Towards *ab initio* Density Functional Theory

from atomic to nuclear systems

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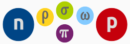
postdoctoral position seminar

2022/01/20 (University of Barcelona)

Context and Motivations

DFT vs *ab initio* description of the many-body problem

$V_2, V_3, \ldots$
$\to$ LECs



[Medvedev et al., Science **55** (2017), Furnstahl, EPJA **56** (2020)]

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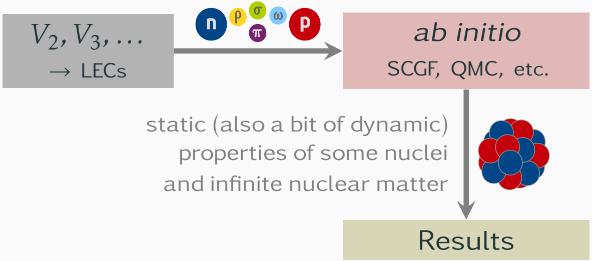

- ✓ relies on bare interaction (recent progresses)
- ✗ costly numerically (many-particle picture)

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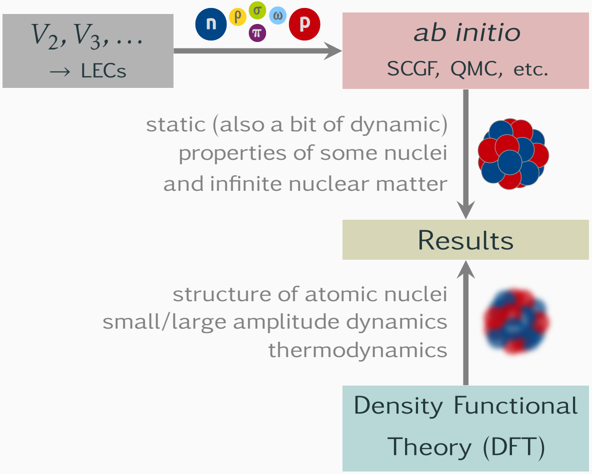

✓ relies on bare interaction (recent progresses)

✗ costly numerically (many-particle picture)

✗ fitted parameters (relative lack of predictive power)

✓ not expansive numerically (single-particle picture)

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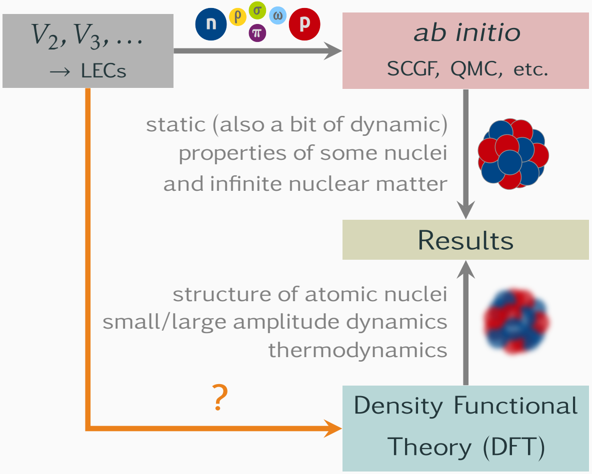

[Medvedev et al., Science **55** (2017), Furnstahl, EPJA **56** (2020)]

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$E[\{\text{densities}\}, \{\text{LECs}\}]$?

✗ fitted parameters (relative lack of predictive power)

✓ not expansive numerically (single-particle picture)

Non-empirical DFT for interacting Fermi systems?

- Low density (perturbative expansion)
- Unitarity (non-perturbative regime)

Dilute Fermi System: EFT guidance and link with ultracold atoms physics

$$\langle \boldsymbol{k}|\hat{V}|\boldsymbol{k}'\rangle = \underbrace{\frac{4\pi}{m}a_s + \frac{2\pi}{m}a_s^2 r_s \frac{\boldsymbol{k}^2 + \boldsymbol{k}'^2}{2}}_{s-wave} + \cdots$$

[Furnstahl, *EFT for DFT*]

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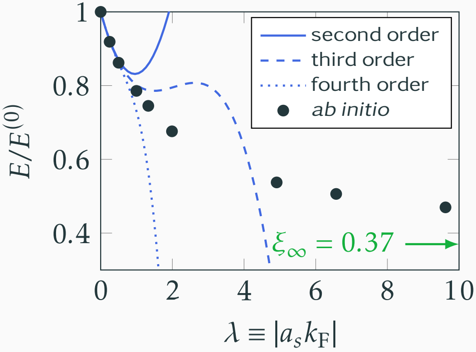

Lee – Yang formula $\lambda \equiv |a_s k_F| \ll 1$

$$E = E^{(0)} + E^{(1)} + E^{(2)} + \cdots$$

$$= E^{(0)}\left[1 - \frac{10}{9\pi}\lambda + \frac{4(11 - 2\ln 2)}{21\pi^2}\lambda^2 + \cdots\right]$$

$$n = \frac{N}{V} = \frac{k_F^3}{3\pi^2} \qquad \frac{E^{(0)}}{V} = \frac{3}{5}n\varepsilon_F \qquad \varepsilon_F = \frac{k_F^2}{2m}$$

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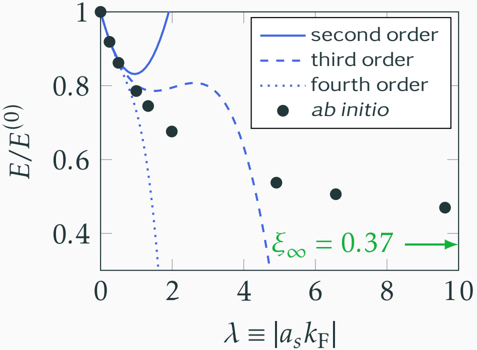

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Unitary Fermi Gas $\lambda \equiv |a_s k_F| \to \infty$

$$E = \xi_\infty E^{(0)} + \mathcal{O}(r_s k_F)$$

$$n = \frac{N}{V} = \frac{k_F^3}{3\pi^2} \qquad \frac{E^{(0)}}{V} = \frac{3}{5}n\varepsilon_F \qquad \varepsilon_F = \frac{k_F^2}{2m}$$

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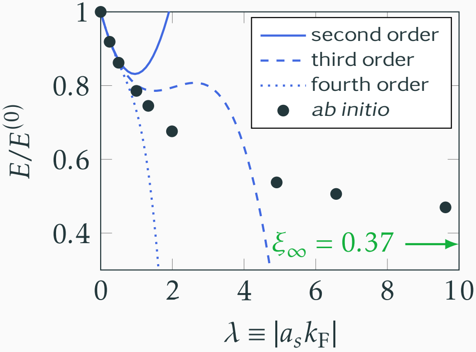

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Neutron Matter $\quad \lambda \equiv |a_s k_F| \sim 30$

$$a_s = -18.9 \text{ fm} \qquad r_s = 2.7 \text{ fm}$$

Unitary Fermi Gas $\quad \lambda \equiv |a_s k_F| \to \infty$

$$E = \xi_\infty E^{(0)} + \mathcal{O}(r_s k_\mathrm{F})$$

$$n = \frac{N}{V} = \frac{k_\mathrm{F}^3}{3\pi^2} \qquad \frac{E^{(0)}}{V} = \frac{3}{5} n \varepsilon_\mathrm{F} \qquad \varepsilon_\mathrm{F} = \frac{k_\mathrm{F}^2}{2m}$$

DFT from EFT resummation

Resumming many-body diagrams

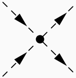
$$E = E^{(0)} + E^{(1)} + E^{(2)} + \cdots$$

[Fetter and Walecka book]

$G(\omega, \boldsymbol{k})$

$$= \frac{n_k}{\omega - e_k + i0^-} + \frac{1 - n_k}{\omega - e_k + i0^+}$$

$\langle \boldsymbol{k} | \hat{V} | \boldsymbol{k}' \rangle$



$$= \frac{4\pi a_s}{m}$$

$n_k = \theta(k_\mathrm{F} - k)$ occupation numbers

$e_k = k^2/2m$ single particle energy

Resummation of many-body diagrams

$$E = E^{(0)} + E^{(1)} + E^{(2)} + \cdots$$

[Fetter and Walecka book]

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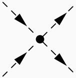
$\langle \boldsymbol{k} | \hat{V} | \boldsymbol{k}' \rangle$  $= \dfrac{4\pi a_s}{m}$

$n_k = \theta(k_F - k)$ occupation numbers

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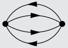
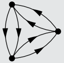
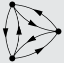
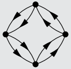
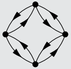
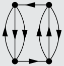
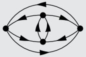
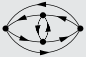
Contributing energy diagrams

$E^{(1)} =$  $\rightarrow \lambda \rightarrow$ Hartree – Fock approximation

$E^{(2)} =$  $\rightarrow \lambda^2 \rightarrow$ Lee – Yang correction

$E^{(3)} =$  $+$ 

$E^{(4)} =$  $+$  $+$  $+$  $+$ 

complexity

Resummation of many-body diagrams

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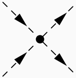
$\langle \boldsymbol{k}|\hat{V}|\boldsymbol{k}'\rangle$  $= \dfrac{4\pi a_s}{m}$

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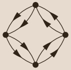
Contributing energy diagrams [Ladder approximation]

$E^{(1)} =$  $\rightarrow$ λ $\rightarrow$ Hartree – Fock approximation

$E^{(2)} =$  $\rightarrow$ λ^2 $\rightarrow$ Lee – Yang correction

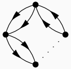
$E^{(3)} =$  + 

$E^{(4)} =$  +  +  +  + 

complexity

Phase-space average approximation

$$\frac{E}{E^{(0)}} = \frac{1}{E^{(0)}} \sum_{n=0}^{\infty}$$



$$= 1 - \frac{80}{\pi k_F^5} \overbrace{\int s^2 \, \mathrm{d}s \int t \, \mathrm{d}\, \mathrm{d}\, t}^{\text{phase space}} \arctan \frac{\lambda \pi I(s,t)}{\pi + \lambda R(s,t)} \underset{\lambda \to \infty}{=} \mathbf{0.51} \neq 0.37$$

[Kaiser NPA **860** (2005), Kaiser EPJA **49** (2013)]

Ladder Ressumation (LR)

- ✓ non-empirical function of $\lambda = |a_s k_{\mathrm{F}}|$
- ✓ match weak coupling limit
- !? complicated expression
- ✗ unitary limit not reproduced

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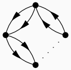
$$\frac{E}{E^{(0)}} = \frac{1}{E^{(0)}} \sum_{n=0}^{\infty}$$  $$= 1 - \frac{80}{\pi k_F^5} \overbrace{\int s^2 \, \mathrm{d}s \int t \, \mathrm{d}\, \mathrm{d}\, t}^{\text{phase space}} \arctan \frac{\lambda \pi I(s,t)}{\pi + \lambda R(s,t)} \underset{\lambda\to\infty}{=} \mathbf{0.51} \neq 0.37$$

$$\simeq 1 - \frac{16}{3\pi} \arctan \frac{\lambda \pi \langle I \rangle}{\pi + \lambda \langle R \rangle} \underset{\lambda\to\infty}{=} \mathbf{0.36} \simeq 0.37$$

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[AB and Lacroix, J. Phys. G **46** (2019)]

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Phase Space Approximation (PSA)

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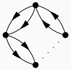
$$\frac{E}{E^{(0)}} = \frac{1}{E^{(0)}} \sum_{n=0}^{\infty}$$  $$= 1 - \frac{80}{\pi k_F^5} \underbrace{\int s^2 \, \mathrm{d}s \int t \, \mathrm{d}\,t}_{\text{phase space}} \arctan \frac{\lambda \pi I(s,t)}{\pi + \lambda R(s,t)} \underset{\lambda\to\infty}{=} \mathbf{0.51} \neq 0.37$$

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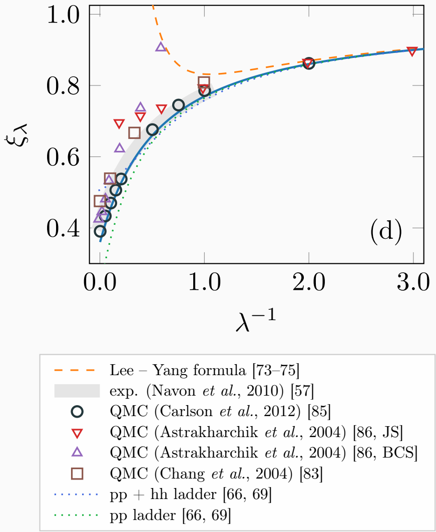
- ▶ self-energy → effective mass $\varepsilon_k \simeq \frac{k^2}{2m^\star} + U_0$


1.0
0.8
0.6
0.4
ξ_λ
0.0
1.0
2.0
3.0
λ^{-1}
(d)
Lee – Yang formula [73–75]
exp. (Navon *et al.*, 2010) [57]
QMC (Carlson *et al.*, 2012) [85]
QMC (Astrakharchik *et al.*, 2004) [86, JS]
QMC (Astrakharchik *et al.*, 2004) [86, BCS]
QMC (Chang *et al.*, 2004) [83]
pp + hh ladder [66, 69]
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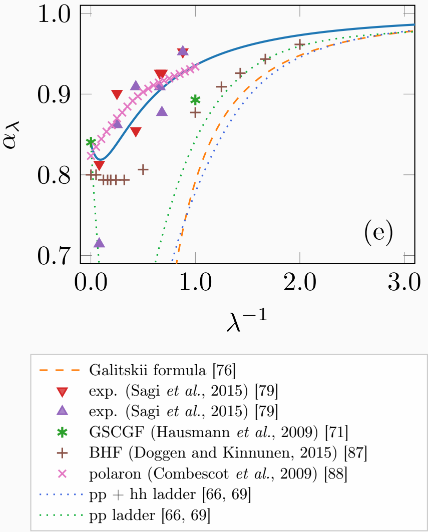
1.0
0.9
0.8
0.7
α_λ
0.0
1.0
2.0
3.0
λ^{-1}
(e)
Galitskii formula [76]
exp. (Sagi *et al.*, 2015) [79]
exp. (Sagi *et al.*, 2015) [79]
GSCGF (Hausmann *et al.*, 2009) [71]
BHF (Doggen and Kinnunen, 2015) [87]
polaron (Combescot *et al.*, 2009) [88]
pp + hh ladder [66, 69]
pp ladder [66, 69]

What about superfluidity and finite-size systems ?

- liquid ^{3}He and ^{4}He, superconductor, etc.
- nuclear systems (atomic nuclei and neutron stars)
- ultra-cold atomic gases (bosonic and fermionic)

Systematic extension of SLDA

DFT for superfluid systems?

1965 Kohn – Sham (+ Holenberg – Kohn)
Self-Consistent Equations Including Exchange and Correlation Effects
→ only normal phase, i.e. no pairing correlation

1988 Oliveira – Gross – Kohn
Density-Functional Theory for Superconductors

1994 Wacker – Kümmel – Gross
Time-Dependent Density-Functional Theory for Superconductors

2002 Bulgac (BCS / weak coupling regime $\lambda = |a_s k_F| \ll 1$)
Local Density *Approximation for Systems with Pairing Correlations*
→ crucial advance for numerical treatment

2007 Bulgac (unitary regime $\lambda = |a_s k_F| = \infty$)
Local Density *Functional Theory for Superfluid Fermionic Systems: The Unitary Gas*
→ lot of successful applications

2022 ...

Local Density Approximation for superfluidity

$$E = \int \mathrm{d}\boldsymbol{r}\,\mathcal{E}(\{n,\nu,\tau\}(\boldsymbol{r})) \quad \overset{\text{B. T.}}{\longrightarrow} \quad E_k \begin{bmatrix} u_k(\boldsymbol{r}) \\ v_k(\boldsymbol{r}) \end{bmatrix} = \begin{bmatrix} +h(\boldsymbol{r}) & \Delta(\boldsymbol{r}) \\ \Delta^*(\boldsymbol{r}) & -h^*(\boldsymbol{r}) \end{bmatrix} \begin{bmatrix} u_k(\boldsymbol{r}) \\ v_k(\boldsymbol{r}) \end{bmatrix}$$

densities (+ proper renormalization with cutoff)

$$n(\boldsymbol{r}) = \sum_k |v_k(\boldsymbol{r})|^2 \qquad \nu(\boldsymbol{r}) = \frac{1}{2}\sum_k u_k(\boldsymbol{r}) v_k^*(\boldsymbol{r}) \qquad \tau(\boldsymbol{r}) = \sum_k |\nabla v_k(\boldsymbol{r})|^2$$

potentials $\boldsymbol{h = h(U, \Delta, m^\star)}$

$$U(\boldsymbol{r}) = \frac{\delta E}{\delta n(\boldsymbol{r})} \qquad \Delta(\boldsymbol{r}) = -\frac{\delta E}{\delta \nu^*(\boldsymbol{r})} \qquad \frac{1}{2m^\star(\boldsymbol{r})} = \frac{\delta E}{\delta \tau(\boldsymbol{r})}$$

- open-source (and user friendly) W-SLDA Toolkit

  @ `https://wslda.fizyka.pw.edu.pl/`

  time-dependent $E_k \to \mathrm{i}\partial_t$, temperature effect, current density $\boldsymbol{j}$, etc.

BdG (HFB) functional

$\lambda \ll 1$

$$\mathcal{E} = \frac{\tau}{2m} + \frac{C_0\lambda}{n^{1/3}}|\nu|$$

$$E = \int \mathrm{d}\boldsymbol{r}\, \mathcal{E}(\{n, \nu, \tau\}(\boldsymbol{r}))$$

$\lambda = |a_s k_F|$

SLDA functional

$\lambda = \infty$

$$\mathcal{E} = A_\infty \frac{\tau}{2m} + \frac{3}{5} B_\infty \varepsilon_F n + \frac{C_\infty}{n^{1/3}}|\nu|$$

$$n(\boldsymbol{r}) = \frac{k_F(\boldsymbol{r})^3}{3\pi^2} \qquad \varepsilon_F(\boldsymbol{r}) = \frac{k_F(\boldsymbol{r})^2}{2m}$$

BdG and SLDA functionals

BdG (HFB) functional $\lambda \ll 1$

$$\mathcal{E} = \frac{\tau}{2m} + \frac{C_0\lambda}{n^{1/3}}|\nu|$$

SLDA extended = SLDAE

$$\mathcal{E} = A_\lambda \frac{\tau}{2m} + \frac{3}{5}B_\lambda \varepsilon_F n + \frac{C_\lambda}{n^{1/3}}|\nu|$$

SLDA functional $\lambda = \infty$

$$\mathcal{E} = A_\infty \frac{\tau}{2m} + \frac{3}{5}B_\infty \varepsilon_F n + \frac{C_\infty}{n^{1/3}}|\nu|$$

$\lambda = |a_s k_F|$

$$E = \int \mathrm{d}\boldsymbol{r}\, \mathcal{E}(\{n, \nu, \tau\}(\boldsymbol{r}))$$

Local energy density functional for superfluid Fermi gases from effective field theory.
AB, G. Wlazłowski, and P. Magierski
submited at PRA, arXiv:2201.07626 (2022)

$$n(\boldsymbol{r}) = \frac{k_F(\boldsymbol{r})^3}{3\pi^2} \qquad \varepsilon_F(\boldsymbol{r}) = \frac{k_F(\boldsymbol{r})^2}{2m}$$

SLDAE from EFT

$$E = \int \mathrm{d}\boldsymbol{r}\,\mathcal{E}(\{n, \nu, \tau\}(\boldsymbol{r})) \qquad \mathcal{E} = A_\lambda \frac{\tau}{2m} + \frac{3}{5} B_\lambda \varepsilon_\mathrm{F} n + \frac{C_\lambda}{n^{1/3}} |\nu|$$

uniform systems $\quad \varepsilon_k = \frac{k^2}{2m^\star} + U_0(B_\lambda, C_\lambda) \quad E_k = \sqrt{(\varepsilon_k - \mu)^2 + \Delta^2} \quad \varepsilon_\mathrm{F}^\star = \frac{k_\mathrm{F}^2}{2m^\star}$

SLDAE from EFT

$$E = \int \mathrm{d}\boldsymbol{r}\, \mathcal{E}(\{n, \nu, \tau\}(\boldsymbol{r}))$$

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uniform systems $\varepsilon_k = \frac{k^2}{2m^\star} + U_0(B_\lambda, C_\lambda)$ $E_k = \sqrt{(\varepsilon_k - \mu)^2 + \Delta^2}$ $\varepsilon_\mathrm{F}^\star = \frac{k_\mathrm{F}^2}{2m^\star}$

$$A_\lambda \quad \leftarrow \quad \frac{m}{m^\star} = A_\lambda + n \frac{\delta A_\lambda}{\delta n}$$

$$B_\lambda \quad \leftarrow \quad U_0 = \mu + \varepsilon_\mathrm{F}^\star \sum_{i=0}^{\infty} \mathcal{B}_i \left(\frac{\Delta}{\varepsilon_\mathrm{F}^\star}\right) \times \left[\frac{\Delta}{\varepsilon_\mathrm{F}^\star}\right]^i$$

$$C_\lambda \quad \leftarrow \quad \frac{1}{C_\lambda} = \frac{m^\star}{m} \times \sum_{i=0}^{\infty} \mathcal{C}_i \left(\frac{\Delta}{\varepsilon_\mathrm{F}^\star}\right) \times \left[\frac{\Delta}{\varepsilon_\mathrm{F}^\star}\right]^i$$

LR + PSA $\longrightarrow m^\star(\lambda), \mu(\lambda)$

ab initio / exp. $\longrightarrow \Delta(\lambda)$

- ✓ **universal expansion in $\Delta/\varepsilon_\mathrm{F}^\star$ of functional parameters!**
- ✓ generalizable systematically

SLDAE from EFT

$$E = \int \mathrm{d}\boldsymbol{r}\, \mathcal{E}(\{n, \nu, \tau\}(\boldsymbol{r}))$$

$$\mathcal{E} = A_\lambda \frac{\tau}{2m} + \frac{3}{5} B_\lambda \varepsilon_\mathrm{F} n + \frac{C_\lambda}{n^{1/3}} |\nu|$$

uniform systems $\varepsilon_k = \frac{k^2}{2m^\star} + U_0(B_\lambda, C_\lambda)$ $E_k = \sqrt{(\varepsilon_k - \mu)^2 + \Delta^2}$ $\varepsilon_\mathrm{F}^\star = \frac{k_\mathrm{F}^2}{2m^\star}$

$$A_\lambda \leftarrow \frac{m}{m^\star} = A_\lambda + n \frac{\delta A_\lambda}{\delta n}$$

$$B_\lambda \leftarrow U_0 = \mu + \varepsilon_\mathrm{F}^\star \sum_{i=0}^{\infty} \mathcal{B}_i \left(\frac{\Delta}{\varepsilon_\mathrm{F}^\star}\right) \times \left[\frac{\Delta}{\varepsilon_\mathrm{F}^\star}\right]^i$$

$$C_\lambda \leftarrow \frac{1}{C_\lambda} = \frac{m^\star}{m} \times \sum_{i=0}^{\infty} \mathcal{C}_i \left(\frac{\Delta}{\varepsilon_\mathrm{F}^\star}\right) \times \left[\frac{\Delta}{\varepsilon_\mathrm{F}^\star}\right]^i$$

LR + PSA $\longrightarrow m^\star(\lambda), \mu(\lambda)$

ab initio / exp. $\longrightarrow \Delta(\lambda)$

✓ universal expansion in $\Delta/\varepsilon_\mathrm{F}^\star$ of functional parameters!

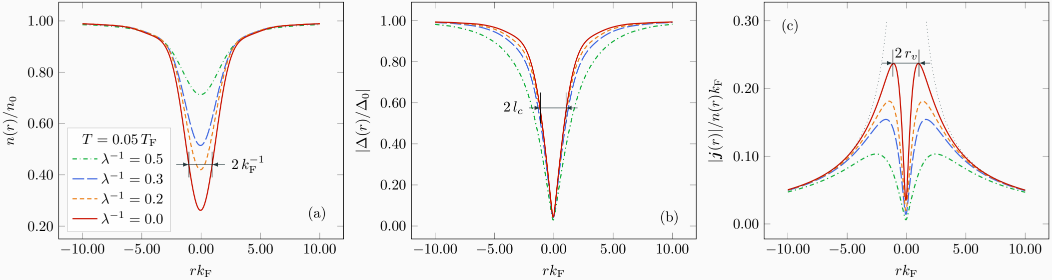
✓ generalizable systematically

non-uniform systems $\lambda = |a_s k_\mathrm{F}| \longrightarrow \lambda(\boldsymbol{r}) = |a_s k_\mathrm{F}(\boldsymbol{r})|$ $\{n, \nu, \tau\} \longrightarrow \{n, \nu, \tau\}(\boldsymbol{r})$

Structure properties

- link with recent experiments

$$\lambda^{-1} = |a_s k_F|^{-1} \lesssim 0.3 \qquad T \simeq 0.05 T_F$$



Applications to superfluid quantum vortex

Structure properties

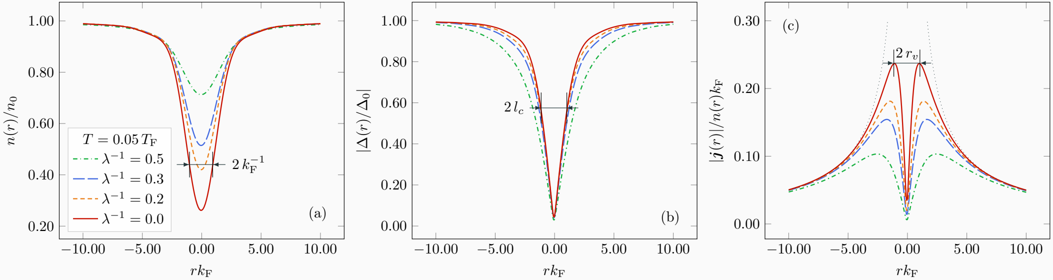
- link with recent experiments

$\lambda^{-1} = |a_s k_F|^{-1} \lesssim 0.3 \qquad T \simeq 0.05 T_F$

EFT correspondence with BCS

- systematic expression of quantities

$Q(\text{BCS}) = f(\Delta/\varepsilon_F) \quad \rightarrow \quad Q \simeq f(\Delta/\varepsilon_F^\star)$



coherence length $\qquad l_c(\text{BCS}) = \dfrac{2\varepsilon_F}{k_F|\Delta(r\to\infty)|} \quad \rightarrow \quad l_c \simeq \dfrac{2\varepsilon_F^\star}{k_F|\Delta(r\to\infty)|}$

Ongoing applications within the time-dependent (local) DFT

many quantum superfluid vortices

- dissipation (even in pure superfluid) during scattering

  A. Barresi, AB, P. Magierski, and G. Wlazłowski (coming soon)

- quantum turbulence and effect of shear viscosity

quantum quenches

- Higgs modes (i.e. $|\Delta(t)|$) and Anderson – Bogoliubov modes (i.e. $\arg \Delta(t)$)

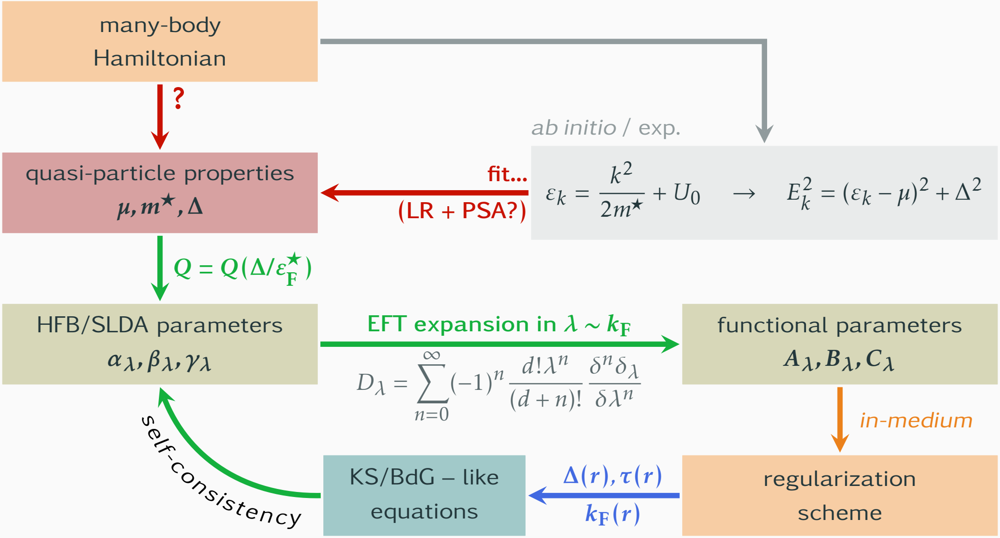
  AB, G. Wlazłowski, and P. Magierski (work in progess)

analogy with gravitation and black hole physics

- high numerical accuracy needed...

Conclusion and Outlook

Summary of the SLDAE method



Example of (long term) project towards *ab initio* DFT *via* VPT

Basic idea of Variational Perturbation Theory

[Kleinert, EJTP 8 (2011)]

$$\mathcal{S} = \mathcal{S}_0 + \mathcal{S}_{\text{int}} \quad \rightarrow \quad \mathcal{S} = \underbrace{(\mathcal{S}_0 + \mathcal{M}[U,\Delta])}_{\text{reference}} + \underbrace{(\mathcal{S}_{\text{int}} - \mathcal{M}[U,\Delta])}_{\text{perturbation}}$$

$$\frac{\delta \mathcal{S}}{\delta U} = \frac{\delta \mathcal{S}}{\delta \Delta} = 0$$

- reference (single particle)
  $\rightarrow$ KS / BdG / HFB like equations
- perturbation (diagramatic)
  $\rightarrow$ self-consistent equations

[project initiated with S. Bogner (MSU)]

✓ systematic improvement of HFB

✓ generalizable (breaking symmetry, etc.)

✓ explicit in terms of densities (Wicks contractions) ≠ Legendre transform

✓ no quantum fluctuations of the collective fields ≠ Hubbard-Stratanovich transform

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- A. Boulet and D. Lacroix, J. Phys. G: Nucl. Part. Phys. **46**, 105104 (2019).
- H. Kleinert, EJTP **8**, 57 (2011).

Towards *ab initio* Density Functional Theory

from atomic to nuclear systems

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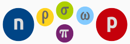
Collaborators:

D. Lacroix (IJCLab)
S. K. Bogner and W. Nazarewicz (MSU)
G. Wlazłowski and P. Magierski (WUT)

postdoctoral position interview
2022/04/07 (University of York)

DFT vs *ab initio* description of the many-body problem

$V_2, V_3, \dots$
$\rightarrow$ LECs



[Medvedev et al., Science **55** (2017), Furnstahl, EPJA **56** (2020)]

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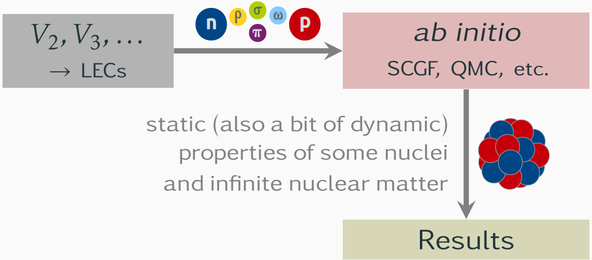

✓ relies on bare interaction (recent progresses)

✗ costly numerically (many-particle picture)

[Medvedev et al., Science **55** (2017), Furnstahl, EPJA **56** (2020)]

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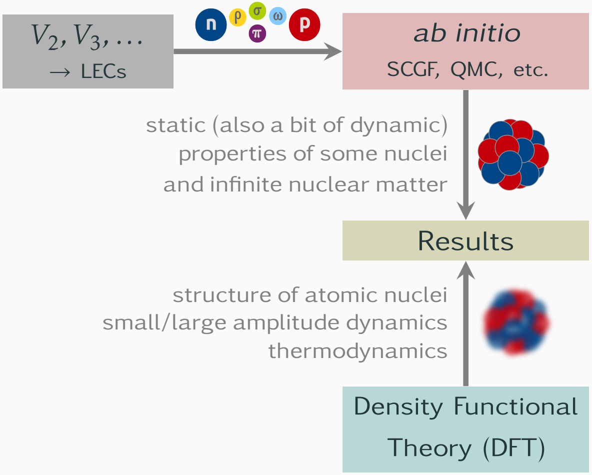

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- ✗ costly numerically (many-particle picture)

- ✗ fitted parameters (relative lack of predictive power)
- ✓ not expansive numerically (single-particle picture)

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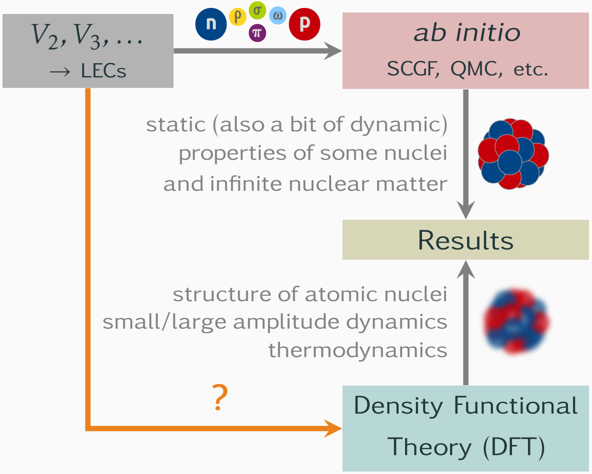

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- ✗ costly numerically (many-particle picture)

$E[\{\text{densities}\},\{\text{LECs}\}]$?

- ✗ fitted parameters (relative lack of predictive power)
- ✓ not expansive numerically (single-particle picture)

Non-empirical DFT for interacting Fermi systems?

- Low density (perturbative expansion)
- Unitarity (non-perturbative regime)

Dilute Fermi System – EFT guidance and link with ultracold atoms physics

$$\langle \boldsymbol{k}|\hat{V}|\boldsymbol{k}'\rangle = \underbrace{\frac{4\pi}{m}a_s + \frac{2\pi}{m}a_s^2 r_s \frac{\boldsymbol{k}^2 + \boldsymbol{k}'^2}{2}}_{s\text{–}wave} + \cdots$$

[Furnstahl, *EFT for DFT*]

$$\langle \boldsymbol{k} | \hat{V} | \boldsymbol{k}' \rangle = \underbrace{\frac{4\pi}{m} a_s + \frac{2\pi}{m} a_s^2 r_s \frac{\boldsymbol{k}^2 + \boldsymbol{k}'^2}{2}}_{s\text{−}wave} + \cdots$$

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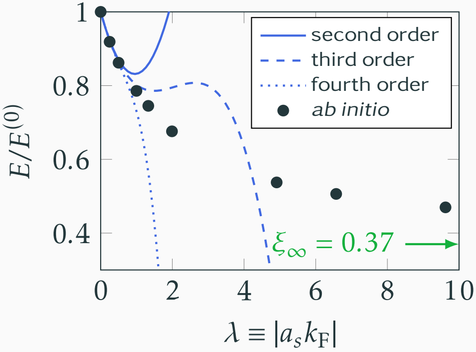

Lee – Yang formula

$\lambda \equiv |a_s k_F| \ll 1$

$$E = E^{(0)} + E^{(1)} + E^{(2)} + \cdots$$

$$= E^{(0)} \left[1 - \frac{10}{9\pi} \lambda + \frac{4(11 - 2\ln 2)}{21\pi^2} \lambda^2 + \cdots \right]$$

$$n = \frac{N}{V} = \frac{k_F^3}{3\pi^2} \qquad \frac{E^{(0)}}{V} = \frac{3}{5} n \varepsilon_F \qquad \varepsilon_F = \frac{k_F^2}{2m}$$

$$\langle \boldsymbol{k}|\hat{V}|\boldsymbol{k}'\rangle = \underbrace{\frac{4\pi}{m}a_s + \frac{2\pi}{m}a_s^2 r_s \frac{\boldsymbol{k}^2+\boldsymbol{k}'^2}{2}}_{s\text{-wave}} + \cdots$$

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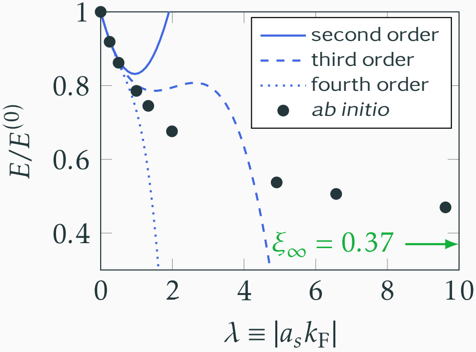

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Unitary Fermi Gas $\quad \lambda \equiv |a_s k_F| \to \infty$

$$E = \xi_\infty E^{(0)} + \mathcal{O}(r_s k_F)$$

$$n = \frac{N}{V} = \frac{k_F^3}{3\pi^2} \qquad \frac{E^{(0)}}{V} = \frac{3}{5} n \varepsilon_F \qquad \varepsilon_F = \frac{k_F^2}{2m}$$

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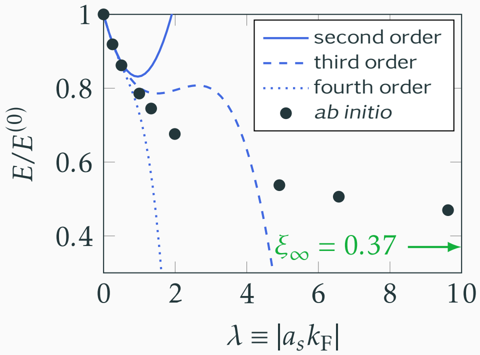

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Neutron Matter $\lambda \equiv |a_s k_F| \sim 30$

$$a_s = -18.9 \text{ fm} \qquad r_s = 2.7 \text{ fm}$$

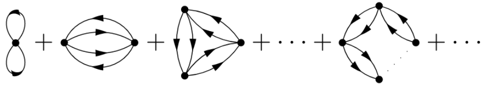
Unitary Fermi Gas $\lambda \equiv |a_s k_F| \to \infty$

$$E = \xi_\infty E^{(0)} + \mathcal{O}(r_s k_F)$$

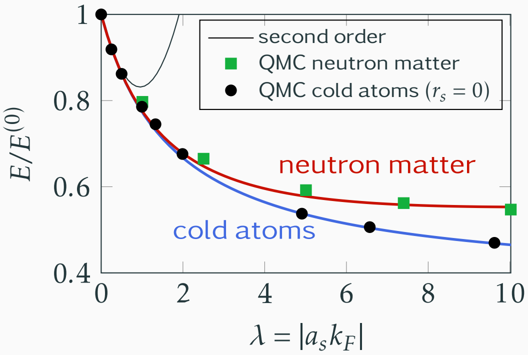
$$n = \frac{N}{V} = \frac{k_F^3}{3\pi^2} \qquad \frac{E^{(0)}}{V} = \frac{3}{5}n\varepsilon_F \qquad \varepsilon_F = \frac{k_F^2}{2m}$$

DFT from EFT resummation

$$\sum_{n=1}^{\infty} E_{(n)}^{ladder} =$$



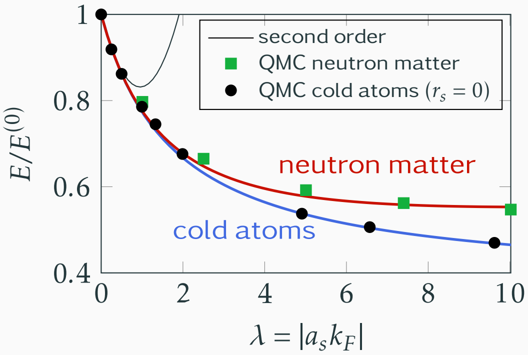
Non-empirical DFT results – dilute neutron matter $r_s \neq 0$



[Lacroix, AB, Grasso, Yang, PRC **95** (2017)]
[AB and Lacroix, PRC **97** (2018)]
[AB and Lacroix, J. Phys. G **46** (2019)]

✓ non-empirical & explicit

$$\frac{E}{E^{(0)}} = 1 - \frac{16}{3\pi}\arctan\left(\frac{5\lambda/24}{1+6(11-2\ln 2)\lambda/35\pi}\right) + f_\lambda(r_s k_F)$$



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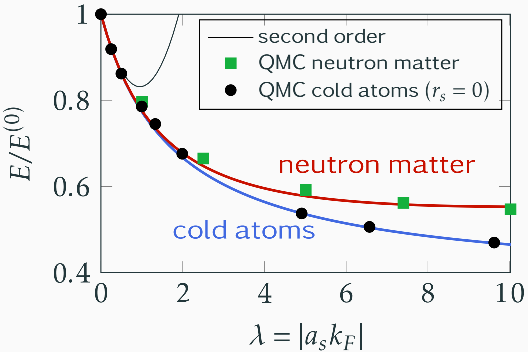
✓ **Successful applications**

- thermodynamics, collective modes, static response vs. ab-initio
- quasi-particles (effective mass, etc.)



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[AB and Lacroix, J. Phys. G **46** (2019)]

✓ non-empirical & explicit

✓ link with standard DFTs

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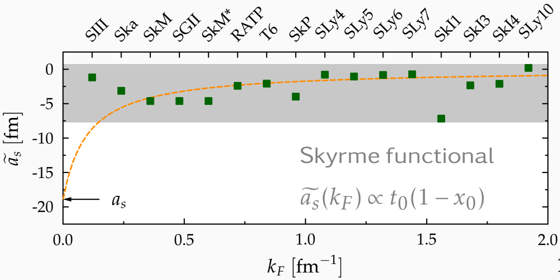
$$= 1 + \frac{10}{9\pi}[\widetilde{a_s}(k_F)k_F] + \cdots \qquad \leftarrow \qquad \text{(HF form)}$$



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- thermodynamics, collective modes, static response vs. ab-initio
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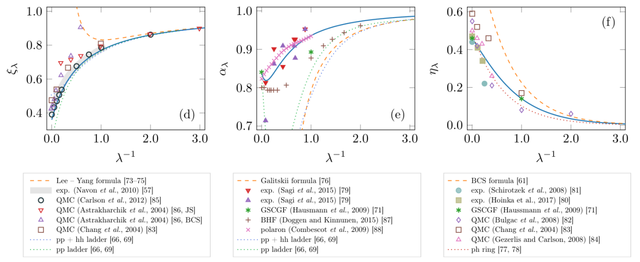
Systematic extension of SLDA



$$E = \int \mathrm{d}\boldsymbol{r}\,\mathcal{E}(\{n, \nu, \tau\}(\boldsymbol{r})) \qquad \mathcal{E} = \frac{\tau}{2m^\star} + \frac{3}{5}B_\lambda \varepsilon_\mathrm{F} n + \frac{C_\lambda}{n^{1/3}}|\nu|^2$$

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LR + PSA $\to m^\star(\lambda)$, $\mu(\lambda)$

ab initio / exp. $\to \Delta(\lambda)$

- ✓ **universal expansion in $\Delta/\varepsilon_\mathrm{F}^\star$ of functional parameters!**
- ✓ generalizable systematically

SLDAE from EFT

[AB, Wlazłowski, Magierski, arXiv:2201.07626 (2022)]

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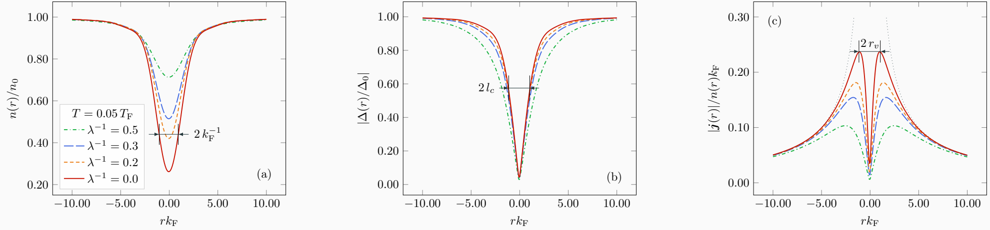
- ✓ universal expansion in $\Delta/\varepsilon_\mathrm{F}^\star$ of functional parameters!
- ✓ generalizable systematically

Implemented in *W-SLDA* toolkit (zero and finite temperature)

non-uniform systems	$\{n, \nu, \tau\} \to \{n, \nu, \tau\}(\boldsymbol{r})$	$\lambda = \lvert a_s k_\mathrm{F}\rvert \to \lambda(\boldsymbol{r})$
time-dependent problems	$\{n, \nu, \tau\} \to \{n, \nu, \tau\}(\boldsymbol{r}, t)$	$\lambda = \lvert a_s k_\mathrm{F}\rvert \to \lambda(\boldsymbol{r}, t)$

Ongoing applications within the time-dependent (local) DFT



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  AB, G. Wlazłowski, and P. Magierski (work in progess)

Summary

open to new opportunities

- formal aspects

  (e.g. MBPT, Green's function, EFT, path integral and effective action, etc.)

- numerical implementations

  (e.g. SLDAE in W-SLDA Toolkit)

- large-scale calculations on HPC

  (e.g. coordinate-space mesh for static and dynamics)

towards *ab initio* DFT via VPT (long term project)

- systematic improvement of HFB

  [project initiated with S. Bogner (MSU)]

Example of (long term) project towards *ab initio* DFT *via* VPT

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