Connecting EFT to EDF for strongly interacting fermions

Bridging nuclear *ab-initio* and density functional theories

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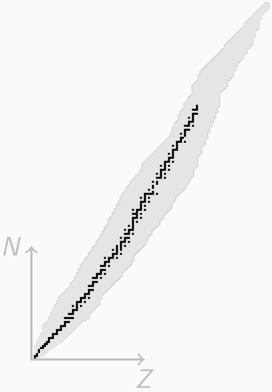
Structure Nucléaire en Ile-de-France (SNIF)
3rd Jully 2019

Context and motivation



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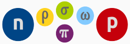
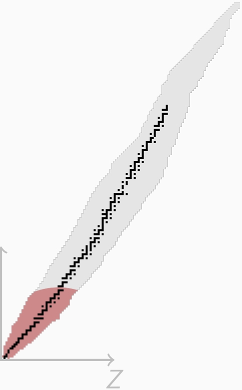


$V_2, V_3, \ldots$
$\rightarrow$ LECs

Ab-initio
BHF,SCGF,QMC,...

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

Results



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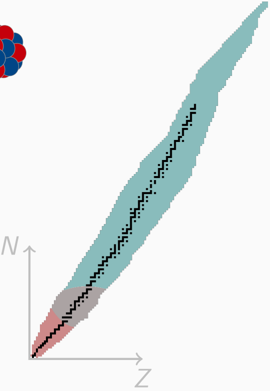
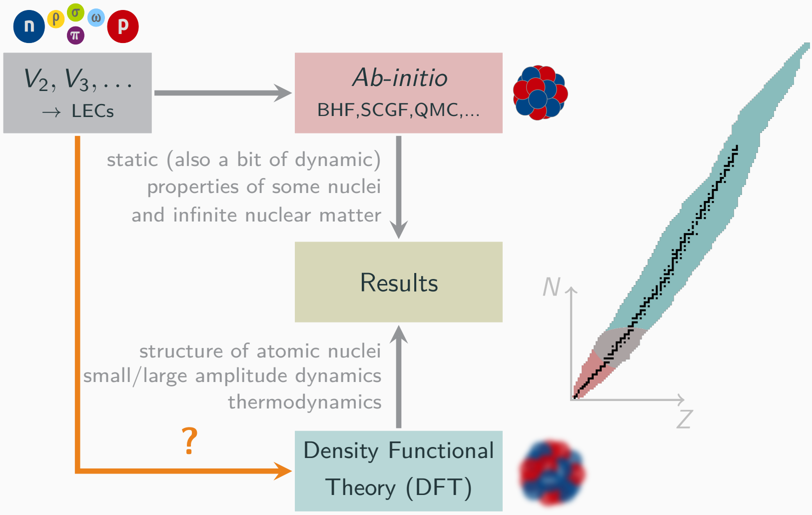


structure of atomic nuclei
small/large amplitude dynamics
thermodynamics

Density Functional Theory (DFT)

Context and motivation



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

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

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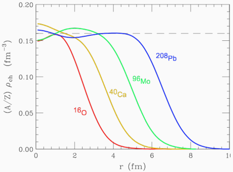
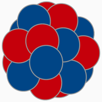
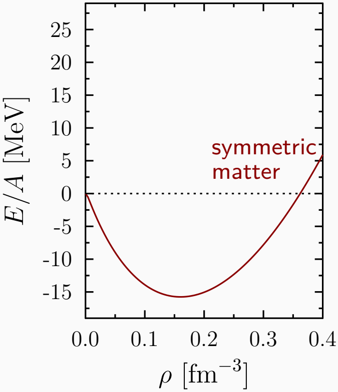
EOS of infinite matter and observations I

Saturation properties $N \simeq Z$

- At equilibrium (and near) point: $\rho_{sat} \simeq 0.16\ \text{fm}^{-3}$ & $E_{sat}/A \simeq -16$ MeV
- Incompressibility/compressibility: $K_\infty \simeq 210 \pm 30$ MeV







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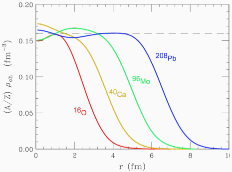
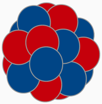
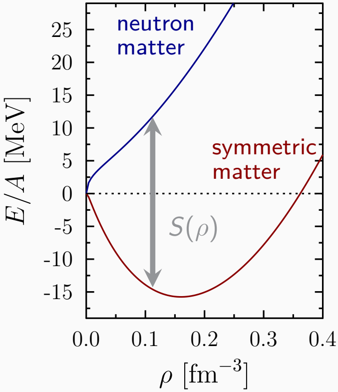
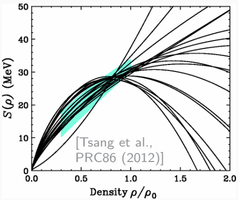


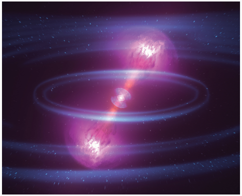




$N \neq Z$ systems

- Symmetry energy $S(\rho)$: astrophysical interest

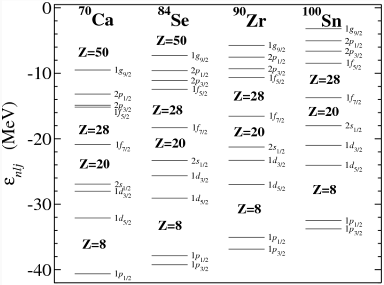




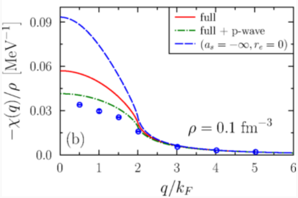
EOS of infinite matter and observations II

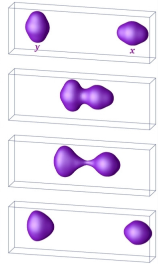
Emergence of single-particle picture of nuclear systems

- Density level (ε_{nlj})
- Quasi-particle properties (effective mass $m^\star$, ...)

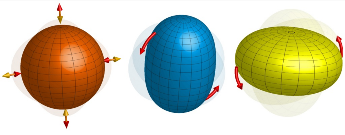


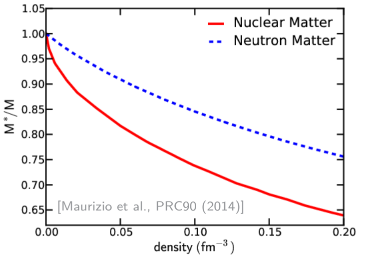
[Roca-Maza et al., PRC87 (2013)]





[Golabek & Simenel, PRL103 (2009)]

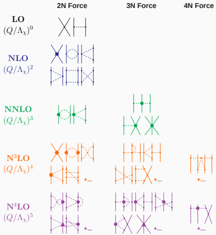


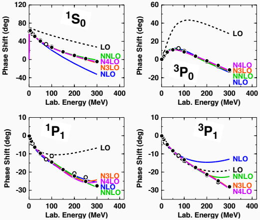


[Maurizio et al., PRC90 (2014)]

Starting point: χEFT

$\rightarrow$ low-energy constants





Epelbaum, Machleidt, van Kolck, ...

Ab initio theories applied to infinite matter

Starting point: χEFT
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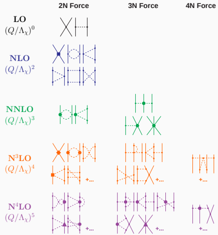

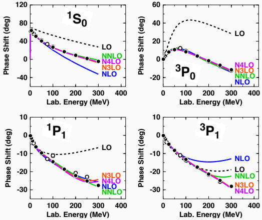

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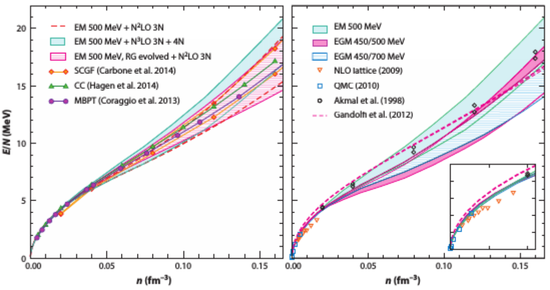

- ✓ Direct link to QCD (chiral)
- ✓ Systematic, Consistent, Constructive
- ✗ Errorbars for saturation points are large

- ✓ Exact caluclations
- ✗ Costly numerically (limitations)
- ✗ Non-explicite in term of the LECs/density

Empirical nuclear EDFs

Nuclear systems $\simeq$ independent nucleons in an external one-body field

Starting point: effective interactions (Skyrme,Gogny,...)

$$E = \langle \Psi | H | \Psi \rangle \rightarrow \langle \phi(\rho) | \mathcal{H}(\rho) | \phi(\rho) \rangle$$

$\sim$ 10 parameters to be adjusted (binding energies, radii, EOS, ...)

- ✓ Correlations Beyond Mean Field
- ✓ Static, dynamic, thermo, ...
- ✓ Accurate and simple to implement
- ✗ Relative lack of predictive power
- ✗ Link to underlying bare Hamiltonian (LECs) is lost

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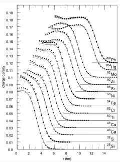

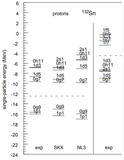

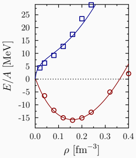

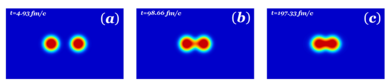

[Ebata et al. (2013)]

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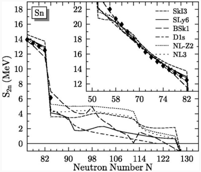
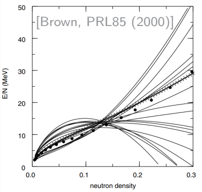
[Bender et al., RMP75 (2003)]





[Brown, PRL85 (2000)]

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

Pionless EFT

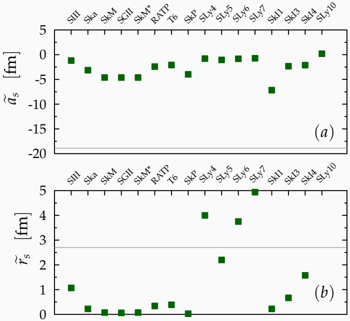
$$\langle \boldsymbol{k'} | V_{nn}^{EFT} | \boldsymbol{k} \rangle = C_0 + \frac{C_2}{2} \left[\boldsymbol{k'}^2 + \boldsymbol{k}^2 \right] + \cdots$$

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

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?

↓

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

One of the solution explored → resummation techniques

[M. Grasso, *Effective density functionals beyond mean field*, PPNP 106 (2019)]

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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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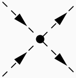
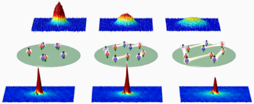
Basics of diagrammatic framework at zero temperature

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

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

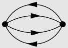
$\langle \boldsymbol{k} | V_{EFT} | \boldsymbol{k'} \rangle =$  $= C_0 = \frac{4\pi a_s}{m} \sim t_0(1 - x_0)$

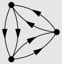
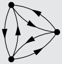
(Directly connected to ultrcold atoms physics)

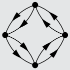
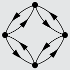
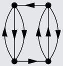
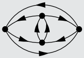
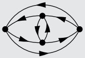


Contributing energy diagrams

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

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

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

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

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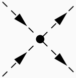
$\langle \boldsymbol{k} | V_{EFT} | \boldsymbol{k'} \rangle =$  $= C_0 = \dfrac{4\pi a_s}{m} \sim t_0(1 - x_0)$

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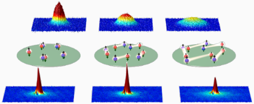

Contributing energy diagrams [Ladder approximation]

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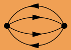
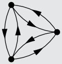
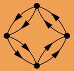
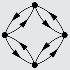
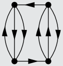
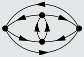
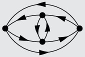
$E_{(2)} =$  $\rightarrow (a_s k_F)^2 \rightarrow Lee - Yang$

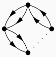
$E_{(3)} =$  $+$ 

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

[Kaiser, NPA860 (2011)]

Phase-space average Approximation (PSA)

$$\frac{E}{E_{FG}} = \sum_{n=0}^{\infty}$$



$$= 1 + \frac{80}{\pi k_F^5} \int s^2 ds \int t dt \,\mathrm{atan} \frac{(a_s k_F) I(s,t)}{1 - (a_s k_F / \pi) R(s,t)}$$

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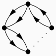
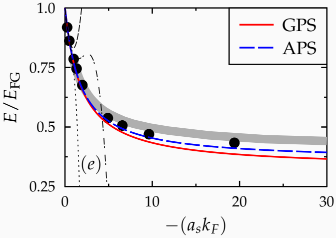
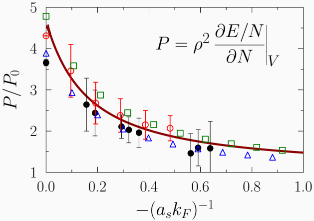

$$= 1 + \frac{80}{\pi k_F^5} \int s^2 ds \int t dt \, \mathrm{atan} \frac{(a_s k_F) I(s,t)}{1 - (a_s k_F/\pi) R(s,t)}$$

APS functional

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

- ✓ All order contributions included
- ✓ Valid at low density (exact up to 2nd order)
- ✓ Depend only on ρ (k_F) and $\boldsymbol{a_s}$: *non-empirical DFT*
- ✓ **No adjustment !**



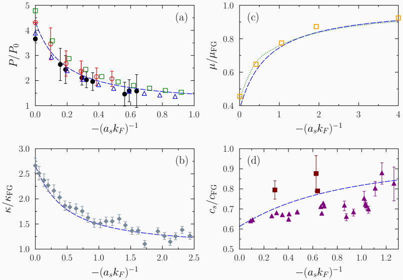


[AB, Lacroix, submitted to J. Phys. G]

Selected applications and/or extensions

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

- thermodynamics of Fermi gas



Including quasi-particle properties

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

- effective mass of Fermi gas

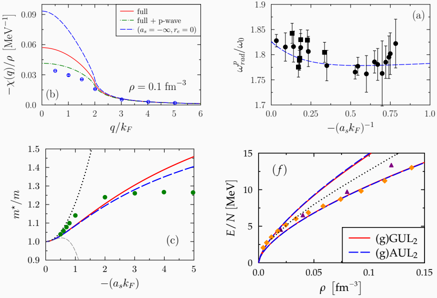
Generalization including effective range effect

- EOS of dilute neutron matter

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

- static and dynamical linear response + collective modes

  [AB, Lacroix, PRC97 (2018)]



Can we understand the empirical Skyrme parameters?

Starting point:

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

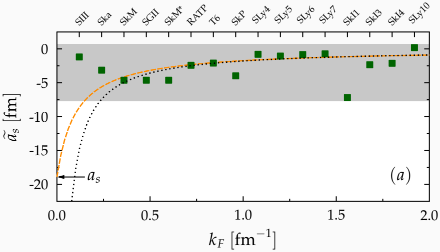
Rewritten as:

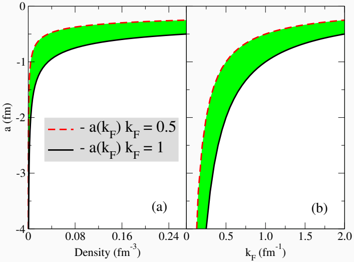
$$\frac{E}{E_{FG}} = 1 + \frac{10}{9\pi}\left[\widetilde{a}_s(k_F)k_F\right]$$

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



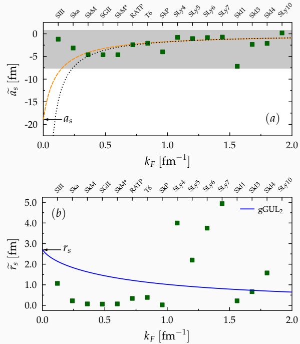


see also: [Lacroix, AB, et al., PRC95 (2017)]

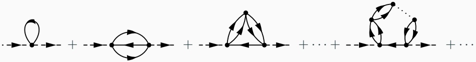
[Grasso et al., PRC95 (2017)]

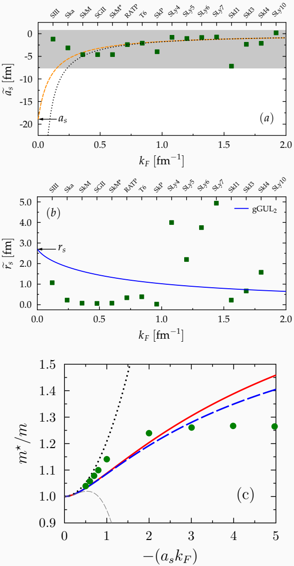
Towards finite systems

- Effective range effects $\widetilde{r}_s(\rho) \sim t_1(\rho)$
  $V = C_0 + (C_2/2)\left[\boldsymbol{k}' + \boldsymbol{k}\right]$



- Effective range effects $\widetilde{r}_s(\rho) \sim t_1(\rho)$
  $V = C_0 + (C_2/2)\left[\boldsymbol{k'} + \boldsymbol{k}\right]$
- Quasi-particle properties
  effective effective mass $m^\star \sim t_1(\rho)$
  $\rightarrow$ self-energy (single particle potential)





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

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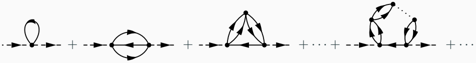
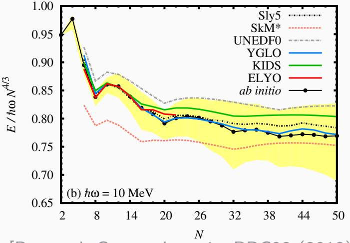
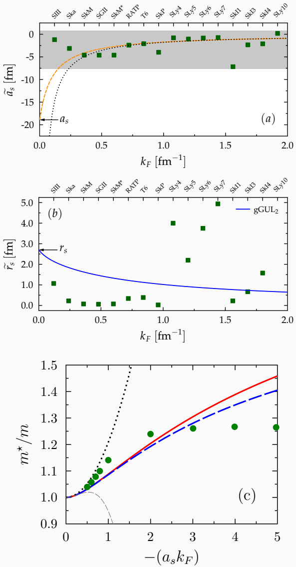


- First step towards finite systems $\rightarrow \nabla\rho, \ldots$
  (Beyond Local Density Approximation)



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



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

Summary and conclusions

- **Phase-space approximation of the energy (simplified model)**
  - ✓ **simple and explicit density dependence = non-empirical EDF**
  - ✓ **predictive from low density to strong coupling limits without adjustment**
  - ✓ **renormalization of the LECs = link with empirical EDF**
- **Inclusion of quasi-particle properties**
  - ✓ **predictive at low and intermediate density**
  - ✓ **towards finite systems: beyond LDA ($\nabla\rho, \ldots$)**
  - ✗ far from expected results in non-perturbative regime: need to be adjusted (see YGLO for instance)
  - ✗ pairing effect: from normal to superfluid

Perspectives and discussions towards non-empirical EDF

- Cross-fertilization: need (pseudo-) data to adjust ($\rightarrow$ experiment or ab-initio)
- Complicated but generalizable (higher order in the interaction, pairing, bound states,...)