\right]$$

Skyrme: $V_{Sk} = t_0(1-x_0)\delta(\boldsymbol{r})$

$$\frac{E}{E_{FG}} = 1 + \frac{10}{9\pi}\left[\widetilde{a}_s k_F\right]$$

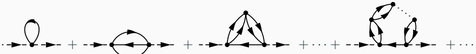
with: $\frac{4\pi}{m}\widetilde{a}_s = t_0(1-x_0)$



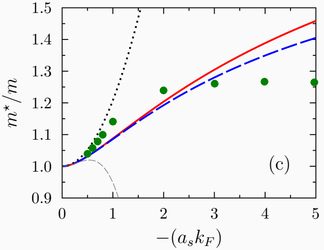
see also: [Lacroix, AB, et al., PRC95 (2017)]

Towards finite systems

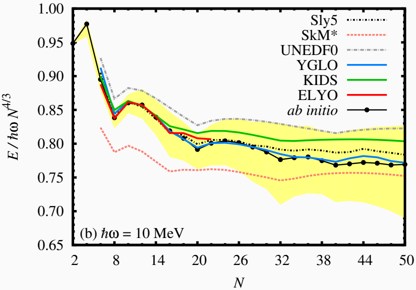
- Quasi-particle properties
  effective effective mass $m^{\star} \sim t_1(\rho)$
  $\rightarrow$ self-energy (single particle potential)

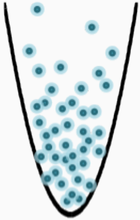


[AB, Lacroix, J. Phys. G]



- First step towards finite systems $\rightarrow \nabla\rho, \ldots$
  (Beyond Local Density Approximation)





[Bonnard, Grasso, Lacroix, PRC98 (2018)]