Quasi-particle properties of Fermi gases from low density to unitary limits

Bridging nuclear *ab-initio* and density functional theories

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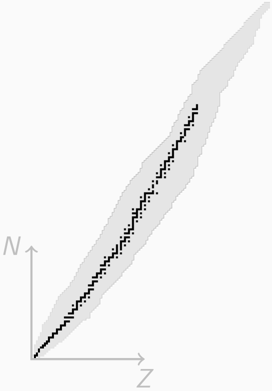
Symposium on Nuclear Structure and Reactions:
The Next Significant Breakthroughs
19th march 2019

Context and motivation



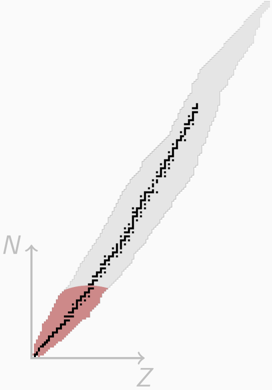
Context and motivation

$V_2, V_3, \ldots$
$\rightarrow$ 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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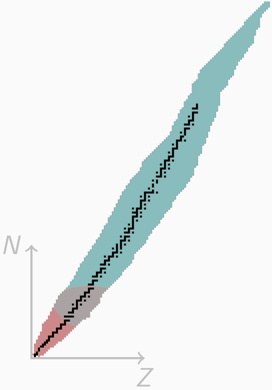
Results

structure of atomic nuclei
small/large amplitude dynamics
thermodynamics

Density Functional Theory (DFT)



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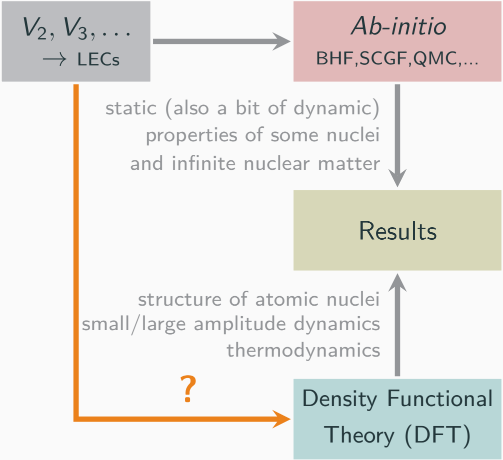
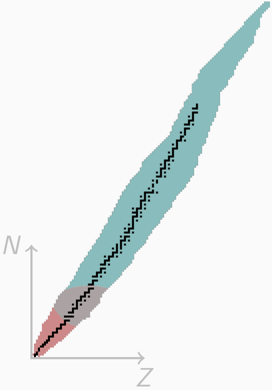




How to relate the bare interaction to DFT and make it less empirical?

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

Contents

1. Many-Body Perturbation Theory for dilute Fermi gas
   in a effective field theory framework
2. Non-perturbative approach: resummation technique

Goal

obtain explicit and simple form for the energy (self-energy)
as function of:

- *the density*
- *the low energy constants of the interaction*

The low-density Fermi gas limit: EFT 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)]

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

Neutron Matter

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

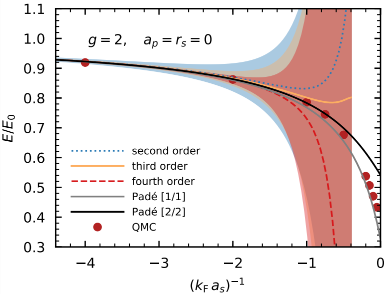
$$r_s = 2.7 \text{ fm}$$

Constructive MBPT

✓ GS energy up to fourth order

[Wellenhofer *et al.*, arXiv (2019)]

UV divergence properly treated
[Kaplan, Savage, Wise, NPB534 (1998)]



Lee-Yang energy density functional

$$E(\rho) = E_{FG} + E^{(1)} + E^{(2)} + \cdots \qquad \left[E_{FG} = \frac{3}{5}\frac{k_F^2}{2m}\rho \;\middle|\; \rho = \frac{k_F^3}{3\pi^2} \right]$$

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

$$= \frac{3(3\pi^2)^{2/3}}{10m}\rho^{5/3} + \frac{\pi a_s}{m}\rho^2 + \frac{6(11 - 2\ln 2)a_s^2}{35(3\pi^2)^{-1/3}m}\rho^{7/3} + \cdots$$

✓ analytical dependence in term of ρ and a_s

Difficulties of the perturbative approach

- Perturbative approach valid if $|a_s k_F| \ll 1$

  Neutron matter: $a_s = -18.9$ fm $\rightarrow \rho \lesssim 10^{-6}$ fm$^{-3} \ll \rho_0 \simeq 0.16$ fm^3

- Non perturbative approaches
  - Standard MB techniques: BHF, SCGF, QMC, AFDMC, ...
    - ✓ very powerful
    - ✗ not explicit in $a_s k_F$
  - Resummation technique
    - ✓ analytical in $a_s k_F$ (compatible with a DFT point of view)

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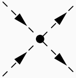
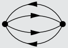
[Hammer and Furnstahl, NPA678 (2000)]

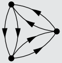
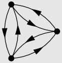
$G(\omega, \boldsymbol{k}) =$  $= \dfrac{n_k}{\omega - e_k + i0^-} + \dfrac{1 - n_k}{\omega - e_k + i0^+}$

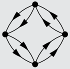
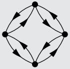
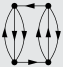
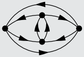
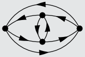
$\langle \boldsymbol{k} | V_{EFT} | \boldsymbol{k'} \rangle =$  $= C_0$ $\quad [n_k = \Theta(k_F - k) \mid e_k = k^2/2m]$

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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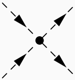
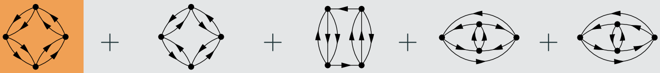
$\langle \boldsymbol{k} | V_{EFT} | \boldsymbol{k'} \rangle =$  $= C_0$ $\qquad [n_k = \Theta(k_F - k) \mid e_k = k^2/2m]$

Contributing energy diagrams [Ladder approximation]

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

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

$E_{(3)} =$ 

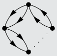
$E_{(4)} =$ 

[Kaiser, NPA860 (2011)]

Ladder approximation for the energy

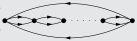
Energy resummation

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



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

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



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

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

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

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

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

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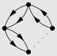

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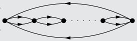
$$E_{int}^{pp} = \sum_{n=1}^{\infty}$$



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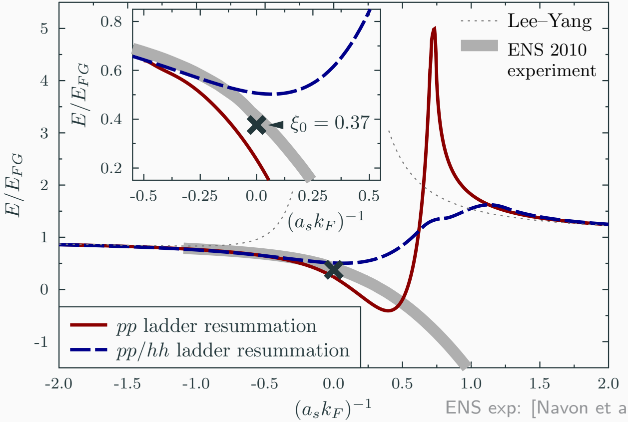
[Kaiser, NPA860 (2011)] (no pairing, no self-consistency)

- ✓ 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



ENS exp: [Navon et al., Science 328 (2010)]

- ✓ 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

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

PSA of *pp* ladder resummation = GPS functional

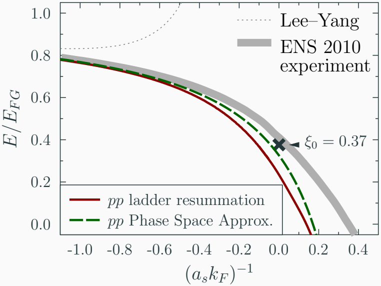
$$\frac{E}{E_{FG}} = 1 + \frac{10}{9\pi} \frac{(a_s k_F)}{1-(a_s k_F/\pi)\langle F \rangle} \underset{a_s k_F \to \infty}{\longrightarrow} 0.32$$

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

✓ Lee–Yang formula

$$\langle F \rangle = \frac{6}{35}(11 - 2\ln 2)$$

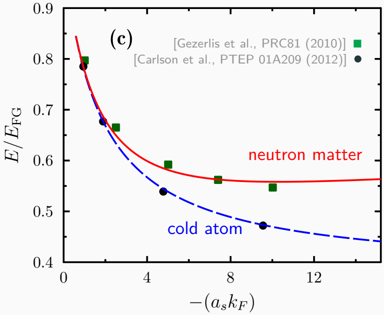
∼ More predictive near unitarity: $\xi_0 = 0.37$ (accepted value)



$$\frac{E}{E_{FG}} = 1 + \frac{\frac{10}{9\pi}(a_s k_F)}{1 - \frac{6}{35\pi}(11 - 2\ln 2)(a_s k_F)} \rightarrow 1 + \frac{\frac{10}{9\pi}(a_s k_F)}{1 - \frac{10}{9\pi}(1-\xi_0)^{-1}(a_s k_F)}$$

[Lacroix, PRA94 (2016)]
[Lacroix, AB, et al., PRC 95 (2017)]

- ✓ unitary limit reproduced
- ✗ Lee-Yang formula



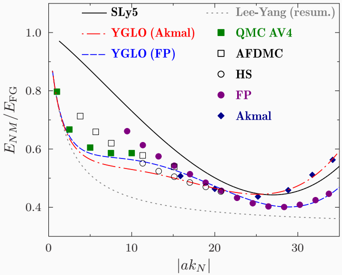
$$\rightarrow \frac{E}{A} = K + \frac{B\rho}{1 - R\rho^{1/3} + C\rho^{2/3}} + D\rho^{5/3} + F\rho^{\alpha+1}$$

YGLO functional

B, R: Lee–Yang (low density)
→ non-empirical

C, D, F: higher correlations (fit)
→ empirical

[Yang, Grasso, Lacroix, PRC94 (2016)]

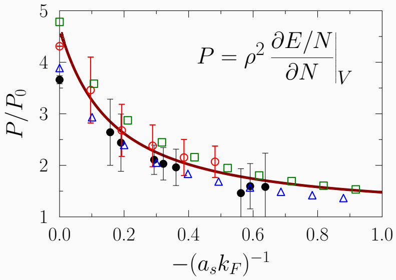


$$\frac{E}{E_{FG}} = 1 + \frac{80}{\pi k_F^5} \underbrace{\int s^2 ds \int t dt}_{\text{accessible phase space}} \operatorname{atan} \frac{(a_s k_F) I(s,t)}{1 - (a_s k_F/\pi) R(s,t)} \underset{a_s k_F \to \infty}{=} 0.51$$

PSA of full ladder resummation = APS functional

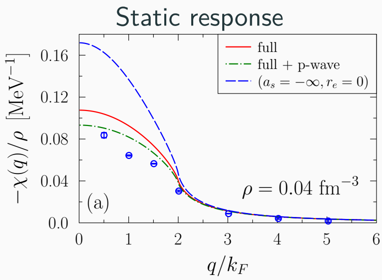
$$\frac{E}{E_{FG}} = 1 + \frac{16}{3\pi} \operatorname{atan} \frac{5/24 (a_s k_F)}{1 - (a_s k_F/\pi) \langle R \rangle} \underset{a_s k_F \to \infty}{=} \mathbf{0.36}$$

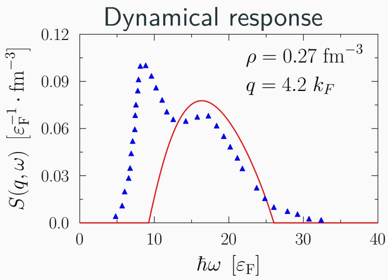
- ✓ Unitary limit well reproduced (accepted value: $\xi_0 = 0.37$)
- ✓ Exact Lee–Yang expansion
- ✓ **No adjustment !**



[AB, Lacroix, submitted to J. Phys. G]

Discussion





✗ effective mass $m^\star$

✗ pairing gap Δ

[AB, Lacroix, PRC97 (2018)]

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

Quasi-particle properties:
Self-Energy Resummation

Ladder Resummation +

Phase-Space average Approximation

Link with Landau theory of Fermi liquid

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

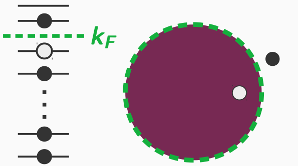
Low-lying excited states $\quad n_k \to n_k + \delta n_k$

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

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

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)]

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

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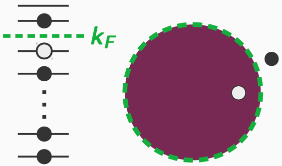


[Landau (1957)]

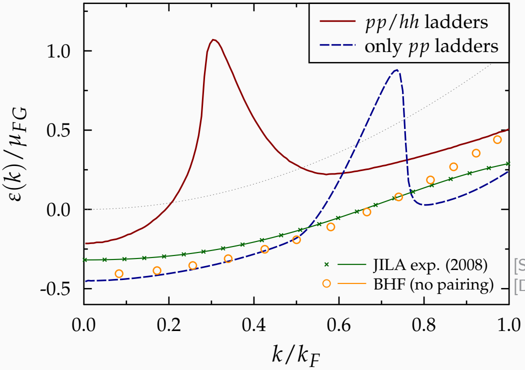
$$\left[\begin{array}{lcl} \epsilon_k & = & \frac{k^2}{2m} + U(k) \\ \frac{1}{2\gamma_k} & = & -W(k) \end{array} \right]$$

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 and Kinnumen, 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 ($a_s k_F \to \infty$)

✗ bad prediction for $a_s k_F \gg 1$: pathological

✗ strong dependence of retained diagrams

Strategy

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

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

Strategy

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

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

$k = k_F$

HvH theorem

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

Strategy

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

PS approx.

Lee-Yang

$$E_{PS}$$

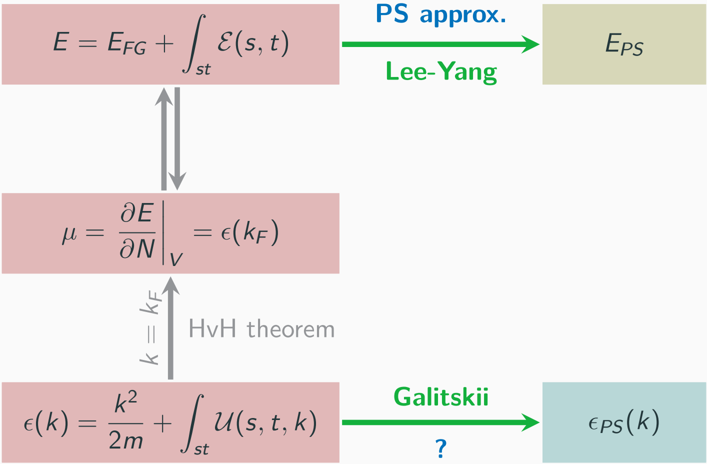
$$\mu = \left.\frac{\partial E}{\partial N}\right|_V = \epsilon(k_F)$$

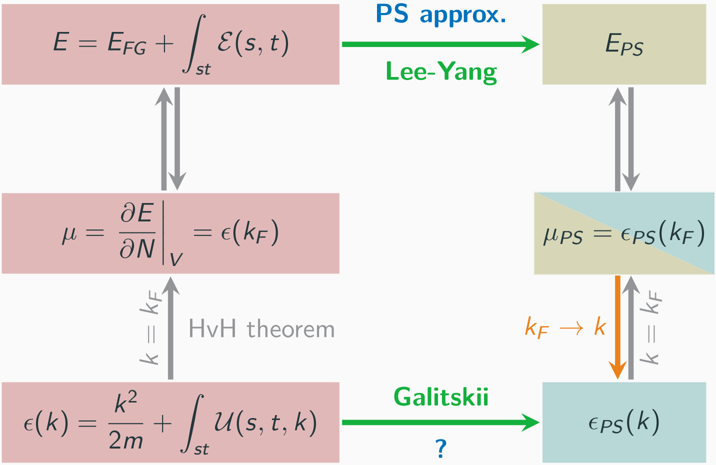
$k = k_F$

HvH theorem

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

Strategy


$E = E_{FG} + \int_{st} \mathcal{E}(s,t)$
PS approx.
Lee-Yang
E_{PS}
$\mu = \left.\frac{\partial E}{\partial N}\right|_V = \epsilon(k_F)$
$k = k_F$
HvH theorem
$\epsilon(k) = \frac{k^2}{2m} + \int_{st} \mathcal{U}(s,t,k)$
Galitskii
?
$\epsilon_{PS}(k)$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PS approx.
Lee-Yang
E_{PS}
$\mu = \left.\frac{\partial E}{\partial N}\right|_V = \epsilon(k_F)$
$\mu_{PS} = \epsilon_{PS}(k_F)$
$k = k_F$
HvH theorem
$k_F \to k$
$k = k_F$
$\epsilon(k) = \frac{k^2}{2m} + \int_{st} \mathcal{U}(s,t,k)$
Galitskii
?
$\epsilon_{PS}(k)$

Phase-space average approximation: GPS case

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

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

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

✓ Lee-Yang Formula

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

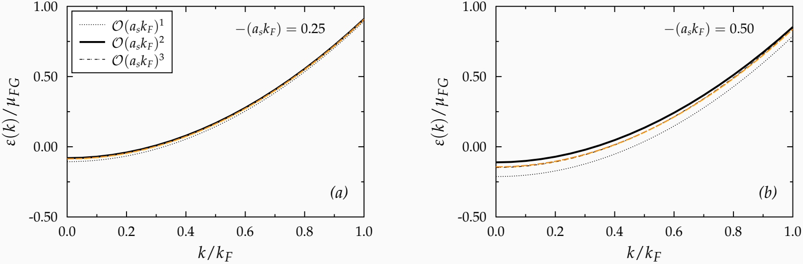
$$\phi_2(k_F) \to \phi_2(k)$$

✓ HvH theorem $\mu = \epsilon(k_F)$

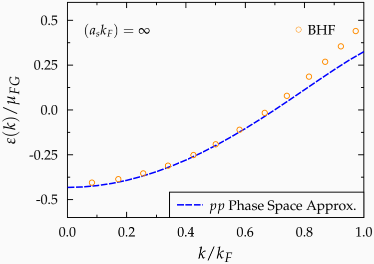
$$\frac{\epsilon(k)}{\mu_{FG}} = 1 + \frac{4}{3}\frac{(a_s k_F)}{\pi-(a_s k_F)\frac{9\pi^2}{14}\phi_2(k)} + \frac{2}{9}\frac{(a_s k_F)^2\frac{9\pi^2}{14}\phi_2(k)}{\left[\pi-(a_s k_F)\frac{9\pi^2}{14}\phi_2(k)\right]^2}$$

✓ Galitskii Formula

Single particle energy



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



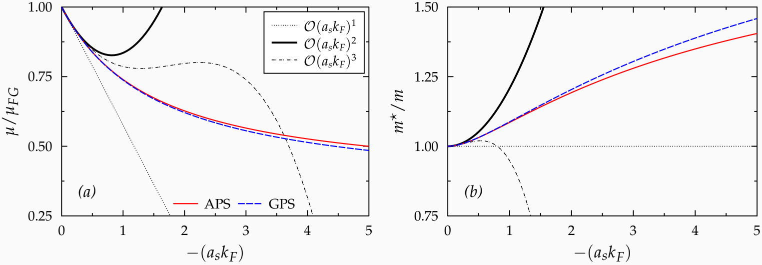
BHF: [Doggen and Kinnumen, Nature (2015)]

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

Chemical potential and effective mass

$\mu = \epsilon(k_F)$

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



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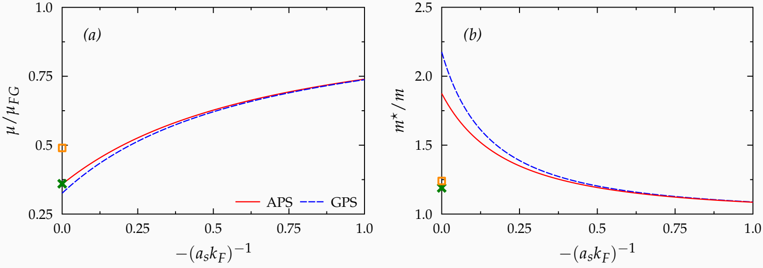
- ✓ Expansion valid up to $(a_s k_F)^2$ → Galitskii formula
- ✓ Simple and explicit dependence in density
- ✓ Finite limit at Unitarity

Discussion

$$\mu = \epsilon(k_F)$$

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



(at unitarity)	superfluid × (expected)	normal □ (expected)	GPS	APS
μ/μ_{FG}	0.37	0.49	0.32	0.36
$m^\star/m$	1.19	1.24	2.18	1.88

It seems difficult to enforce unitarity without adjustment

Summary

- 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

Perspective

Make explicit the link with density functional theory

$\rightarrow$ *apply to finite systems*